



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 08:07 AM UTC

PDB ID : 2JOF / pdb_00002jof
BMRB ID : 15169
Title : The Trp-cage: Optimizing the Stability of a Globular Miniprotein
Authors : Barua, B.; Andersen, N.H.
Deposited on : 2007-03-09

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

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A user guide is available at

<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

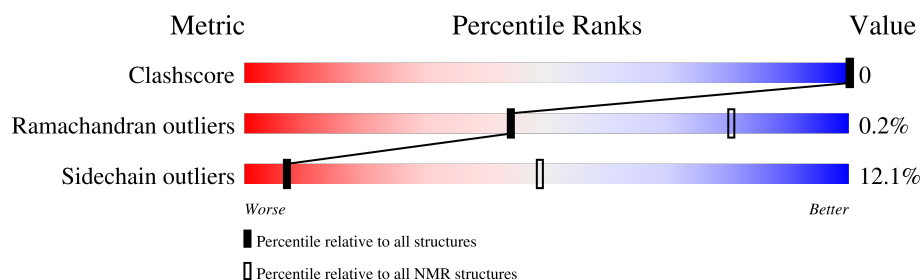
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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	20	

2 Ensemble composition and analysis

This entry contains 28 models. Model 27 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:19 (18)	0.35	27

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

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

The models can be grouped into 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	3, 7, 10, 11, 14, 16, 21, 22, 24, 25, 26, 27
2	2, 5, 6, 8
3	1, 4, 17, 19
4	20, 23, 28
5	9, 13, 18
Single-model clusters	12; 15

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 284 atoms, of which 136 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TRP-CAGE.

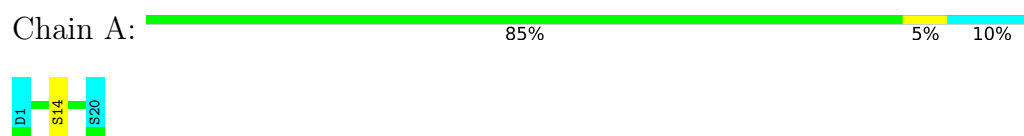
Mol	Chain	Residues	Atoms					Trace
1	A	20	Total	C	H	N	O	0
			284	92	136	26	30	

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: TRP-CAGE

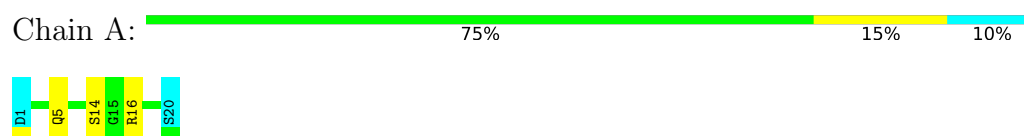


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

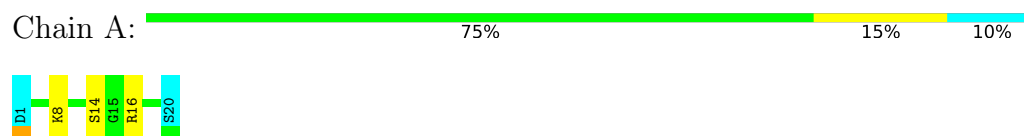
4.2.1 Score per residue for model 1

- Molecule 1: TRP-CAGE



4.2.2 Score per residue for model 2

- Molecule 1: TRP-CAGE



4.2.3 Score per residue for model 3

- Molecule 1: TRP-CAGE

Chain A:  85% 5% 10%



4.2.4 Score per residue for model 4

- Molecule 1: TRP-CAGE

Chain A:  70% 15% 5% 10%



4.2.5 Score per residue for model 5

- Molecule 1: TRP-CAGE

Chain A:  90% 10%



4.2.6 Score per residue for model 6

- Molecule 1: TRP-CAGE

Chain A:  80% 5% 5% 10%



4.2.7 Score per residue for model 7

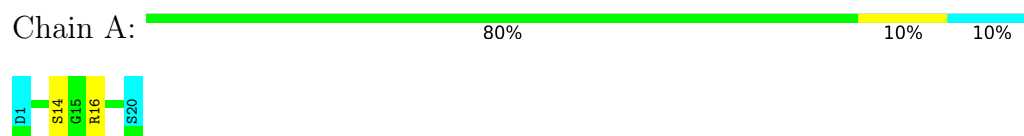
- Molecule 1: TRP-CAGE

Chain A:  80% 10% 10%



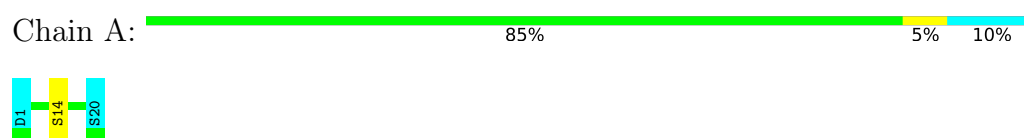
4.2.8 Score per residue for model 8

- Molecule 1: TRP-CAGE



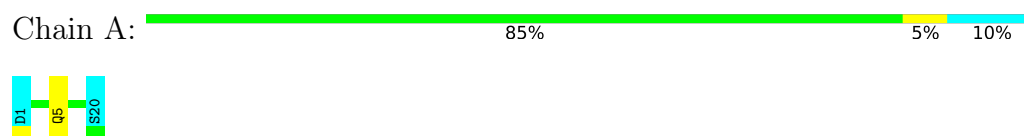
4.2.9 Score per residue for model 9

- Molecule 1: TRP-CAGE



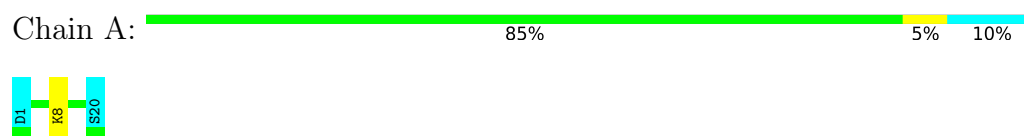
4.2.10 Score per residue for model 10

- Molecule 1: TRP-CAGE



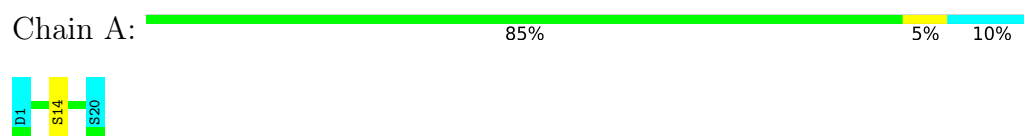
4.2.11 Score per residue for model 11

- Molecule 1: TRP-CAGE



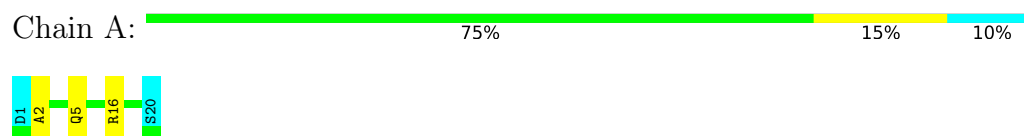
4.2.12 Score per residue for model 12

- Molecule 1: TRP-CAGE



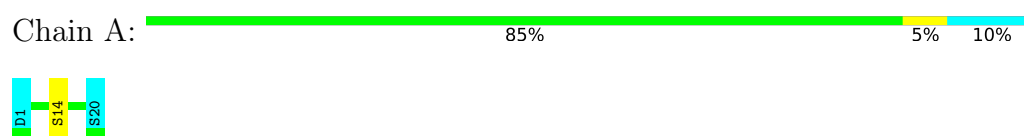
4.2.13 Score per residue for model 13

- Molecule 1: TRP-CAGE



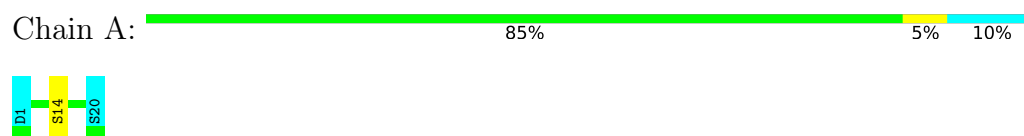
4.2.14 Score per residue for model 14

- Molecule 1: TRP-CAGE



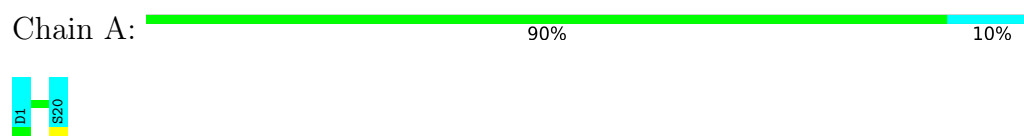
4.2.15 Score per residue for model 15

- Molecule 1: TRP-CAGE



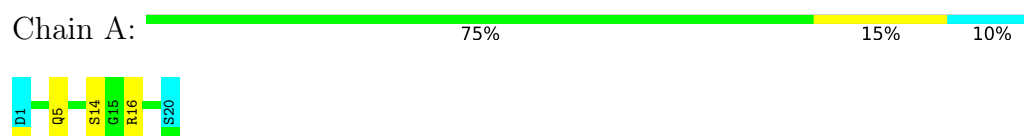
4.2.16 Score per residue for model 16

- Molecule 1: TRP-CAGE



4.2.17 Score per residue for model 17

- Molecule 1: TRP-CAGE



4.2.18 Score per residue for model 18

- Molecule 1: TRP-CAGE

Chain A:  90% 10%



4.2.19 Score per residue for model 19

- Molecule 1: TRP-CAGE

Chain A:  75% 15% 10%



4.2.20 Score per residue for model 20

- Molecule 1: TRP-CAGE

Chain A:  85% 5% 10%



4.2.21 Score per residue for model 21

- Molecule 1: TRP-CAGE

Chain A:  75% 15% 10%



4.2.22 Score per residue for model 22

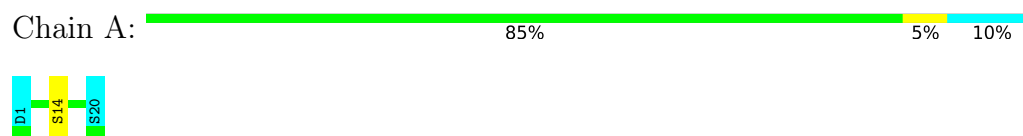
- Molecule 1: TRP-CAGE

Chain A:  70% 20% 10%



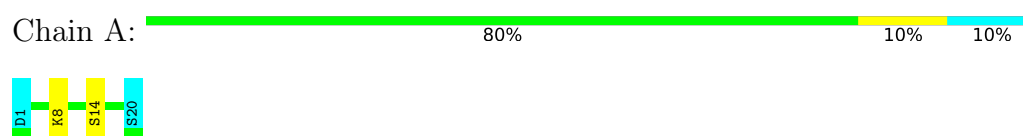
4.2.23 Score per residue for model 23

- Molecule 1: TRP-CAGE



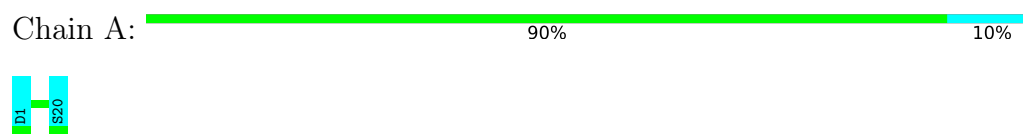
4.2.24 Score per residue for model 24

- Molecule 1: TRP-CAGE



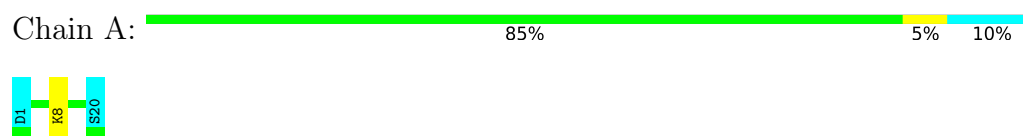
4.2.25 Score per residue for model 25

- Molecule 1: TRP-CAGE



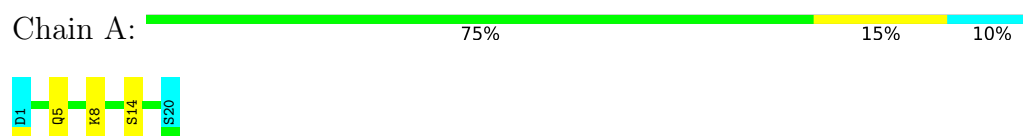
4.2.26 Score per residue for model 26

- Molecule 1: TRP-CAGE



4.2.27 Score per residue for model 27 (medoid)

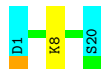
- Molecule 1: TRP-CAGE



4.2.28 Score per residue for model 28

- Molecule 1: TRP-CAGE

Chain A:  85% 5% 10%



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 28 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
Amber	refinement	6
CNS	structure solution	1.1

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	109
Number of shifts mapped to atoms	109
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.92±0.02	0±0/140 (0.0± 0.0%)	1.41±0.07	0±0/193 (0.0± 0.1%)
All	All	0.92	0/3920 (0.0%)	1.41	2/5404 (0.0%)

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	0.1±0.3
All	All	0	3

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	GLN	OE1-CD-NE2	-5.31	117.29	122.60	4	2

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	16	ARG	Sidechain	3

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	3724	3500	3500	-

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	18/20 (90%)	17±1 (93±4%)	1±1 (7±4%)	0±0 (0±1%)	44	80
All	All	504/560 (90%)	470 (93%)	33 (7%)	1 (0%)	44	80

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	2	ALA	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	13/15 (87%)	11±1 (88±8%)	2±1 (12±8%)	7	49
All	All	364/420 (87%)	320 (88%)	44 (12%)	7	49

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	14	SER	19

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Mol	Chain	Res	Type	Models (Total)
1	A	5	GLN	9
1	A	8	LYS	9
1	A	16	ARG	7

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 46% for the well-defined parts and 46% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	109
Number of shifts mapped to atoms	109
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 46%, i.e. 102 atoms were assigned a chemical shift out of a possible 220. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	32/85 (38%)	32/35 (91%)	0/36 (0%)	0/14 (0%)
Sidechain	60/114 (53%)	60/74 (81%)	0/35 (0%)	0/5 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	102/220 (46%)	102/119 (86%)	0/81 (0%)	0/20 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 109 atoms were assigned a chemical shift out of a possible 237. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	35/95 (37%)	35/39 (90%)	0/40 (0%)	0/16 (0%)
Sidechain	64/121 (53%)	64/78 (82%)	0/38 (0%)	0/5 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	109/237 (46%)	109/127 (86%)	0/88 (0%)	0/22 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

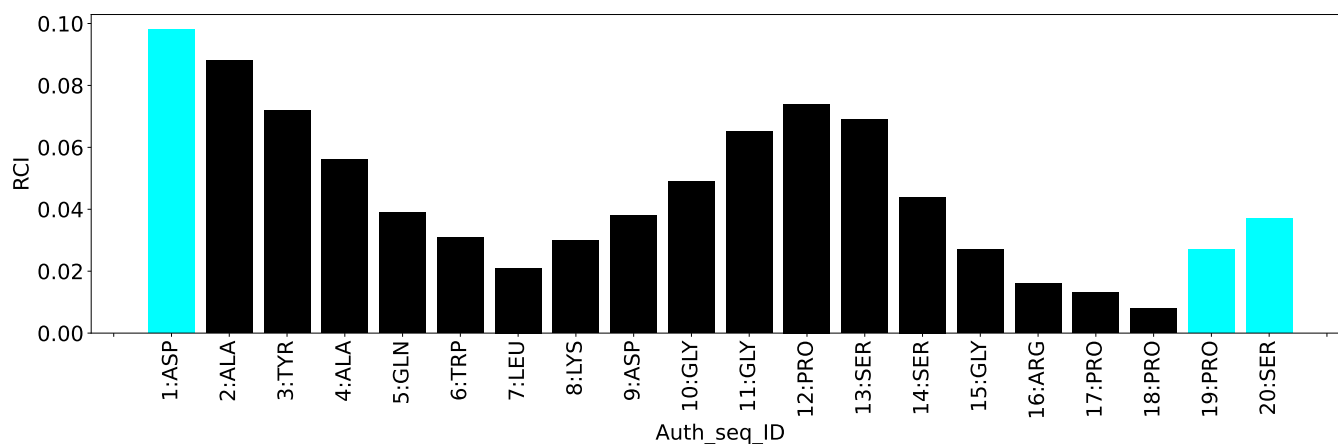
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	18	PRO	HA	2.40	2.78 – 6.00	-6.2
1	A	18	PRO	HB3	0.21	0.25 – 3.76	-5.1

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	186
Intra-residue ($ i-j =0$)	85
Sequential ($ i-j =1$)	52
Medium range ($ i-j >1$ and $ i-j <5$)	21
Long range ($ i-j \geq 5$)	28
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.3
Number of long range restraints per residue ¹	1.4

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)	9.9	0.2
0.2-0.5 (Medium)	19.0	0.5
>0.5 (Large)	7.0	1.1

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

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

9 Distance violation analysis ⓘ

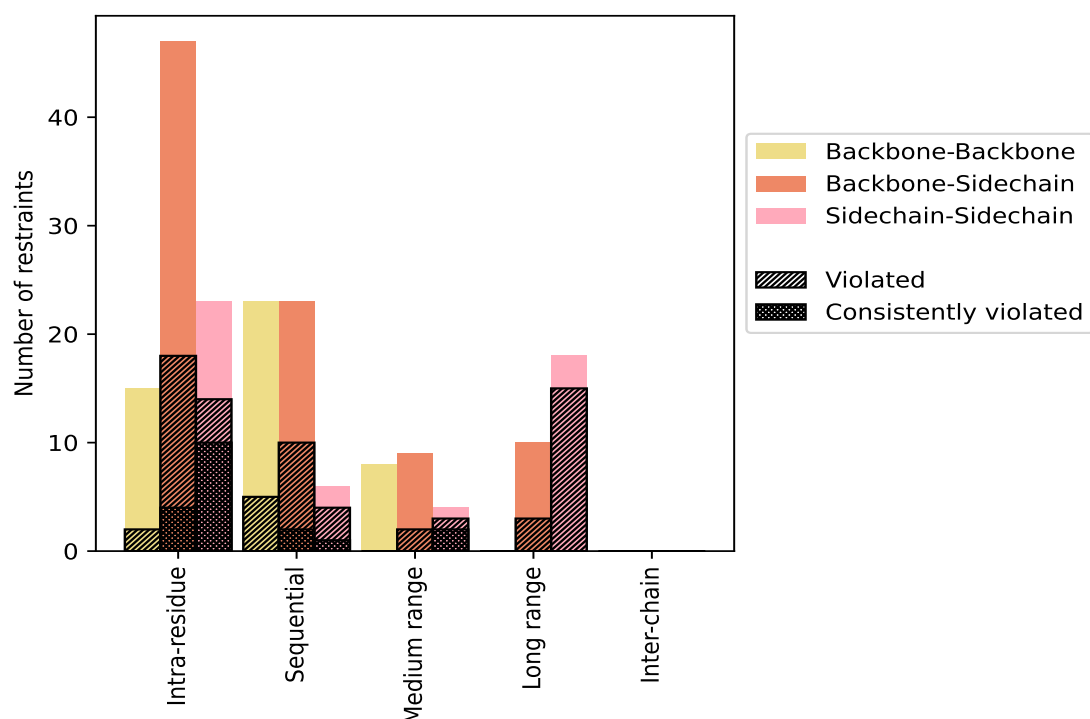
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	85	45.7	34	40.0	18.3	14	16.5	7.5
Backbone-Backbone	15	8.1	2	13.3	1.1	0	0.0	0.0
Backbone-Sidechain	47	25.3	18	38.3	9.7	4	8.5	2.2
Sidechain-Sidechain	23	12.4	14	60.9	7.5	10	43.5	5.4
Sequential (i-j =1)	52	28.0	19	36.5	10.2	3	5.8	1.6
Backbone-Backbone	23	12.4	5	21.7	2.7	0	0.0	0.0
Backbone-Sidechain	23	12.4	10	43.5	5.4	2	8.7	1.1
Sidechain-Sidechain	6	3.2	4	66.7	2.2	1	16.7	0.5
Medium range (i-j >1 & i-j <5)	21	11.3	5	23.8	2.7	2	9.5	1.1
Backbone-Backbone	8	4.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	9	4.8	2	22.2	1.1	0	0.0	0.0
Sidechain-Sidechain	4	2.2	3	75.0	1.6	2	50.0	1.1
Long range (i-j ≥5)	28	15.1	18	64.3	9.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	10	5.4	3	30.0	1.6	0	0.0	0.0
Sidechain-Sidechain	18	9.7	15	83.3	8.1	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	186	100.0	76	40.9	40.9	19	10.2	10.2
Backbone-Backbone	46	24.7	7	15.2	3.8	0	0.0	0.0
Backbone-Sidechain	89	47.8	33	37.1	17.7	6	6.7	3.2
Sidechain-Sidechain	51	27.4	36	70.6	19.4	13	25.5	7.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	19	10	3	3	0	35	0.35	1.02	0.23	0.29
2	19	9	4	5	0	37	0.37	1.02	0.22	0.28
3	20	9	3	1	0	33	0.35	1.02	0.23	0.28
4	21	9	4	3	0	37	0.35	1.0	0.22	0.28
5	23	9	4	5	0	41	0.35	0.98	0.21	0.3
6	21	10	4	2	0	37	0.35	0.98	0.22	0.3
7	24	7	4	2	0	37	0.34	1.05	0.22	0.28
8	19	10	3	3	0	35	0.36	1.0	0.22	0.31
9	21	11	3	4	0	39	0.36	1.05	0.21	0.28
10	23	8	3	2	0	36	0.35	1.04	0.22	0.3

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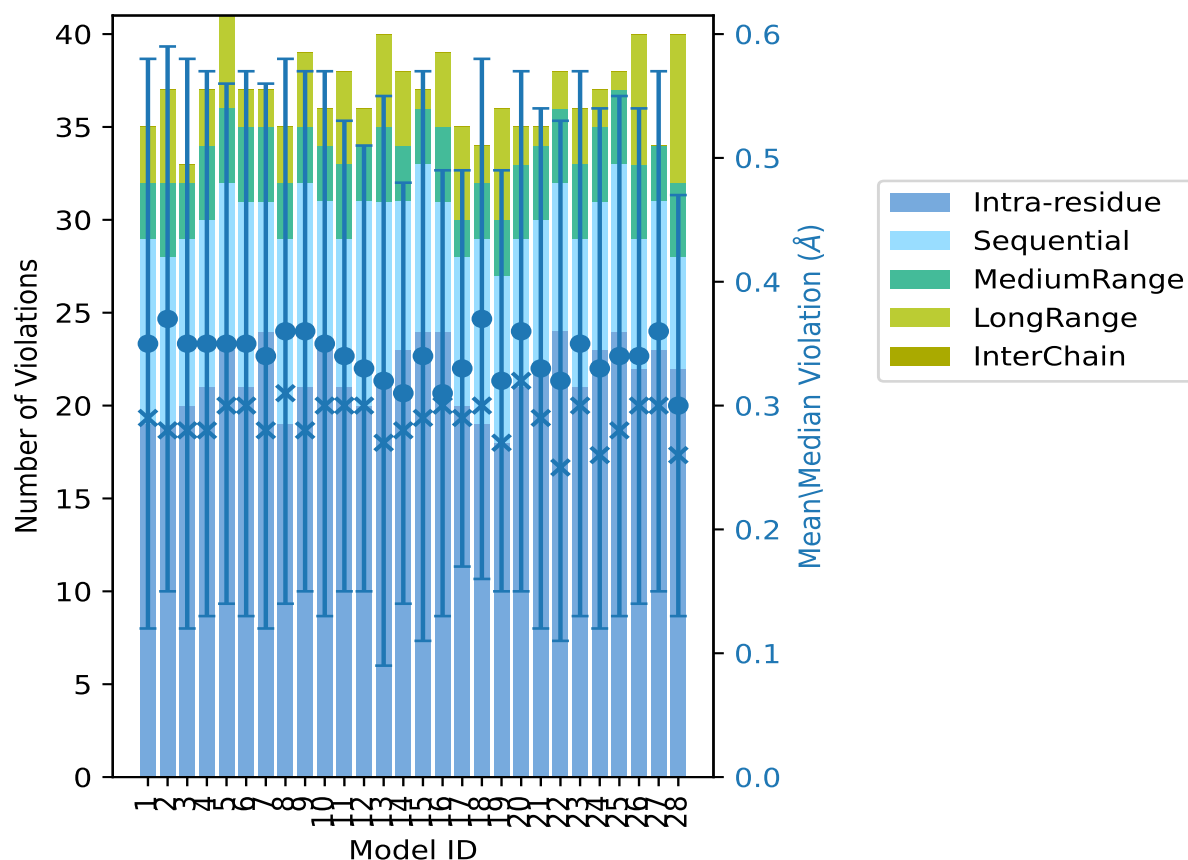
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	21	8	4	5	0	38	0.34	0.81	0.19	0.3
12	20	11	3	2	0	36	0.33	0.82	0.18	0.3
13	21	10	4	5	0	40	0.32	1.1	0.23	0.27
14	23	8	3	4	0	38	0.31	0.76	0.17	0.28
15	24	9	3	1	0	37	0.34	1.0	0.23	0.29
16	24	7	4	4	0	39	0.31	0.78	0.18	0.3
17	20	8	2	5	0	35	0.33	0.68	0.16	0.29
18	19	10	3	2	0	34	0.37	0.9	0.21	0.3
19	18	9	3	6	0	36	0.32	0.72	0.17	0.27
20	21	8	4	2	0	35	0.36	0.93	0.21	0.32
21	22	8	4	1	0	35	0.33	1.0	0.21	0.29
22	24	8	4	2	0	38	0.32	0.9	0.21	0.25
23	21	8	4	3	0	36	0.35	1.04	0.22	0.3
24	23	8	4	2	0	37	0.33	0.97	0.21	0.26
25	24	9	4	1	0	38	0.34	0.96	0.21	0.28
26	22	7	4	7	0	40	0.34	0.87	0.2	0.3
27	23	8	3	0	0	34	0.36	0.99	0.21	0.3
28	22	6	4	8	0	40	0.3	0.7	0.17	0.26

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, 110(IR:51, SQ:33, MR:16, LR:10, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	3	0	3	0	7	1	3.6
1	3	0	1	0	5	2	7.1
1	1	1	3	0	6	3	10.7
2	1	0	2	0	5	4	14.3
0	0	0	1	0	1	5	17.9
2	0	0	2	0	4	6	21.4

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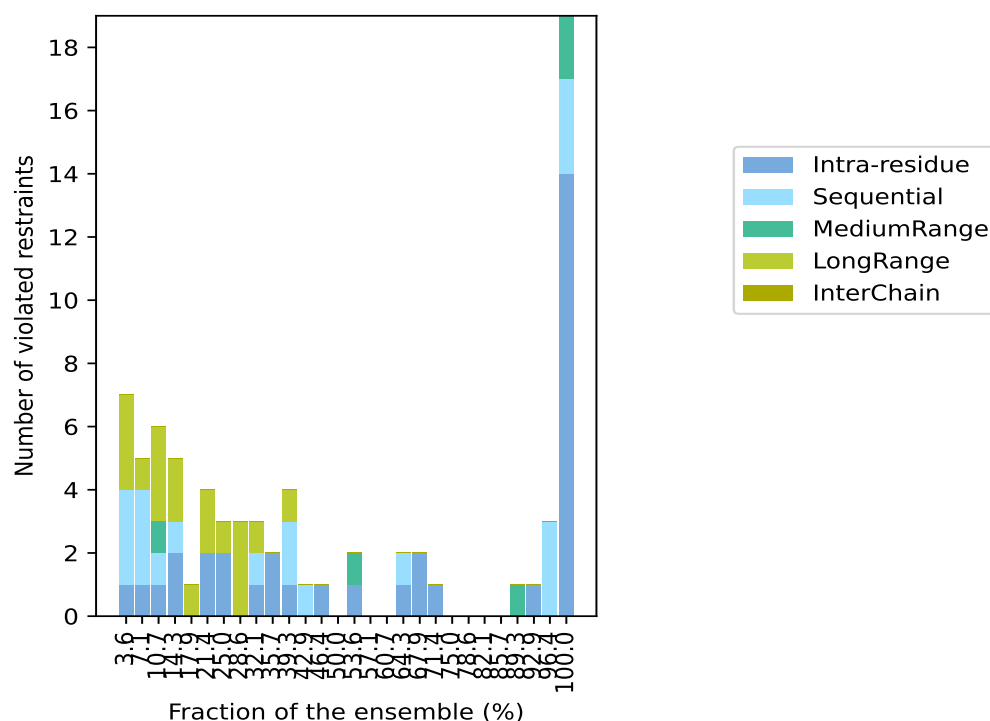
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	0	0	1	0	3	7	25.0
0	0	0	3	0	3	8	28.6
1	1	0	1	0	3	9	32.1
2	0	0	0	0	2	10	35.7
1	2	0	1	0	4	11	39.3
0	1	0	0	0	1	12	42.9
1	0	0	0	0	1	13	46.4
0	0	0	0	0	0	14	50.0
1	0	1	0	0	2	15	53.6
0	0	0	0	0	0	16	57.1
0	0	0	0	0	0	17	60.7
1	1	0	0	0	2	18	64.3
2	0	0	0	0	2	19	67.9
1	0	0	0	0	1	20	71.4
0	0	0	0	0	0	21	75.0
0	0	0	0	0	0	22	78.6
0	0	0	0	0	0	23	82.1
0	0	0	0	0	0	24	85.7
0	0	1	0	0	1	25	89.3
1	0	0	0	0	1	26	92.9
0	3	0	0	0	3	27	96.4
14	3	2	0	0	19	28	100.0

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

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

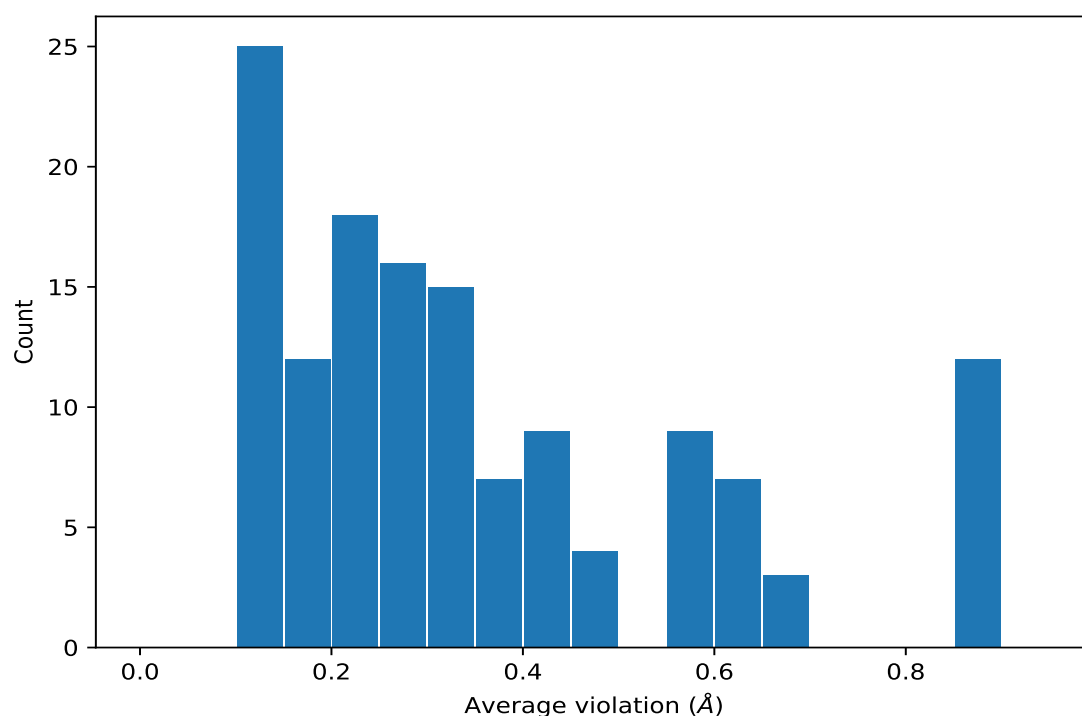
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	28	0.86	0.17	0.94
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	28	0.86	0.17	0.94
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	28	0.86	0.17	0.94
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	28	0.86	0.17	0.94
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	28	0.86	0.17	0.94
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	28	0.86	0.17	0.94
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	28	0.66	0.01	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	28	0.66	0.01	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	28	0.66	0.01	0.67
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	28	0.63	0.03	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	28	0.63	0.03	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	28	0.63	0.03	0.62
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	28	0.6	0.04	0.62
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	28	0.6	0.04	0.62
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	28	0.6	0.04	0.62
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	28	0.6	0.04	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	28	0.58	0.19	0.59
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	28	0.58	0.19	0.59
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	28	0.58	0.19	0.59
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	28	0.58	0.19	0.59
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	28	0.58	0.19	0.59
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	28	0.58	0.19	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	28	0.57	0.01	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	28	0.57	0.01	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	28	0.57	0.01	0.57
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	28	0.45	0.02	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	28	0.45	0.02	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	28	0.45	0.02	0.45
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	28	0.43	0.06	0.44
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	28	0.43	0.06	0.44
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	28	0.43	0.06	0.44
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	28	0.36	0.01	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	28	0.36	0.01	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	28	0.36	0.01	0.36
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	28	0.32	0.01	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	28	0.32	0.01	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	28	0.32	0.01	0.32
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	28	0.32	0.06	0.32
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	28	0.32	0.03	0.32
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	28	0.32	0.03	0.32
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	28	0.26	0.01	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	28	0.26	0.01	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	28	0.26	0.01	0.26
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	28	0.25	0.03	0.26
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	28	0.25	0.04	0.26
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	28	0.24	0.04	0.24
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	28	0.24	0.04	0.24
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	28	0.24	0.04	0.24
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	28	0.24	0.12	0.18
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	28	0.24	0.12	0.18
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	28	0.15	0.01	0.15
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	28	0.13	0.01	0.13
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	27	0.4	0.1	0.43
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	27	0.4	0.1	0.43
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	27	0.4	0.1	0.43
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	27	0.34	0.07	0.35
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	27	0.34	0.07	0.35
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	27	0.34	0.07	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	27	0.2	0.04	0.2
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	26	0.18	0.03	0.18
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	26	0.18	0.03	0.18
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	25	0.87	0.25	0.96
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	25	0.87	0.25	0.96
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	25	0.87	0.25	0.96
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	25	0.87	0.25	0.96
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	25	0.87	0.25	0.96
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	25	0.87	0.25	0.96
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	20	0.11	0.0	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	20	0.11	0.0	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	20	0.11	0.0	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	20	0.11	0.0	0.11
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	19	0.26	0.01	0.26
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	19	0.13	0.01	0.13
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	18	0.37	0.11	0.44
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	18	0.37	0.11	0.44
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	18	0.21	0.08	0.2
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	18	0.21	0.08	0.2
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	15	0.32	0.13	0.32
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	15	0.32	0.13	0.32
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	15	0.32	0.13	0.32
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	15	0.27	0.08	0.31
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	15	0.27	0.08	0.31
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	13	0.25	0.01	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	13	0.25	0.01	0.25
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	12	0.41	0.09	0.4
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	12	0.41	0.09	0.4
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	12	0.41	0.09	0.4
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	11	0.35	0.04	0.36
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	11	0.32	0.1	0.36
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	11	0.32	0.1	0.36
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	11	0.25	0.07	0.22
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	11	0.14	0.03	0.14
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	10	0.29	0.11	0.27
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	10	0.13	0.02	0.12
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	10	0.13	0.02	0.12
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	9	0.31	0.04	0.32
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	9	0.29	0.01	0.29
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	9	0.22	0.06	0.2
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	9	0.22	0.06	0.2
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	8	0.29	0.21	0.22

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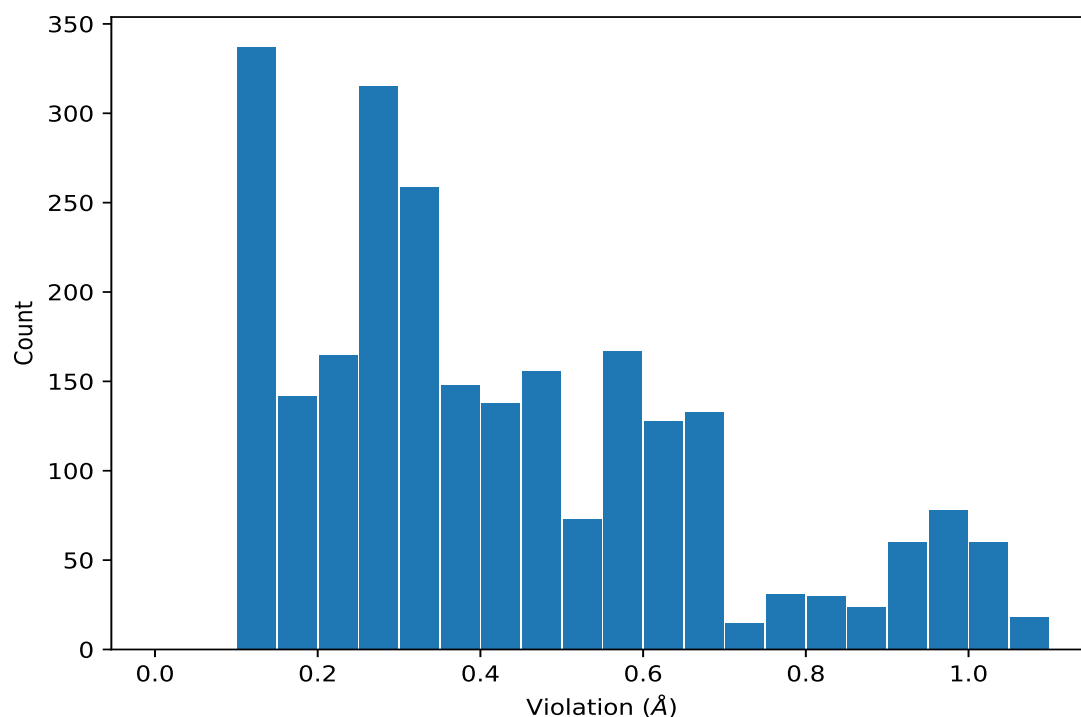
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	8	0.24	0.05	0.24
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	8	0.24	0.05	0.24
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	8	0.22	0.08	0.2
(1,38)	1:14:A:SER:HB3	1:9:A:ASP:HB2	7	0.39	0.17	0.37
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB2	7	0.14	0.04	0.12
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB3	7	0.14	0.04	0.12
(1,125)	1:5:A:GLN:HA	1:5:A:GLN:HB2	7	0.14	0.03	0.14
(1,97)	1:3:A:TYR:HA	1:19:A:PRO:HG2	6	0.16	0.03	0.16
(1,60)	1:17:A:PRO:HA	1:17:A:PRO:HG3	6	0.16	0.04	0.17
(1,19)	1:12:A:PRO:HD3	1:6:A:TRP:HH2	6	0.14	0.02	0.15
(1,167)	1:7:A:LEU:HD11	1:7:A:LEU:H	6	0.12	0.02	0.12
(1,167)	1:7:A:LEU:HD12	1:7:A:LEU:H	6	0.12	0.02	0.12
(1,167)	1:7:A:LEU:HD13	1:7:A:LEU:H	6	0.12	0.02	0.12
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE1	5	0.28	0.16	0.19
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE2	5	0.28	0.16	0.19
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB2	4	0.17	0.01	0.18
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB3	4	0.17	0.01	0.18
(1,53)	1:16:A:ARG:HB2	1:6:A:TRP:HE1	4	0.16	0.06	0.14
(1,53)	1:16:A:ARG:HB3	1:6:A:TRP:HE1	4	0.16	0.06	0.14
(1,169)	1:7:A:LEU:H	1:8:A:LYS:H	4	0.11	0.02	0.11
(1,22)	1:12:A:PRO:HA	1:6:A:TRP:HH2	4	0.1	0.0	0.1
(1,175)	1:8:A:LYS:HA	1:8:A:LYS:H	4	0.1	0.0	0.1
(1,128)	1:6:A:TRP:HD1	1:16:A:ARG:HE	3	0.46	0.08	0.5
(1,68)	1:18:A:PRO:HB3	1:3:A:TYR:HE1	3	0.23	0.12	0.17
(1,68)	1:18:A:PRO:HB3	1:3:A:TYR:HE2	3	0.23	0.12	0.17
(1,83)	1:19:A:PRO:HB2	1:20:A:SER:H	3	0.23	0.04	0.21
(1,143)	1:6:A:TRP:HA	1:9:A:ASP:HB3	3	0.18	0.04	0.2
(1,87)	1:20:A:SER:HA	1:20:A:SER:HB2	3	0.13	0.0	0.13
(1,87)	1:20:A:SER:HA	1:20:A:SER:HB3	3	0.13	0.0	0.13
(1,51)	1:16:A:ARG:HG2	1:6:A:TRP:HD1	3	0.12	0.02	0.12
(1,51)	1:16:A:ARG:HG3	1:6:A:TRP:HD1	3	0.12	0.02	0.12
(1,23)	1:13:A:SER:HA	1:13:A:SER:HB2	2	0.2	0.01	0.2
(1,23)	1:13:A:SER:HA	1:13:A:SER:HB3	2	0.2	0.01	0.2
(1,37)	1:14:A:SER:HB2	1:9:A:ASP:HB2	2	0.16	0.01	0.16
(1,9)	1:12:A:PRO:HD2	1:11:A:GLY:H	2	0.15	0.0	0.15
(1,2)	1:10:A:GLY:H	1:11:A:GLY:H	2	0.12	0.01	0.12
(1,140)	1:6:A:TRP:HB3	1:7:A:LEU:H	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	13	1.1
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	13	1.1
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	13	1.1
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	13	1.1
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	13	1.1
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	13	1.1
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	7	1.05
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	7	1.05
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	7	1.05
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	7	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	7	1.05
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	7	1.05
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	9	1.05
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	9	1.05
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	9	1.05
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	9	1.05
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	9	1.05
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	9	1.05
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	10	1.04
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	10	1.04
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	10	1.04
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	10	1.04
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	10	1.04
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	10	1.04
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	23	1.04
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	23	1.04
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	23	1.04
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	23	1.04
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	23	1.04
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	23	1.04
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	1	1.02
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	1	1.02
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	1	1.02
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	1	1.02
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	1	1.02
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	1	1.02
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	2	1.02
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	2	1.02
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	2	1.02
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	2	1.02
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	2	1.02
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	2	1.02
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	3	1.02
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	3	1.02
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	3	1.02
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	3	1.02
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	3	1.02
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	3	1.02
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	13	1.0
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	13	1.0
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	13	1.0
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	13	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	13	1.0
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	13	1.0
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	21	1.0
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	21	1.0
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	21	1.0
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	21	1.0
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	21	1.0
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	21	1.0
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	4	1.0
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	4	1.0
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	4	1.0
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	4	1.0
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	4	1.0
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	4	1.0
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	8	1.0
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	8	1.0
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	8	1.0
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	8	1.0
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	8	1.0
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	8	1.0
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	15	1.0
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	15	1.0
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	15	1.0
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	15	1.0
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	15	1.0
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	15	1.0
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	27	0.99
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	27	0.99
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	27	0.99
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	27	0.99
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	27	0.99
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	27	0.99
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	5	0.98
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	5	0.98
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	5	0.98
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	5	0.98
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	5	0.98
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	5	0.98
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	7	0.98
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	7	0.98
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	7	0.98
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	7	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	7	0.98
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	7	0.98
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	8	0.98
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	8	0.98
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	8	0.98
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	8	0.98
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	8	0.98
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	8	0.98
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	23	0.98
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	23	0.98
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	23	0.98
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	23	0.98
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	23	0.98
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	23	0.98
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	6	0.98
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	6	0.98
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	6	0.98
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	6	0.98
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	6	0.98
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	6	0.98
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	10	0.97
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	10	0.97
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	10	0.97
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	10	0.97
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	10	0.97
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	10	0.97
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	24	0.97
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	24	0.97
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	24	0.97
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	24	0.97
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	24	0.97
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	24	0.97
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	4	0.96
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	4	0.96
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	4	0.96
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	4	0.96
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	4	0.96
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	4	0.96
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	9	0.96
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	9	0.96
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	9	0.96
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	9	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	9	0.96
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	9	0.96
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	25	0.96
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	25	0.96
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	25	0.96
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	25	0.96
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	25	0.96
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	25	0.96
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	5	0.96
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	5	0.96
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	5	0.96
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	5	0.96
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	5	0.96
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	5	0.96
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	27	0.96
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	27	0.96
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	27	0.96
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	27	0.96
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	27	0.96
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	27	0.96
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	1	0.95
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	1	0.95
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	1	0.95
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	1	0.95
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	1	0.95
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	1	0.95
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	2	0.95
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	2	0.95
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	2	0.95
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	2	0.95
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	2	0.95
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	2	0.95
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	25	0.95
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	25	0.95
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	25	0.95
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	25	0.95
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	25	0.95
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	25	0.95
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	20	0.93
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	20	0.93
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	20	0.93
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	20	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	20	0.93
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	20	0.93
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	6	0.92
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	6	0.92
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	6	0.92
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	6	0.92
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	6	0.92
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	6	0.92
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	15	0.92
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	15	0.92
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	15	0.92
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	15	0.92
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	15	0.92
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	15	0.92
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	18	0.9
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	18	0.9
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	18	0.9
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	18	0.9
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	18	0.9
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	18	0.9
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	22	0.9
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	22	0.9
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	22	0.9
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	22	0.9
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	22	0.9
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	22	0.9
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	21	0.9
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	21	0.9
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	21	0.9
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	21	0.9
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	21	0.9
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	21	0.9
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	24	0.9
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	24	0.9
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	24	0.9
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	24	0.9
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	24	0.9
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	24	0.9
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	20	0.89
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	20	0.89
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	20	0.89
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	20	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	20	0.89
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	20	0.89
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	3	0.88
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	3	0.88
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	3	0.88
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	3	0.88
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	3	0.88
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	3	0.88
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	26	0.87
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	26	0.87
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	26	0.87
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	26	0.87
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	26	0.87
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	26	0.87
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	26	0.86
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	26	0.86
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	26	0.86
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	26	0.86
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	26	0.86
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	26	0.86
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	18	0.84
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	18	0.84
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	18	0.84
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	18	0.84
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	18	0.84
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	18	0.84
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	12	0.82
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	12	0.82
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	12	0.82
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	12	0.82
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	12	0.82
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	12	0.82
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	15	0.82
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	15	0.82
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	15	0.82
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	15	0.82
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	15	0.82
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	15	0.82
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	11	0.81
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	11	0.81
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	11	0.81
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	11	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	11	0.81
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	11	0.81
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	6	0.8
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	6	0.8
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	6	0.8
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	6	0.8
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	6	0.8
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	6	0.8
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	22	0.78
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	22	0.78
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	22	0.78
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	22	0.78
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	22	0.78
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	22	0.78
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	11	0.78
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	11	0.78
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	11	0.78
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	11	0.78
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	11	0.78
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	11	0.78
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	16	0.78
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	16	0.78
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	16	0.78
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	16	0.78
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	16	0.78
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	16	0.78
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	22	0.77
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	22	0.77
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	22	0.77
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	22	0.77
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	22	0.77
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	22	0.77
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	14	0.76
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	14	0.76
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	14	0.76
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	14	0.76
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	14	0.76
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	14	0.76
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	2	0.76
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	26	0.73
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	26	0.73
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	26	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	26	0.73
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	26	0.73
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	26	0.73
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	12	0.72
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	12	0.72
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	12	0.72
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	19	0.72
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	19	0.72
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	19	0.72
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	19	0.72
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	19	0.72
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	19	0.72
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	28	0.7
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	28	0.7
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	28	0.7
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	28	0.7
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	28	0.7
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	28	0.7
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	15	0.69
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	15	0.69
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	15	0.69
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	26	0.69
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	26	0.69
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	26	0.69
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.68
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.68
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	5	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	5	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	5	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	11	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	11	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	11	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	16	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	16	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	16	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	23	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	23	0.68
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	23	0.68
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	17	0.68
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	17	0.68
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	17	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	17	0.68
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	17	0.68
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	17	0.68
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.67
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.67
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.67
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	17	0.67
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	17	0.67
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	17	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	4	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	4	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	4	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	7	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	7	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	7	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	8	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	8	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	8	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	9	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	9	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	9	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	13	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	13	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	13	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	20	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	20	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	20	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	21	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	21	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	21	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	22	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	22	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	22	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	25	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	25	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	25	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	28	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	28	0.67
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	28	0.67
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	11	0.66
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	11	0.66
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	11	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	28	0.66
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	28	0.66
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	28	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	1	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	1	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	1	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	2	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	2	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	2	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	6	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	6	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	6	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	14	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	14	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	14	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	18	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	18	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	18	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	19	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	19	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	19	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	24	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	24	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	24	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	27	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	27	0.66
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	27	0.66
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	3	0.66
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	3	0.66
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	3	0.66
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	3	0.66
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	3	0.66
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	3	0.66
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	14	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	14	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	14	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	16	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	16	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	19	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	19	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	19	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	22	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	22	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	22	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	26	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	26	0.65
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	26	0.65
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	15	0.65
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	15	0.65
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	15	0.65
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	17	0.65
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	17	0.65
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	17	0.65
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	16	0.65
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	16	0.65
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	16	0.65
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	16	0.65
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	3	0.64
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	3	0.64
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	3	0.64
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	16	0.64
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	16	0.64
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	16	0.64
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	16	0.64
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	16	0.64
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	16	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	8	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	8	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	8	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	8	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	9	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	9	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	9	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	9	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	12	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	12	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	12	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	12	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	14	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	14	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	14	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	14	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	18	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	18	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	18	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	18	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	23	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	23	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	23	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	23	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	28	0.64
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	28	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	28	0.64
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	28	0.64
(1,38)	1:14:A:SER:HB3	1:9:A:ASP:HB2	5	0.64
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	25	0.63
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	25	0.63
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	25	0.63
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	27	0.63
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	27	0.63
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	27	0.63
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	7	0.63
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	7	0.63
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	7	0.63
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	7	0.63
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	10	0.63
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	10	0.63
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	10	0.63
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	10	0.63
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	11	0.63
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	11	0.63
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	11	0.63
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	11	0.63
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	20	0.63
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	20	0.63
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	20	0.63
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	20	0.63
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	20	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	20	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	20	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	24	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	24	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	24	0.62
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	12	0.62
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	12	0.62
(1,162)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	12	0.62
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	2	0.62
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	2	0.62
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	2	0.62
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	2	0.62
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	2	0.62
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	2	0.62
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	1	0.62
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	1	0.62
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	1	0.62
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	1	0.62
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	19	0.62
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	19	0.62
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	19	0.62
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	19	0.62
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.61
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	12	0.61
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	12	0.61
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	12	0.61
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	12	0.61
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	12	0.61
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	12	0.61
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	14	0.61
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	14	0.61
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	14	0.61
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	14	0.61
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	14	0.61
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	19	0.61
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	19	0.61
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	19	0.61
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	19	0.61
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	19	0.61
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	19	0.61
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	9	0.61
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	9	0.61
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	9	0.61
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	9	0.61
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	9	0.61
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	9	0.61
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	2	0.61
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	2	0.61
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	2	0.61
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	2	0.61
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	17	0.61
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	17	0.61
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	17	0.61
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	17	0.61
(1,38)	1:14:A:SER:HB3	1:9:A:ASP:HB2	18	0.61
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	13	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	13	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	13	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	18	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	18	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	18	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	21	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	21	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	21	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	23	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	23	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	23	0.6
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	7	0.6
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	7	0.6
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	7	0.6
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	4	0.6
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	4	0.6
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	4	0.6
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	25	0.6
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	25	0.6
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	25	0.6
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	25	0.6
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.59
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.59
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	5	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	5	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	5	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	8	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	8	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	8	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	23	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	23	0.59
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	23	0.59
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.58
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.58
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.58
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.58
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.58
(1,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	1	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	1	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	1	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	4	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	4	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	4	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	9	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	9	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	9	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	13	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	13	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	13	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	20	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	20	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	20	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	21	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	21	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	21	0.58
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	2	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	2	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	2	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	14	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	14	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	14	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	18	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	18	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	18	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	24	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	24	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	24	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	25	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	25	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	25	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	26	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	26	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	26	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	27	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	27	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	27	0.57
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	4	0.57
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	4	0.57
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	4	0.57
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	4	0.57
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	4	0.57
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	4	0.57
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	1	0.57
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	1	0.57
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	1	0.57
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	22	0.57
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	22	0.57
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	22	0.57
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	22	0.57
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	5	0.57
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	3	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	3	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	3	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	6	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	6	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	11	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	11	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	11	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	16	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	16	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	16	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	17	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	17	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	17	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	19	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	19	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	19	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	22	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	22	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	22	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	28	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	28	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	28	0.56
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	18	0.56
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	18	0.56
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	18	0.56
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	18	0.56
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	18	0.56
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	18	0.56
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	3	0.56
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	3	0.56
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	3	0.56
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	3	0.56
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	13	0.56
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	13	0.56
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	13	0.56
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	13	0.56
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	15	0.56
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	15	0.56
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	15	0.56
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	15	0.56
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	24	0.56
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	24	0.56
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	24	0.56
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	24	0.56
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	15	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	15	0.55
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	15	0.55
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	1	0.55
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	1	0.55
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	1	0.55
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	1	0.55
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	1	0.55
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	1	0.55
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	10	0.55
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	10	0.55
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	10	0.55
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	10	0.55
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	10	0.55
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	10	0.55
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE1	20	0.55
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE2	20	0.55
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	6	0.55
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	6	0.55
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	6	0.55
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	6	0.55
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	12	0.54
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	12	0.54
(1,161)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	12	0.54
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	18	0.54
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	18	0.54
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	18	0.54
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	20	0.54
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	20	0.54
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	20	0.54
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	20	0.54
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	20	0.54
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	20	0.54
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	25	0.54
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	25	0.54
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	25	0.54
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	25	0.54
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	25	0.54
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	25	0.54
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	7	0.54
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	7	0.54
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	18	0.53
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	18	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	18	0.53
(1,128)	1:6:A:TRP:HD1	1:16:A:ARG:HE	8	0.53
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	4	0.53
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	4	0.53
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	5	0.53
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	5	0.53
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	5	0.53
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	5	0.53
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	27	0.53
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	27	0.53
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	27	0.53
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	27	0.53
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	8	0.52
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	8	0.52
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	8	0.52
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	8	0.52
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	8	0.52
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	8	0.52
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	11	0.52
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	11	0.52
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	11	0.52
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	11	0.52
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	11	0.52
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	11	0.52
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	22	0.52
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	22	0.52
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	22	0.52
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	21	0.52
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	21	0.52
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	21	0.52
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	21	0.52
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG2	26	0.52
(1,47)	1:16:A:ARG:HD2	1:16:A:ARG:HG3	26	0.52
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG2	26	0.52
(1,47)	1:16:A:ARG:HD3	1:16:A:ARG:HG3	26	0.52
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	9	0.51
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	9	0.51
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	9	0.51
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	26	0.51
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	26	0.51
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	26	0.51
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	1	0.5
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	1	0.5
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	5	0.5
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	5	0.5
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	5	0.5
(1,128)	1:6:A:TRP:HD1	1:16:A:ARG:HE	18	0.5
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	28	0.5
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	28	0.5
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	28	0.5
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	2	0.49
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	2	0.49
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	2	0.49
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	13	0.49
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	13	0.49
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	13	0.49
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	13	0.49
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	13	0.49
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	13	0.49
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	13	0.49
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	13	0.49
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	13	0.49
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	27	0.49
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	27	0.49
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	27	0.49
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	27	0.49
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	27	0.49
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	27	0.49
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	4	0.49
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	4	0.49
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	4	0.49
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	16	0.49
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	16	0.49
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.48
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.48
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.48
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	12	0.48
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	12	0.48
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	12	0.48
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	12	0.48
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	12	0.48
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	12	0.48
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	20	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	20	0.48
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	20	0.48
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	25	0.48
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	25	0.48
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.47
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.47
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.47
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	15	0.47
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	15	0.47
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	15	0.47
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	20	0.47
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	20	0.47
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	20	0.47
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	5	0.47
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	5	0.47
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	5	0.47
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	9	0.47
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	9	0.47
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	9	0.47
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	10	0.47
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	10	0.47
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	15	0.47
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	15	0.47
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	17	0.47
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	17	0.47
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	24	0.47
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	24	0.47
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	26	0.47
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	26	0.47
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	14	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	14	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	14	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	17	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	17	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	17	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	18	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	18	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	18	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	20	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	20	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	20	0.46
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	23	0.46
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	23	0.46
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	23	0.46
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	27	0.46
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	27	0.46
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	27	0.46
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	1	0.46
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	1	0.46
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	1	0.46
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	19	0.46
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	19	0.46
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	19	0.46
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	23	0.46
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	23	0.46
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	23	0.46
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	28	0.46
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	28	0.46
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	28	0.46
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	28	0.46
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	28	0.46
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	28	0.46
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	23	0.46
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	23	0.46
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	23	0.46
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	23	0.46
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	23	0.46
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	23	0.46
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	11	0.46
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	11	0.46
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	11	0.46
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	5	0.46
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	5	0.46
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	11	0.46
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	11	0.46
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	13	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	13	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	13	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	22	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	22	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	22	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	24	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	24	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	24	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	25	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	25	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	25	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	27	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	27	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	27	0.45
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	10	0.45
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	10	0.45
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	10	0.45
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	21	0.45
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	21	0.45
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	21	0.45
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	24	0.45
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	24	0.45
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	24	0.45
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	6	0.45
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	6	0.45
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	6	0.45
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	17	0.45
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	17	0.45
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	17	0.45
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	6	0.45
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	6	0.45
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	6	0.45
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	19	0.45
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	19	0.45
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	28	0.45
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	19	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	19	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	19	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	21	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	21	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	21	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	23	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	23	0.44
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	23	0.44
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	11	0.44
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	11	0.44
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	11	0.44
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	13	0.44
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	13	0.44
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	13	0.44
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	28	0.44
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	28	0.44
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	28	0.44
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	9	0.44
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	9	0.44
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	9	0.44
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	10	0.44
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	10	0.44
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	10	0.44
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	26	0.44
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	26	0.44
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	26	0.44
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	9	0.44
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	9	0.44
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	9	0.44
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	14	0.44
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	14	0.44
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	6	0.43
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	6	0.43
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	6	0.43
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	15	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	15	0.43
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	15	0.43
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	17	0.43
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	17	0.43
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	17	0.43
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	2	0.43
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	2	0.43
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	2	0.43
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	24	0.43
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	24	0.43
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	24	0.43
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	25	0.43
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	25	0.43
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	25	0.43
(1,38)	1:14:A:SER:HB3	1:9:A:ASP:HB2	8	0.43
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	19	0.43
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	19	0.43
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	11	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	11	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	11	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	16	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	16	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	16	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	26	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	26	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	26	0.42
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	3	0.42
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	3	0.42
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	3	0.42
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	19	0.42
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	19	0.42
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	19	0.42
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	25	0.42
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	25	0.42
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	25	0.42
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	18	0.42
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	18	0.42
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	18	0.42
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	8	0.42
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	8	0.42
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	25	0.42
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	25	0.42
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD21	28	0.41
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD22	28	0.41
(1,158)	1:7:A:LEU:HA	1:7:A:LEU:HD23	28	0.41
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	4	0.41
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	4	0.41
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	4	0.41
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	1	0.41
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	1	0.41
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	1	0.41
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	3	0.41
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	3	0.41
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	3	0.41
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	8	0.41
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	8	0.41
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	8	0.41
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	7	0.41
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	7	0.41
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	13	0.41
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	13	0.41
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	16	0.4
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	16	0.4
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	16	0.4
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	7	0.4
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	7	0.4
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	7	0.4
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD1	17	0.4
(1,149)	1:7:A:LEU:HD11	1:3:A:TYR:HD2	17	0.4
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD1	17	0.4
(1,149)	1:7:A:LEU:HD12	1:3:A:TYR:HD2	17	0.4
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD1	17	0.4
(1,149)	1:7:A:LEU:HD13	1:3:A:TYR:HD2	17	0.4
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	7	0.4
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	7	0.4
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	7	0.4
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	21	0.4
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	21	0.4
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	21	0.4
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	2	0.4
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	2	0.4
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	7	0.4
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	7	0.4
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	7	0.4
(1,68)	1:18:A:PRO:HB3	1:3:A:TYR:HE1	26	0.4
(1,68)	1:18:A:PRO:HB3	1:3:A:TYR:HE2	26	0.4
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	3	0.4
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	28	0.4
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	24	0.39
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	24	0.39
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	24	0.39
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	24	0.39
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	24	0.39
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	24	0.39
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	23	0.39
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	23	0.39
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	23	0.39
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	22	0.39
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	22	0.39
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	22	0.39
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	14	0.39
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	14	0.39
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	14	0.39
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	23	0.39
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	1	0.39
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	1	0.39
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	13	0.39
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	14	0.38
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	14	0.38
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	14	0.38
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	16	0.38
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	16	0.38
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	16	0.38
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	11	0.38
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	11	0.38
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	11	0.38
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	17	0.38
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	17	0.38
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	17	0.38
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	2	0.38
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	2	0.38
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	5	0.38
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	5	0.38
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	5	0.38
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	13	0.38
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	13	0.38
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	13	0.38
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	16	0.38
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	25	0.38
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	23	0.38
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	16	0.38
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	27	0.38
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	7	0.37
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	7	0.37
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	7	0.37
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	21	0.37
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	21	0.37
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	21	0.37
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	4	0.37
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	4	0.37
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	4	0.37
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	12	0.37
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	12	0.37
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	12	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	11	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	11	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	11	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	19	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	19	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	19	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	24	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	24	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	24	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	28	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	28	0.37
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	28	0.37
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE1	23	0.37
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE2	23	0.37
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	23	0.37
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	23	0.37
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	26	0.37
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	27	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	4	0.37
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	4	0.37
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	14	0.37
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	14	0.37
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	27	0.37
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	27	0.37
(1,38)	1:14:A:SER:HB3	1:9:A:ASP:HB2	9	0.37
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	5	0.37
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	14	0.37
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	12	0.37
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	7	0.37
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	9	0.37
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	10	0.37
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	11	0.37
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	26	0.37
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	12	0.36
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	12	0.36
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	12	0.36
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	16	0.36
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	16	0.36
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	16	0.36
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	16	0.36
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	16	0.36
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	16	0.36
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	7	0.36
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	7	0.36
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	7	0.36
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	15	0.36
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	15	0.36
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	15	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	3	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	3	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	3	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	4	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	4	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	4	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	12	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	12	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	12	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	16	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	16	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	17	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	17	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	17	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	20	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	20	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	20	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	21	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	21	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	21	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	23	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	23	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	23	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	25	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	25	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	25	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	26	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	26	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	26	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	27	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	27	0.36
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	27	0.36
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	22	0.36
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	22	0.36
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	3	0.36
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	20	0.36
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	11	0.36
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	11	0.36
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	6	0.36
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	6	0.36
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	20	0.36
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	24	0.36
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	5	0.35
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	5	0.35
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	4	0.35
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	4	0.35
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	4	0.35
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	11	0.35
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	11	0.35
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	11	0.35
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	8	0.35
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	8	0.35
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	8	0.35
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	8	0.35
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	8	0.35
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	24	0.35
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	24	0.35
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	24	0.35
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	25	0.35
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	25	0.35
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	25	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	1	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	1	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	1	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	2	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	2	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	2	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	6	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	6	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	6	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	8	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	8	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	8	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	9	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	9	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	9	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	10	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	10	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	10	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	15	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	15	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	15	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	18	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	18	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	18	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB1	22	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB2	22	0.35
(1,89)	1:2:A:ALA:HA	1:2:A:ALA:HB3	22	0.35
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	26	0.35
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	26	0.35
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	24	0.35
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	20	0.35
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	20	0.35
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	15	0.35
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	2	0.35
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	21	0.35
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	12	0.34
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	12	0.34
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	15	0.34
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	15	0.34
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	15	0.34
(1,128)	1:6:A:TRP:HD1	1:16:A:ARG:HE	9	0.34
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	16	0.34
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	16	0.34
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	16	0.34
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	15	0.34
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	15	0.34
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	15	0.34
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	2	0.34
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	2	0.34
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	3	0.34
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	3	0.34
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	20	0.34
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	20	0.34
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	21	0.34
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	21	0.34
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	24	0.34
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	24	0.34
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	27	0.34
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	27	0.34
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	21	0.34
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	13	0.34
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	13	0.34
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	26	0.34
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	9	0.34
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	17	0.34
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	17	0.34
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	1	0.34
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	5	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	5	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	5	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	7	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	7	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	7	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	8	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	8	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	9	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	9	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	9	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	13	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	13	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	13	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	21	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	21	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	21	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	22	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	22	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	22	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	23	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	23	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	23	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	26	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	26	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	26	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	28	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	28	0.33
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	28	0.33
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	12	0.33
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	12	0.33
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	12	0.33
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	12	0.33
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	12	0.33
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	12	0.33
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	6	0.33
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	6	0.33
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	6	0.33
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	13	0.33
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	13	0.33
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	13	0.33
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	20	0.33
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	20	0.33
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	20	0.33
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	28	0.33
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	28	0.33
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	28	0.33
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	10	0.33
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	10	0.33
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	11	0.33
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	11	0.33
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	12	0.33
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	12	0.33
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	25	0.33
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	25	0.33
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	28	0.33
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	28	0.33
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	28	0.33
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	19	0.33
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	19	0.33
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	27	0.33
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	17	0.33
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	17	0.33
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	21	0.33
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	21	0.33
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	6	0.33
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	14	0.33
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	11	0.32
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	11	0.32
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	11	0.32
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	16	0.32
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	16	0.32
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	16	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	1	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	1	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	1	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	2	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	2	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	2	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	3	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	3	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	3	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	4	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	4	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	4	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	6	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	6	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	6	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	10	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	10	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	11	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	11	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	11	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	14	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	14	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	14	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	16	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	16	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	16	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	17	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	17	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	17	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	18	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	18	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	18	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	19	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	19	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	19	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	20	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	20	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	20	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	24	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	24	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	24	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	25	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	25	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	25	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	27	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	27	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	27	0.32
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	8	0.32
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	5	0.32
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	5	0.32
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	5	0.32
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	14	0.32
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	14	0.32
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	14	0.32
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	4	0.32
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	4	0.32
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	6	0.32
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	15	0.32
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	15	0.32
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	16	0.32
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	16	0.32
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	14	0.32
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	14	0.32
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	26	0.32
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	26	0.32
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	10	0.32
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	5	0.32
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	17	0.32
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	23	0.32
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	12	0.31
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	12	0.31
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	12	0.31
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	15	0.31
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	15	0.31
(1,166)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	15	0.31
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	21	0.31
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	21	0.31
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	21	0.31
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	28	0.31
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	5	0.31
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	5	0.31
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	10	0.31
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	10	0.31
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	18	0.31
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	18	0.31
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	12	0.31
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	12	0.31
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	22	0.31
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	22	0.31
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	8	0.31
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	5	0.31
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	25	0.31
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	6	0.31
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	12	0.31
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	19	0.3
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	19	0.3
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	27	0.3
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	27	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	26	0.3
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	26	0.3
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	26	0.3
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	27	0.3
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	27	0.3
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	27	0.3
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	28	0.3
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	28	0.3
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	28	0.3
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	14	0.3
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	14	0.3
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	14	0.3
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	16	0.3
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	16	0.3
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	16	0.3
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	27	0.3
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	27	0.3
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	27	0.3
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	10	0.3
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	14	0.3
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	14	0.3
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	14	0.3
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	16	0.3
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	16	0.3
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	22	0.3
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	22	0.3
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	10	0.3
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	8	0.3
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	8	0.3
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	17	0.3
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	17	0.3
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	19	0.3
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	19	0.3
(1,63)	1:18:A:PRO:HD2	1:17:A:PRO:HB3	18	0.3
(1,63)	1:18:A:PRO:HD3	1:17:A:PRO:HB3	18	0.3
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	26	0.3
(1,38)	1:14:A:SER:HB3	1:9:A:ASP:HB2	6	0.3
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	6	0.3
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	15	0.3
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	5	0.3
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	3	0.29
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	3	0.29
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	7	0.29
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	23	0.29
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	5	0.29
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	5	0.29
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	5	0.29
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	19	0.29
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	19	0.29
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	19	0.29
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	9	0.29
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	9	0.29
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	9	0.29
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	6	0.29
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	15	0.29
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	17	0.29
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	18	0.29
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	25	0.29
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	1	0.29
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	1	0.29
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	10	0.29
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	10	0.29
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	21	0.29
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	12	0.29
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	1	0.29
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	2	0.29
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	4	0.29
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	8	0.29
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	17	0.29
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	15	0.28
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	15	0.28
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	15	0.28
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	22	0.28
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	22	0.28
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	22	0.28
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	28	0.28
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	28	0.28
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	28	0.28
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	5	0.28
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	9	0.28
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	13	0.28
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	12	0.28
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	12	0.28
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	4	0.28
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	4	0.28
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	4	0.28
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	7	0.28
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	7	0.28
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	7	0.28
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	12	0.28
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	12	0.28
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	12	0.28
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	14	0.28
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	14	0.28
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	14	0.28
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	22	0.28
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	22	0.28
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	22	0.28
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	26	0.28
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	26	0.28
(1,83)	1:19:A:PRO:HB2	1:20:A:SER:H	9	0.28
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	9	0.28
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	20	0.28
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	26	0.28
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	7	0.28
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	7	0.28
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	9	0.28
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	9	0.28
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	13	0.28
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	13	0.28
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	3	0.28
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	9	0.28
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	9	0.28
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	2	0.28
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	2	0.28
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	27	0.28
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	1	0.28
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	18	0.28
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	13	0.28
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	25	0.27
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	25	0.27
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	25	0.27
(1,153)	1:7:A:LEU:HD21	1:6:A:TRP:HE3	26	0.27
(1,153)	1:7:A:LEU:HD22	1:6:A:TRP:HE3	26	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:7:A:LEU:HD23	1:6:A:TRP:HE3	26	0.27
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	2	0.27
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	10	0.27
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	14	0.27
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	20	0.27
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	2	0.27
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	2	0.27
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	2	0.27
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	10	0.27
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	10	0.27
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	10	0.27
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	11	0.27
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	11	0.27
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	11	0.27
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	17	0.27
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	17	0.27
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	17	0.27
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	19	0.27
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	19	0.27
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	19	0.27
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	26	0.27
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	26	0.27
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	26	0.27
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	27	0.27
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	27	0.27
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	27	0.27
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	7	0.27
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	13	0.27
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	14	0.27
(1,53)	1:16:A:ARG:HB2	1:6:A:TRP:HE1	17	0.27
(1,53)	1:16:A:ARG:HB3	1:6:A:TRP:HE1	17	0.27
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	13	0.27
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	13	0.27
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	7	0.27
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	21	0.27
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	27	0.27
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	27	0.27
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	2	0.27
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	2	0.27
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	8	0.27
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	17	0.27
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	7	0.27
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	16	0.27
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	18	0.27
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	26	0.27
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	9	0.26
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	9	0.26
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	10	0.26
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	10	0.26
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	18	0.26
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	18	0.26
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	18	0.26
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	4	0.26
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	1	0.26
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	4	0.26
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	17	0.26
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	18	0.26
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	21	0.26
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	28	0.26
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	22	0.26
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	22	0.26
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	22	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	1	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	1	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	1	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	3	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	3	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	3	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	15	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	15	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	15	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	16	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	16	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	16	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	18	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	18	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	18	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	20	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	20	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	20	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	23	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	23	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	23	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	24	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	24	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	24	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	25	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	25	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	25	0.26
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	28	0.26
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	28	0.26
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	28	0.26
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	4	0.26
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	16	0.26
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	23	0.26
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	9	0.26
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	9	0.26
(1,52)	1:16:A:ARG:HB2	1:6:A:TRP:HD1	5	0.26
(1,52)	1:16:A:ARG:HB3	1:6:A:TRP:HD1	5	0.26
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	24	0.26
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	24	0.26
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	5	0.26
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	5	0.26
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	11	0.26
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	11	0.26
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	19	0.26
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	19	0.26
(1,38)	1:14:A:SER:HB3	1:9:A:ASP:HB2	2	0.26
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	11	0.26
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	18	0.26
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	18	0.26
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	28	0.26
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	28	0.26
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	6	0.26
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	6	0.26
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	12	0.26
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	12	0.26
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	2	0.26
(1,14)	1:12:A:PRO:HD2	1:12:A:PRO:HB2	19	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	3	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	9	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	10	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	14	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	15	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	22	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	23	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	24	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	25	0.26
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	27	0.26
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	23	0.25
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	23	0.25
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	6	0.25
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	6	0.25
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	6	0.25
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	12	0.25
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	12	0.25
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	12	0.25
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	17	0.25
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	17	0.25
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	17	0.25
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	19	0.25
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	19	0.25
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	19	0.25
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	19	0.25
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	24	0.25
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	26	0.25
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	26	0.25
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	26	0.25
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	5	0.25
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	5	0.25
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	5	0.25
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	6	0.25
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	6	0.25
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	6	0.25
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	8	0.25
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	8	0.25
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	8	0.25
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	13	0.25
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	13	0.25
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	13	0.25
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	11	0.25
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	11	0.25
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	12	0.25
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	19	0.25
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	27	0.25
(1,66)	1:18:A:PRO:HD2	1:18:A:PRO:HB3	14	0.25
(1,66)	1:18:A:PRO:HD3	1:18:A:PRO:HB3	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	3	0.25
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	3	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	4	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	4	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	7	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	7	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	8	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	8	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	10	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	10	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	18	0.25
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	18	0.25
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	15	0.25
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	4	0.25
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	11	0.25
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	20	0.25
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	21	0.25
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	21	0.24
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	21	0.24
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	21	0.24
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	24	0.24
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	24	0.24
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	24	0.24
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	6	0.24
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	7	0.24
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	15	0.24
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	27	0.24
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	6	0.24
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	25	0.24
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	27	0.24
(1,114)	1:4:A:ALA:HB1	1:4:A:ALA:H	21	0.24
(1,114)	1:4:A:ALA:HB2	1:4:A:ALA:H	21	0.24
(1,114)	1:4:A:ALA:HB3	1:4:A:ALA:H	21	0.24
(1,91)	1:2:A:ALA:HB1	1:3:A:TYR:H	7	0.24
(1,91)	1:2:A:ALA:HB2	1:3:A:TYR:H	7	0.24
(1,91)	1:2:A:ALA:HB3	1:3:A:TYR:H	7	0.24
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	14	0.24
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	14	0.24
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	5	0.24
(1,59)	1:17:A:PRO:HD2	1:17:A:PRO:HB2	22	0.24
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	2	0.24
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	1	0.24
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	1	0.24
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	9	0.24
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	9	0.24
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB2	14	0.24
(1,45)	1:16:A:ARG:HA	1:16:A:ARG:HB3	14	0.24
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	2	0.24
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	9	0.24
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	9	0.24
(1,17)	1:12:A:PRO:HB2	1:13:A:SER:H	19	0.24
(1,13)	1:12:A:PRO:HA	1:12:A:PRO:HG3	28	0.24
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	1	0.23
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	1	0.23
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	1	0.23
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	5	0.23
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	5	0.23
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	5	0.23
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	22	0.23
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	22	0.23
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	22	0.23
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	1	0.23
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	25	0.23
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	12	0.23
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	15	0.23
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	16	0.23
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	13	0.23
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	13	0.23
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	13	0.23
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	3	0.23
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	24	0.23
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	10	0.23
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	10	0.23
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB2	2	0.22
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB3	2	0.22
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	2	0.22
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	2	0.22
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	2	0.22
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	13	0.22
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	13	0.22
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	13	0.22
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	20	0.22
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	20	0.22
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	23	0.22
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	19	0.22
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	19	0.22
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	19	0.22
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	2	0.22
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	8	0.22
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	11	0.22
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	24	0.22
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	25	0.22
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	5	0.22
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	5	0.22
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	11	0.22
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	11	0.22
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	12	0.22
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	12	0.22
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	14	0.22
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	14	0.22
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	21	0.22
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	21	0.22
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	22	0.22
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	22	0.22
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	20	0.21
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	20	0.21
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	9	0.21
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	9	0.21
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	9	0.21
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	10	0.21
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	10	0.21
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	10	0.21
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	23	0.21
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	23	0.21
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	23	0.21
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	3	0.21
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	3	0.21
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	3	0.21
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	2	0.21
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	13	0.21
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	17	0.21
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	20	0.21
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	7	0.21
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	7	0.21
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	7	0.21
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	7	0.21
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	7	0.21
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	21	0.21
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	21	0.21
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	21	0.21
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	21	0.21
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	21	0.21
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	21	0.21
(1,143)	1:6:A:TRP:HA	1:9:A:ASP:HB3	2	0.21
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	3	0.21
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	11	0.21
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	22	0.21
(1,139)	1:6:A:TRP:HB2	1:6:A:TRP:HE3	26	0.21
(1,97)	1:3:A:TYR:HA	1:19:A:PRO:HG2	17	0.21
(1,83)	1:19:A:PRO:HB2	1:20:A:SER:H	6	0.21
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	1	0.21
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	16	0.21
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	16	0.21
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	16	0.21
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	23	0.21
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	23	0.21
(1,29)	1:14:A:SER:HA	1:14:A:SER:HB2	5	0.21
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	4	0.21
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	4	0.21
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	11	0.21
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	11	0.21
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	26	0.21
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	26	0.21
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	18	0.2
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	14	0.2
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	14	0.2
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	7	0.2
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	7	0.2
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	7	0.2
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	9	0.2
(1,143)	1:6:A:TRP:HA	1:9:A:ASP:HB3	4	0.2
(1,60)	1:17:A:PRO:HA	1:17:A:PRO:HG3	12	0.2
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	1	0.2
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	1	0.2
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	20	0.2
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	9	0.2
(1,23)	1:13:A:SER:HA	1:13:A:SER:HB2	22	0.2
(1,23)	1:13:A:SER:HA	1:13:A:SER:HB3	22	0.2
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	4	0.2
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	4	0.2
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	5	0.2
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	5	0.2
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	9	0.2
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	9	0.2
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	15	0.2
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	15	0.2
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	27	0.2
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	27	0.2
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	3	0.19
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	3	0.19
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	8	0.19
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	8	0.19
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	8	0.19
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	5	0.19
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	21	0.19
(1,125)	1:5:A:GLN:HA	1:5:A:GLN:HB2	25	0.19
(1,97)	1:3:A:TYR:HA	1:19:A:PRO:HG2	26	0.19
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB2	11	0.19
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB3	11	0.19
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	19	0.19
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	19	0.19
(1,83)	1:19:A:PRO:HB2	1:20:A:SER:H	8	0.19
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE1	13	0.19
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE2	13	0.19
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE1	24	0.19
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE2	24	0.19
(1,60)	1:17:A:PRO:HA	1:17:A:PRO:HG3	6	0.19
(1,60)	1:17:A:PRO:HA	1:17:A:PRO:HG3	15	0.19
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	22	0.19
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	3	0.19
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	3	0.19
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	26	0.19
(1,23)	1:13:A:SER:HA	1:13:A:SER:HB2	4	0.19
(1,23)	1:13:A:SER:HA	1:13:A:SER:HB3	4	0.19
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	2	0.19
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	7	0.19
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	7	0.19
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	20	0.19
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	20	0.19
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	28	0.19
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	28	0.19
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	4	0.18
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	4	0.18
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	4	0.18
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	16	0.18
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	19	0.18
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB2	8	0.18
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB3	8	0.18
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	24	0.18
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	13	0.18
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	13	0.18
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	5	0.18
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	5	0.18
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	8	0.18
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	8	0.18
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	16	0.18
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	16	0.18
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	23	0.18
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	23	0.18
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	25	0.18
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	25	0.18
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	15	0.17
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	15	0.17
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB2	17	0.17
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB3	17	0.17
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	18	0.17
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	24	0.17
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	26	0.17
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	28	0.17
(1,125)	1:5:A:GLN:HA	1:5:A:GLN:HB2	6	0.17
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	25	0.17
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	25	0.17
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	25	0.17
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	13	0.17
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	13	0.17
(1,97)	1:3:A:TYR:HA	1:19:A:PRO:HG2	28	0.17
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB2	25	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB3	25	0.17
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	17	0.17
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	17	0.17
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	15	0.17
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	28	0.17
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	21	0.17
(1,68)	1:18:A:PRO:HB3	1:3:A:TYR:HE1	22	0.17
(1,68)	1:18:A:PRO:HB3	1:3:A:TYR:HE2	22	0.17
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	6	0.17
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	6	0.17
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	10	0.17
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	10	0.17
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	17	0.17
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	17	0.17
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	16	0.17
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	16	0.17
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	17	0.17
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	22	0.17
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	8	0.17
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	8	0.17
(1,19)	1:12:A:PRO:HD3	1:6:A:TRP:HH2	7	0.17
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	6	0.17
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	6	0.17
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	24	0.17
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	24	0.17
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	5	0.16
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	8	0.16
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	1	0.16
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	1	0.16
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	13	0.16
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	13	0.16
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	25	0.16
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	25	0.16
(1,168)	1:7:A:LEU:HD21	1:7:A:LEU:H	14	0.16
(1,168)	1:7:A:LEU:HD22	1:7:A:LEU:H	14	0.16
(1,168)	1:7:A:LEU:HD23	1:7:A:LEU:H	14	0.16
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	8	0.16
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	14	0.16
(1,125)	1:5:A:GLN:HA	1:5:A:GLN:HB2	7	0.16
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	20	0.16
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	20	0.16
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	5	0.16
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	5	0.16
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	27	0.16
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	27	0.16
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD1	28	0.16
(1,84)	1:19:A:PRO:HD2	1:3:A:TYR:HD2	28	0.16
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	6	0.16
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	9	0.16
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	10	0.16
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	22	0.16
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	20	0.16
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	8	0.16
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	8	0.16
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	12	0.16
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	12	0.16
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	21	0.16
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	21	0.16
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	22	0.16
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	22	0.16
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	23	0.16
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	23	0.16
(1,37)	1:14:A:SER:HB2	1:9:A:ASP:HB2	11	0.16
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	28	0.16
(1,24)	1:13:A:SER:HB2	1:13:A:SER:H	22	0.16
(1,24)	1:13:A:SER:HB3	1:13:A:SER:H	22	0.16
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	1	0.16
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	1	0.16
(1,19)	1:12:A:PRO:HD3	1:6:A:TRP:HH2	28	0.16
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	4	0.16
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	22	0.16
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	11	0.15
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	13	0.15
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	18	0.15
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	18	0.15
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB2	16	0.15
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB3	16	0.15
(1,167)	1:7:A:LEU:HD11	1:7:A:LEU:H	22	0.15
(1,167)	1:7:A:LEU:HD12	1:7:A:LEU:H	22	0.15
(1,167)	1:7:A:LEU:HD13	1:7:A:LEU:H	22	0.15
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	12	0.15
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE1	5	0.15
(1,147)	1:7:A:LEU:HD11	1:3:A:TYR:HE2	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE1	5	0.15
(1,147)	1:7:A:LEU:HD12	1:3:A:TYR:HE2	5	0.15
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE1	5	0.15
(1,147)	1:7:A:LEU:HD13	1:3:A:TYR:HE2	5	0.15
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	23	0.15
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	23	0.15
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	23	0.15
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	4	0.15
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	4	0.15
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB2	14	0.15
(1,86)	1:1:A:ASP:HA	1:1:A:ASP:HB3	14	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	1	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	3	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	4	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	5	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	7	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	8	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	11	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	12	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	17	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	18	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	19	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	21	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	24	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	25	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	26	0.15
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	27	0.15
(1,60)	1:17:A:PRO:HA	1:17:A:PRO:HG3	17	0.15
(1,53)	1:16:A:ARG:HB2	1:6:A:TRP:HE1	26	0.15
(1,53)	1:16:A:ARG:HB3	1:6:A:TRP:HE1	26	0.15
(1,51)	1:16:A:ARG:HG2	1:6:A:TRP:HD1	19	0.15
(1,51)	1:16:A:ARG:HG3	1:6:A:TRP:HD1	19	0.15
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	15	0.15
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	15	0.15
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	18	0.15
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	18	0.15
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	24	0.15
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	24	0.15
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	26	0.15
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	26	0.15
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	27	0.15
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	27	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:14:A:SER:HB2	1:9:A:ASP:HB2	28	0.15
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	16	0.15
(1,31)	1:14:A:SER:HB2	1:14:A:SER:H	20	0.15
(1,19)	1:12:A:PRO:HD3	1:6:A:TRP:HH2	13	0.15
(1,15)	1:12:A:PRO:HD2	1:13:A:SER:H	22	0.15
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	22	0.15
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	28	0.15
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	11	0.15
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	21	0.15
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	24	0.15
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	28	0.15
(1,9)	1:12:A:PRO:HD2	1:11:A:GLY:H	4	0.15
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	4	0.15
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	4	0.15
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	12	0.15
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	12	0.15
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	19	0.15
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	19	0.15
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	24	0.14
(1,169)	1:7:A:LEU:H	1:8:A:LYS:H	14	0.14
(1,167)	1:7:A:LEU:HD11	1:7:A:LEU:H	11	0.14
(1,167)	1:7:A:LEU:HD12	1:7:A:LEU:H	11	0.14
(1,167)	1:7:A:LEU:HD13	1:7:A:LEU:H	11	0.14
(1,125)	1:5:A:GLN:HA	1:5:A:GLN:HB2	21	0.14
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD11	24	0.14
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD12	24	0.14
(1,120)	1:4:A:ALA:HA	1:7:A:LEU:HD13	24	0.14
(1,99)	1:3:A:TYR:HA	1:19:A:PRO:HB3	15	0.14
(1,97)	1:3:A:TYR:HA	1:19:A:PRO:HG2	25	0.14
(1,87)	1:20:A:SER:HA	1:20:A:SER:HB2	6	0.14
(1,87)	1:20:A:SER:HA	1:20:A:SER:HB3	6	0.14
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	2	0.14
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	13	0.14
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	14	0.14
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	20	0.14
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	23	0.14
(1,74)	1:19:A:PRO:HD2	1:18:A:PRO:HA	22	0.14
(1,50)	1:16:A:ARG:HA	1:17:A:PRO:HD2	12	0.14
(1,48)	1:16:A:ARG:HD2	1:16:A:ARG:HE	28	0.14
(1,48)	1:16:A:ARG:HD3	1:16:A:ARG:HE	28	0.14
(1,20)	1:12:A:PRO:HG2	1:6:A:TRP:HH2	19	0.14
(1,20)	1:12:A:PRO:HG3	1:6:A:TRP:HH2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:12:A:PRO:HD3	1:6:A:TRP:HH2	14	0.14
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	11	0.14
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	20	0.14
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	21	0.14
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	24	0.14
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	3	0.14
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	7	0.14
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	14	0.14
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	16	0.14
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	20	0.14
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	25	0.14
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	26	0.14
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	27	0.14
(1,9)	1:12:A:PRO:HD2	1:11:A:GLY:H	3	0.14
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	17	0.14
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	17	0.14
(1,167)	1:7:A:LEU:HD11	1:7:A:LEU:H	5	0.13
(1,167)	1:7:A:LEU:HD12	1:7:A:LEU:H	5	0.13
(1,167)	1:7:A:LEU:HD13	1:7:A:LEU:H	5	0.13
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	3	0.13
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE1	28	0.13
(1,148)	1:7:A:LEU:HD21	1:3:A:TYR:HE2	28	0.13
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE1	28	0.13
(1,148)	1:7:A:LEU:HD22	1:3:A:TYR:HE2	28	0.13
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE1	28	0.13
(1,148)	1:7:A:LEU:HD23	1:3:A:TYR:HE2	28	0.13
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	9	0.13
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	9	0.13
(1,97)	1:3:A:TYR:HA	1:19:A:PRO:HG2	16	0.13
(1,87)	1:20:A:SER:HA	1:20:A:SER:HB2	7	0.13
(1,87)	1:20:A:SER:HA	1:20:A:SER:HB3	7	0.13
(1,87)	1:20:A:SER:HA	1:20:A:SER:HB2	10	0.13
(1,87)	1:20:A:SER:HA	1:20:A:SER:HB3	10	0.13
(1,80)	1:19:A:PRO:HD2	1:19:A:PRO:HG2	16	0.13
(1,53)	1:16:A:ARG:HB2	1:6:A:TRP:HE1	28	0.13
(1,53)	1:16:A:ARG:HB3	1:6:A:TRP:HE1	28	0.13
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	25	0.13
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	25	0.13
(1,46)	1:16:A:ARG:HB2	1:16:A:ARG:H	28	0.13
(1,46)	1:16:A:ARG:HB3	1:16:A:ARG:H	28	0.13
(1,39)	1:15:A:GLY:H	1:14:A:SER:H	19	0.13
(1,38)	1:14:A:SER:HB3	1:9:A:ASP:HB2	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	23	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	3	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	7	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	9	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	10	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	14	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	15	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	16	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	23	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	25	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	26	0.13
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	27	0.13
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	9	0.13
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	10	0.13
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	15	0.13
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	23	0.13
(1,2)	1:10:A:GLY:H	1:11:A:GLY:H	18	0.13
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB2	7	0.12
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB3	7	0.12
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB2	13	0.12
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB3	13	0.12
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB2	14	0.12
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB3	14	0.12
(1,150)	1:7:A:LEU:H	1:6:A:TRP:H	22	0.12
(1,143)	1:6:A:TRP:HA	1:9:A:ASP:HB3	6	0.12
(1,140)	1:6:A:TRP:HB3	1:7:A:LEU:H	9	0.12
(1,125)	1:5:A:GLN:HA	1:5:A:GLN:HB2	16	0.12
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	10	0.12
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	10	0.12
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	23	0.12
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	23	0.12
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	24	0.12
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	24	0.12
(1,97)	1:3:A:TYR:HA	1:19:A:PRO:HG2	19	0.12
(1,85)	1:19:A:PRO:HD2	1:6:A:TRP:HD1	24	0.12
(1,51)	1:16:A:ARG:HG2	1:6:A:TRP:HD1	1	0.12
(1,51)	1:16:A:ARG:HG3	1:6:A:TRP:HD1	1	0.12
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	13	0.12
(1,19)	1:12:A:PRO:HD3	1:6:A:TRP:HH2	20	0.12
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	13	0.12
(1,12)	1:12:A:PRO:HD2	1:12:A:PRO:HG2	18	0.12
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	2	0.12
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	4	0.12
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	8	0.12
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	13	0.12
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	18	0.12
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	19	0.12
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	2	0.11
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	9	0.11
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	12	0.11
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	25	0.11
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	6	0.11
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	6	0.11
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	17	0.11
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	17	0.11
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB2	15	0.11
(1,176)	1:8:A:LYS:HA	1:8:A:LYS:HB3	15	0.11
(1,169)	1:7:A:LEU:H	1:8:A:LYS:H	15	0.11
(1,167)	1:7:A:LEU:HD11	1:7:A:LEU:H	28	0.11
(1,167)	1:7:A:LEU:HD12	1:7:A:LEU:H	28	0.11
(1,167)	1:7:A:LEU:HD13	1:7:A:LEU:H	28	0.11
(1,152)	1:7:A:LEU:HD21	1:6:A:TRP:HZ3	22	0.11
(1,152)	1:7:A:LEU:HD22	1:6:A:TRP:HZ3	22	0.11
(1,152)	1:7:A:LEU:HD23	1:6:A:TRP:HZ3	22	0.11
(1,140)	1:6:A:TRP:HB3	1:7:A:LEU:H	10	0.11
(1,125)	1:5:A:GLN:HA	1:5:A:GLN:HB2	28	0.11
(1,116)	1:4:A:ALA:HB1	1:5:A:GLN:H	27	0.11
(1,116)	1:4:A:ALA:HB2	1:5:A:GLN:H	27	0.11
(1,116)	1:4:A:ALA:HB3	1:5:A:GLN:H	27	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	3	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	3	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	3	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	3	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	5	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	5	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	5	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	5	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	6	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	6	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	6	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	6	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	7	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	7	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	7	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	10	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	10	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	10	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	10	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	13	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	13	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	13	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	13	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	15	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	15	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	15	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	15	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	18	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	18	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	18	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	18	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	20	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	20	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	20	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	20	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	21	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	21	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	21	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	21	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	23	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	23	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	23	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	23	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	24	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	24	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	24	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	24	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	25	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	25	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	25	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	25	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	27	0.11
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	27	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	27	0.11
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	27	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	25	0.11
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	25	0.11
(1,68)	1:18:A:PRO:HB3	1:3:A:TYR:HE1	11	0.11
(1,68)	1:18:A:PRO:HB3	1:3:A:TYR:HE2	11	0.11
(1,60)	1:17:A:PRO:HA	1:17:A:PRO:HG3	4	0.11
(1,53)	1:16:A:ARG:HB2	1:6:A:TRP:HE1	12	0.11
(1,53)	1:16:A:ARG:HB3	1:6:A:TRP:HE1	12	0.11
(1,35)	1:14:A:SER:HB3	1:9:A:ASP:HB3	4	0.11
(1,22)	1:12:A:PRO:HA	1:6:A:TRP:HH2	28	0.11
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	5	0.11
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	6	0.11
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	12	0.11
(1,11)	1:12:A:PRO:HD3	1:12:A:PRO:HG3	17	0.11
(1,2)	1:10:A:GLY:H	1:11:A:GLY:H	13	0.11
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	1	0.11
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	1	0.11
(1,181)	1:9:A:ASP:H	1:8:A:LYS:H	1	0.1
(1,177)	1:8:A:LYS:HB2	1:9:A:ASP:H	11	0.1
(1,177)	1:8:A:LYS:HB3	1:9:A:ASP:H	11	0.1
(1,175)	1:8:A:LYS:HA	1:8:A:LYS:H	1	0.1
(1,175)	1:8:A:LYS:HA	1:8:A:LYS:H	10	0.1
(1,175)	1:8:A:LYS:HA	1:8:A:LYS:H	16	0.1
(1,175)	1:8:A:LYS:HA	1:8:A:LYS:H	22	0.1
(1,169)	1:7:A:LEU:H	1:8:A:LYS:H	11	0.1
(1,169)	1:7:A:LEU:H	1:8:A:LYS:H	13	0.1
(1,167)	1:7:A:LEU:HD11	1:7:A:LEU:H	8	0.1
(1,167)	1:7:A:LEU:HD12	1:7:A:LEU:H	8	0.1
(1,167)	1:7:A:LEU:HD13	1:7:A:LEU:H	8	0.1
(1,167)	1:7:A:LEU:HD11	1:7:A:LEU:H	26	0.1
(1,167)	1:7:A:LEU:HD12	1:7:A:LEU:H	26	0.1
(1,167)	1:7:A:LEU:HD13	1:7:A:LEU:H	26	0.1
(1,125)	1:5:A:GLN:HA	1:5:A:GLN:HB2	15	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	1	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	1	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	1	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	1	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	2	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	2	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	2	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	2	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	12	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	12	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	12	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	14	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	14	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	14	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	14	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	16	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	16	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	16	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	16	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	26	0.1
(1,102)	1:3:A:TYR:HB2	1:3:A:TYR:HD2	26	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	26	0.1
(1,102)	1:3:A:TYR:HB3	1:3:A:TYR:HD2	26	0.1
(1,101)	1:3:A:TYR:HB2	1:3:A:TYR:H	7	0.1
(1,101)	1:3:A:TYR:HB3	1:3:A:TYR:H	7	0.1
(1,75)	1:19:A:PRO:HD2	1:18:A:PRO:HB2	21	0.1
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE1	3	0.1
(1,67)	1:18:A:PRO:HB2	1:3:A:TYR:HE2	3	0.1
(1,60)	1:17:A:PRO:HA	1:17:A:PRO:HG3	5	0.1
(1,54)	1:16:A:ARG:HG2	1:6:A:TRP:HE1	2	0.1
(1,54)	1:16:A:ARG:HG3	1:6:A:TRP:HE1	2	0.1
(1,51)	1:16:A:ARG:HG2	1:6:A:TRP:HD1	14	0.1
(1,51)	1:16:A:ARG:HG3	1:6:A:TRP:HD1	14	0.1
(1,36)	1:14:A:SER:HB2	1:9:A:ASP:HB3	16	0.1
(1,22)	1:12:A:PRO:HA	1:6:A:TRP:HH2	13	0.1
(1,22)	1:12:A:PRO:HA	1:6:A:TRP:HH2	23	0.1
(1,22)	1:12:A:PRO:HA	1:6:A:TRP:HH2	26	0.1
(1,19)	1:12:A:PRO:HD3	1:6:A:TRP:HH2	21	0.1
(1,1)	1:10:A:GLY:HA2	1:10:A:GLY:H	3	0.1
(1,1)	1:10:A:GLY:HA3	1:10:A:GLY:H	3	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found