



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 01:36 PM UTC

PDB ID : 1L2Y / pdb_00001l2y
BMRB ID : 5292
Title : NMR Structure of Trp-Cage Miniprotein Construct TC5b
Authors : Neidigh, J.W.; Fesinmeyer, R.M.; Andersen, N.H.
Deposited on : 2002-02-25

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

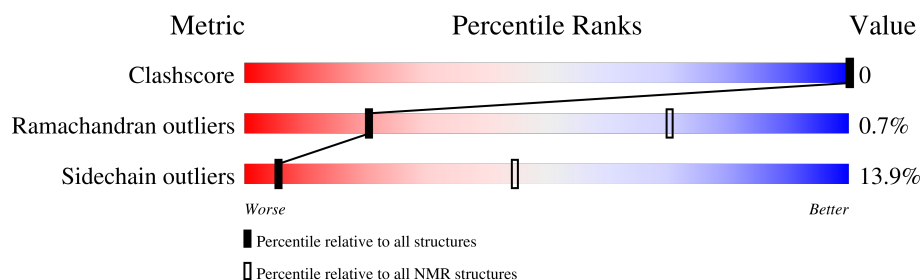
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 53%.

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 38 models. Model 5 is the overall representative, medoid model (most similar to other models).

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	5

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 6 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 304 atoms, of which 150 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TC5b.

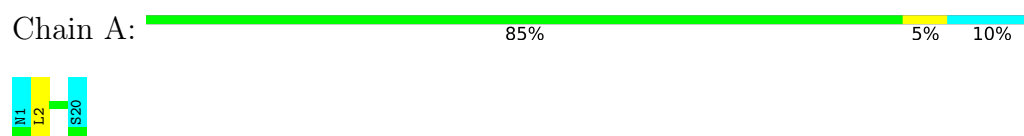
Mol	Chain	Residues	Atoms					Trace
1	A	20	Total	C	H	N	O	0
			304	98	150	27	29	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: TC5b

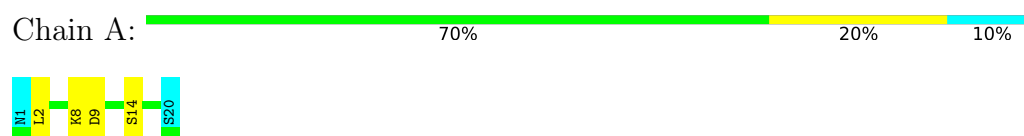


4.2 Scores per residue for each member of the ensemble

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

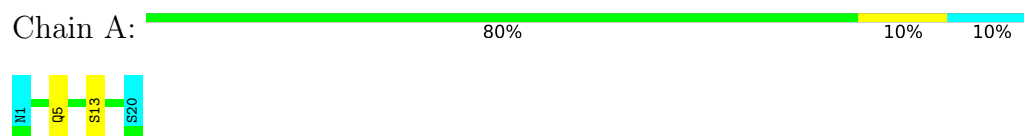
4.2.1 Score per residue for model 1

- Molecule 1: TC5b



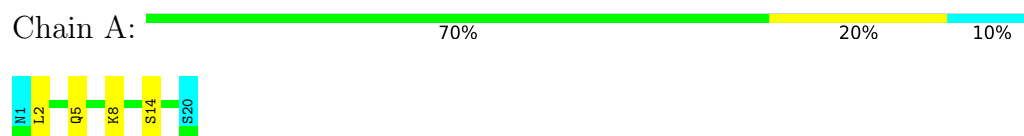
4.2.2 Score per residue for model 2

- Molecule 1: TC5b



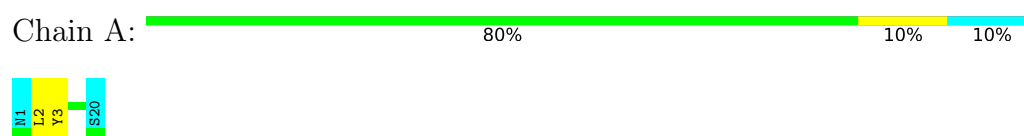
4.2.3 Score per residue for model 3

- Molecule 1: TC5b



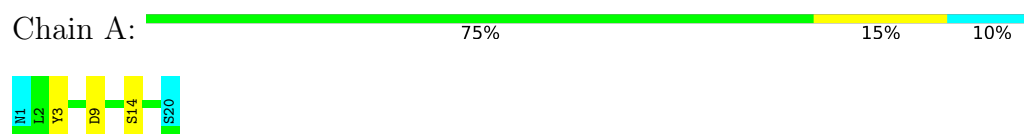
4.2.4 Score per residue for model 4

- Molecule 1: TC5b



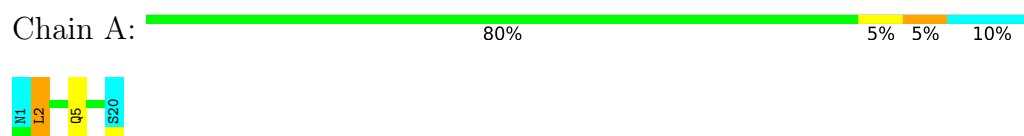
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: TC5b



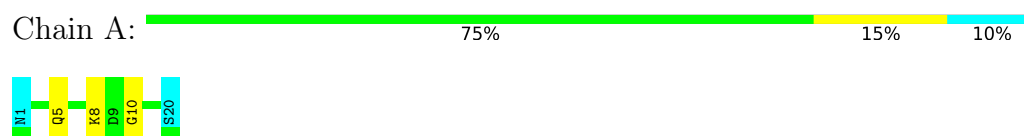
4.2.6 Score per residue for model 6

- Molecule 1: TC5b



4.2.7 Score per residue for model 7

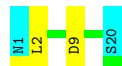
- Molecule 1: TC5b



4.2.8 Score per residue for model 8

- Molecule 1: TC5b

Chain A:  80% 10% 10%



4.2.9 Score per residue for model 9

- Molecule 1: TC5b

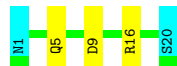
Chain A:  80% 10% 10%



4.2.10 Score per residue for model 10

- Molecule 1: TC5b

Chain A:  75% 15% 10%



4.2.11 Score per residue for model 11

- Molecule 1: TC5b

Chain A:  90% 10%



4.2.12 Score per residue for model 12

- Molecule 1: TC5b

Chain A:  75% 15% 10%



4.2.13 Score per residue for model 13

- Molecule 1: TC5b

Chain A:  85% 5% 10%



4.2.14 Score per residue for model 14

- Molecule 1: TC5b

Chain A:  85% 5% 10%



4.2.15 Score per residue for model 15

- Molecule 1: TC5b

Chain A:  80% 10% 10%



4.2.16 Score per residue for model 16

- Molecule 1: TC5b

Chain A:  70% 20% 10%



4.2.17 Score per residue for model 17

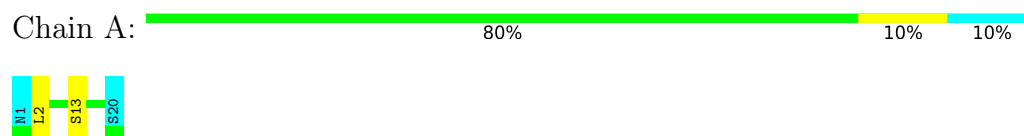
- Molecule 1: TC5b

Chain A:  80% 10% 10%



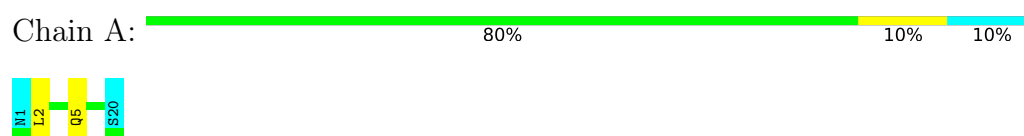
4.2.18 Score per residue for model 18

- Molecule 1: TC5b



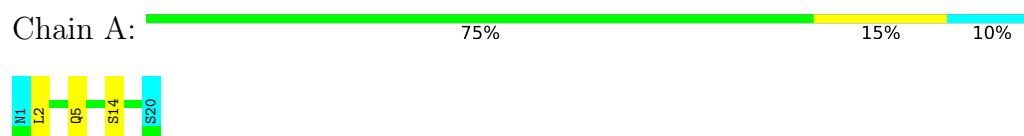
4.2.19 Score per residue for model 19

- Molecule 1: TC5b



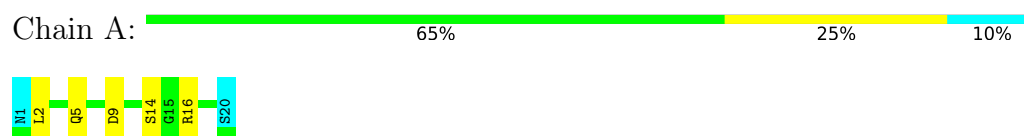
4.2.20 Score per residue for model 20

- Molecule 1: TC5b



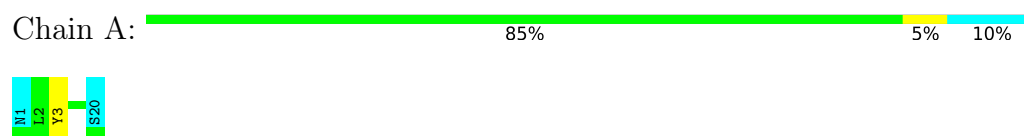
4.2.21 Score per residue for model 21

- Molecule 1: TC5b



4.2.22 Score per residue for model 22

- Molecule 1: TC5b



4.2.23 Score per residue for model 23

- Molecule 1: TC5b

Chain A:  90% 10%



4.2.24 Score per residue for model 24

- Molecule 1: TC5b

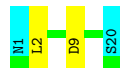
Chain A:  75% 15% 10%



4.2.25 Score per residue for model 25

- Molecule 1: TC5b

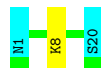
Chain A:  80% 10% 10%



4.2.26 Score per residue for model 26

- Molecule 1: TC5b

Chain A:  85% 5% 10%



4.2.27 Score per residue for model 27

- Molecule 1: TC5b

Chain A:  75% 15% 10%



4.2.28 Score per residue for model 28

- Molecule 1: TC5b

Chain A:  85% 5% 10%



4.2.29 Score per residue for model 29

- Molecule 1: TC5b

Chain A:  75% 15% 10%



4.2.30 Score per residue for model 30

- Molecule 1: TC5b

Chain A:  90% 10%



4.2.31 Score per residue for model 31

- Molecule 1: TC5b

Chain A:  80% 10% 10%



4.2.32 Score per residue for model 32

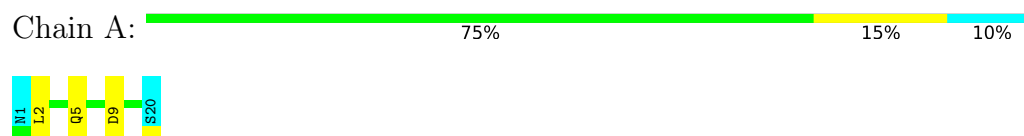
- Molecule 1: TC5b

Chain A:  80% 10% 10%



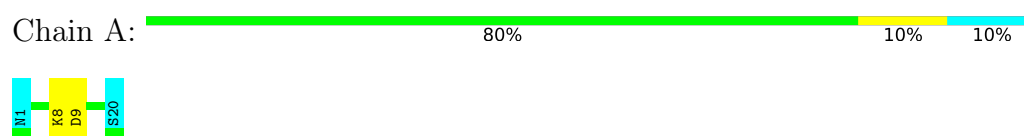
4.2.33 Score per residue for model 33

- Molecule 1: TC5b



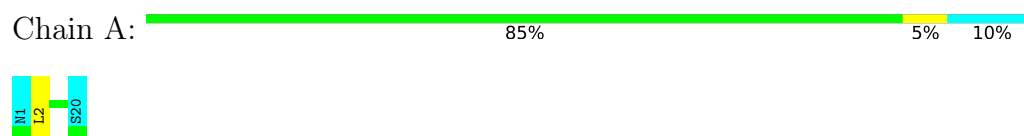
4.2.34 Score per residue for model 34

- Molecule 1: TC5b



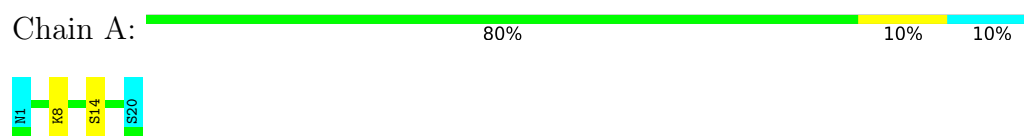
4.2.35 Score per residue for model 35

- Molecule 1: TC5b



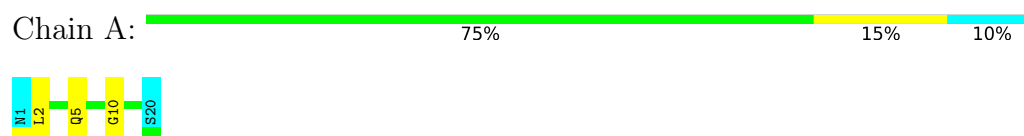
4.2.36 Score per residue for model 36

- Molecule 1: TC5b



4.2.37 Score per residue for model 37

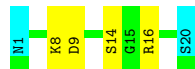
- Molecule 1: TC5b



4.2.38 Score per residue for model 38

- Molecule 1: TC5b

Chain A: 70% 20% 10%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Simulated annealing from random structures followed by steepest descent minimization.*

Of the 50 calculated structures, 38 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with the least restraint violations.*

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

Software name	Classification	Version
CNS	structure solution	1.0
Amber	structure solution	6.0
Amber	refinement	6.0

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	276
Number of shifts mapped to atoms	276
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	53%

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±0/146 (0.0± 0.0%)	1.41±0.05	0±0/201 (0.0± 0.2%)
All	All	0.92	0/5548 (0.0%)	1.41	3/7638 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	2	LEU	CA-C-N	5.61	128.57	120.38	6	1
1	A	2	LEU	C-N-CA	5.61	128.57	120.38	6	1
1	A	18	PRO	N-CA-CB	5.39	106.02	103.22	29	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	5282	5206	5206	-

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 (94±4%)	1±1 (5±4%)	0±0 (1±2%)	20	70
All	All	684/760 (90%)	642 (94%)	37 (5%)	5 (1%)	20	70

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

Mol	Chain	Res	Type	Models (Total)
1	A	10	GLY	4
1	A	2	LEU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	15/17 (88%)	13±1 (86±8%)	2±1 (14±8%)	5	45
All	All	570/646 (88%)	491 (86%)	79 (14%)	5	45

All 8 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	2	LEU	19
1	A	5	GLN	14
1	A	8	LYS	13
1	A	9	ASP	12
1	A	14	SER	12
1	A	16	ARG	4
1	A	3	TYR	3
1	A	13	SER	2

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 53% for the well-defined parts and 53% 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	139
Number of shifts mapped to atoms	139
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 53%, i.e. 127 atoms were assigned a chemical shift out of a possible 238. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	35/85 (41%)	35/35 (100%)	0/36 (0%)	0/14 (0%)
Sidechain	82/132 (62%)	82/86 (95%)	0/41 (0%)	0/5 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	127/238 (53%)	127/131 (97%)	0/87 (0%)	0/20 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 53%, i.e. 136 atoms were assigned a chemical shift out of a possible 258. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	38/95 (40%)	38/39 (97%)	0/40 (0%)	0/16 (0%)
Sidechain	88/142 (62%)	88/92 (96%)	0/44 (0%)	0/6 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	136/258 (53%)	136/141 (96%)	0/94 (0%)	0/23 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

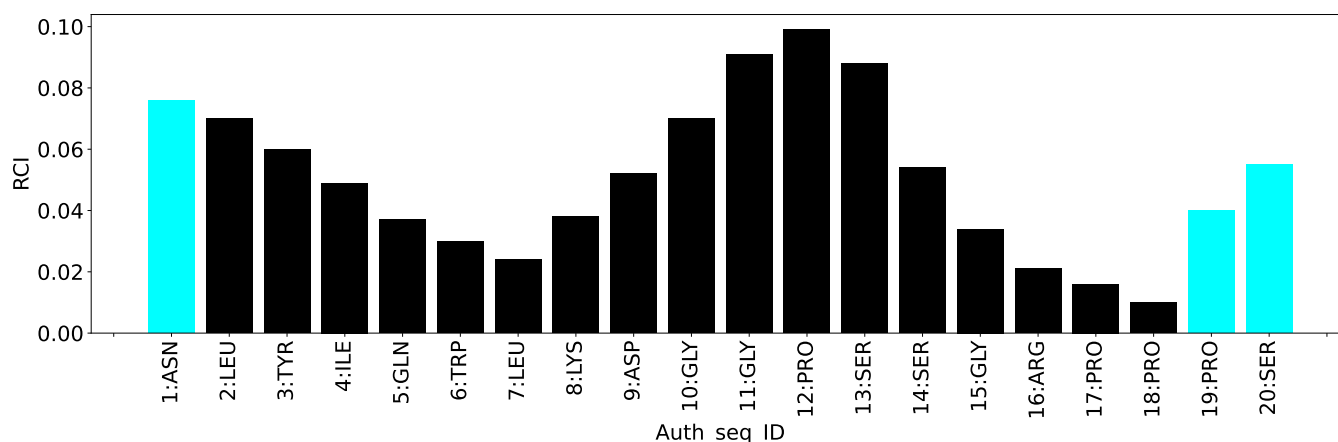
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	11	GLY	HA2	1.05	2.15 – 5.77	-8.1
1	A	18	PRO	HA	2.66	2.78 – 6.00	-5.4

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping [i](#)

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

Total number of shifts	137
Number of shifts mapped to atoms	137
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

7.2.2 Chemical shift referencing [i](#)

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

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 53%, i.e. 127 atoms were assigned a chemical shift out of a possible 238. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	35/85 (41%)	35/35 (100%)	0/36 (0%)	0/14 (0%)
Sidechain	82/132 (62%)	82/86 (95%)	0/41 (0%)	0/5 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	127/238 (53%)	127/131 (97%)	0/87 (0%)	0/20 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 53%, i.e. 136 atoms were assigned a chemical shift out of a possible 258. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	38/95 (40%)	38/39 (97%)	0/40 (0%)	0/16 (0%)
Sidechain	88/142 (62%)	88/92 (96%)	0/44 (0%)	0/6 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	136/258 (53%)	136/141 (96%)	0/94 (0%)	0/23 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

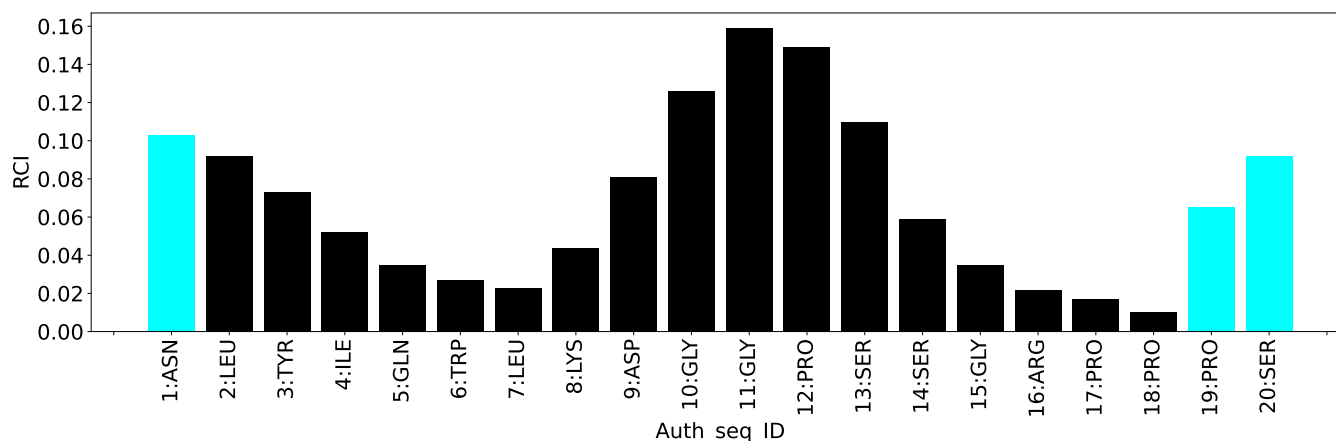
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	11	GLY	HA2	0.95	2.15 – 5.77	-8.3
2	A	18	PRO	HA	2.65	2.78 – 6.00	-5.4

7.2.5 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	169
Intra-residue ($ i-j =0$)	43
Sequential ($ i-j =1$)	62
Medium range ($ i-j >1$ and $ i-j <5$)	36
Long range ($ 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	8.4
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)	7.4	0.2
0.2-0.5 (Medium)	9.7	0.5
>0.5 (Large)	2.4	0.75

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 ⓘ

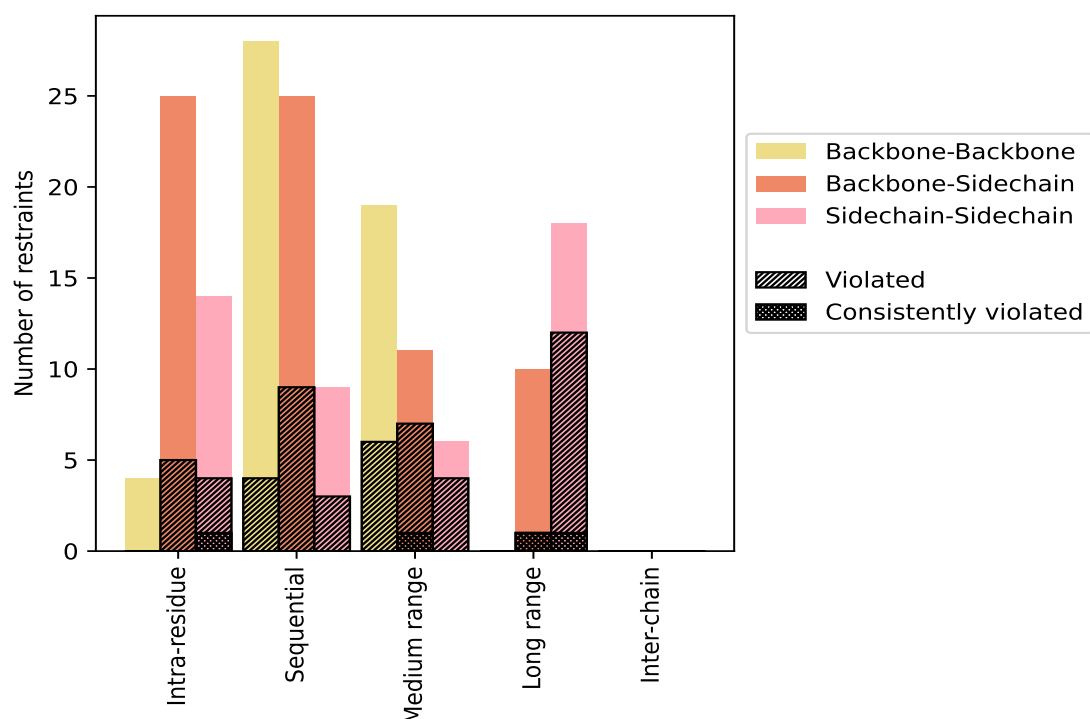
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	43	25.4	9	20.9	5.3	1	2.3	0.6
Backbone-Backbone	4	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	25	14.8	5	20.0	3.0	0	0.0	0.0
Sidechain-Sidechain	14	8.3	4	28.6	2.4	1	7.1	0.6
Sequential ($i-j =1$)	62	36.7	16	25.8	9.5	0	0.0	0.0
Backbone-Backbone	28	16.6	4	14.3	2.4	0	0.0	0.0
Backbone-Sidechain	25	14.8	9	36.0	5.3	0	0.0	0.0
Sidechain-Sidechain	9	5.3	3	33.3	1.8	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	36	21.3	17	47.2	10.1	1	2.8	0.6
Backbone-Backbone	19	11.2	6	31.6	3.6	0	0.0	0.0
Backbone-Sidechain	11	6.5	7	63.6	4.1	1	9.1	0.6
Sidechain-Sidechain	6	3.6	4	66.7	2.4	0	0.0	0.0
Long range ($i-j \geq 5$)	28	16.6	13	46.4	7.7	2	7.1	1.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	10	5.9	1	10.0	0.6	1	10.0	0.6
Sidechain-Sidechain	18	10.7	12	66.7	7.1	1	5.6	0.6
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	169	100.0	55	32.5	32.5	4	2.4	2.4
Backbone-Backbone	51	30.2	10	19.6	5.9	0	0.0	0.0
Backbone-Sidechain	71	42.0	22	31.0	13.0	2	2.8	1.2
Sidechain-Sidechain	47	27.8	23	48.9	13.6	2	4.3	1.2

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

9.1.1 Bar chart : Distribution of distance restraints and violations [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	5	6	7	6	0	24	0.28	0.59	0.15	0.26
2	5	4	6	4	0	19	0.32	0.69	0.17	0.24
3	3	4	6	3	0	16	0.34	0.71	0.18	0.34
4	4	7	6	4	0	21	0.27	0.65	0.14	0.21
5	4	6	6	4	0	20	0.26	0.48	0.15	0.2
6	4	4	6	6	0	20	0.35	0.7	0.17	0.38
7	5	2	7	4	0	18	0.3	0.63	0.16	0.24
8	5	5	8	4	0	22	0.26	0.59	0.16	0.18
9	4	5	7	5	0	21	0.28	0.63	0.17	0.2
10	3	4	7	5	0	19	0.32	0.65	0.16	0.25

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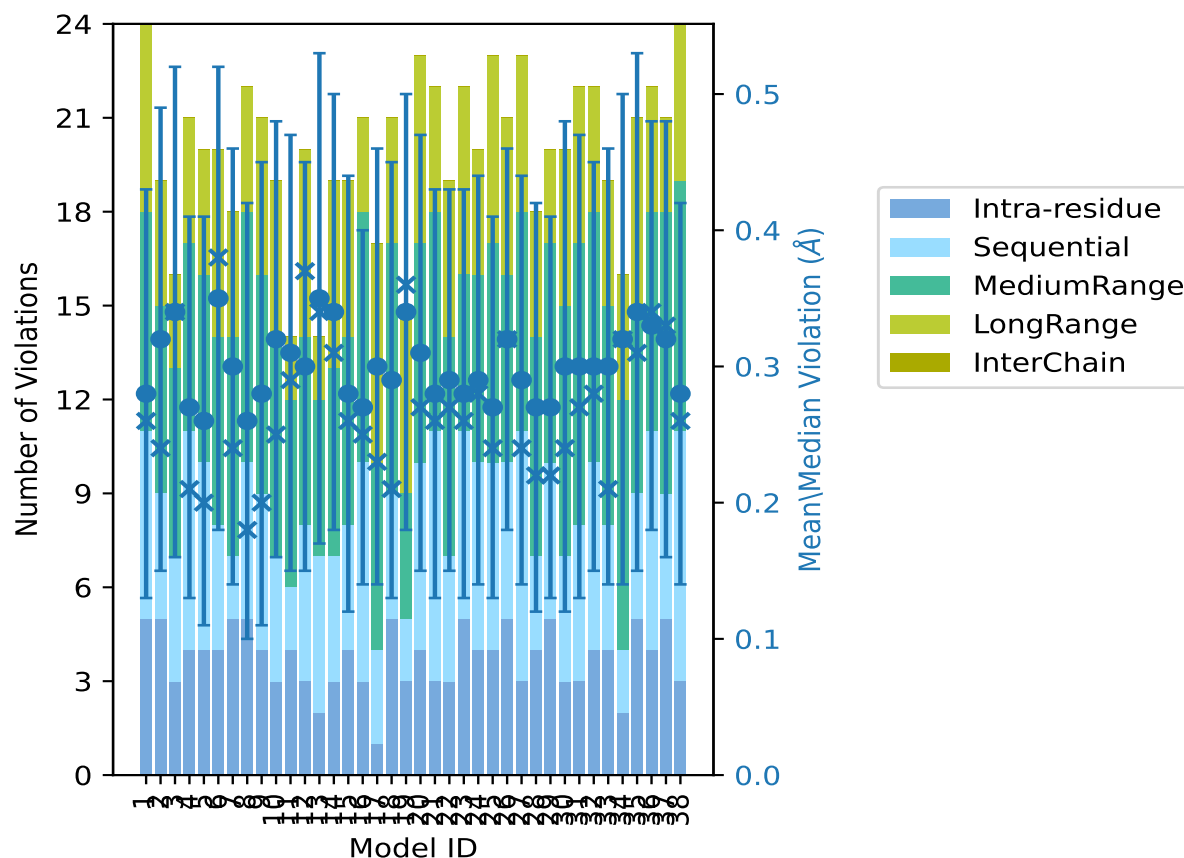
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	4	2	6	2	0	14	0.31	0.74	0.16	0.29
12	3	5	6	6	0	20	0.3	0.57	0.15	0.37
13	2	5	5	2	0	14	0.35	0.67	0.18	0.34
14	3	4	6	6	0	19	0.34	0.68	0.16	0.31
15	4	4	6	5	0	19	0.28	0.65	0.16	0.26
16	3	7	8	3	0	21	0.27	0.55	0.13	0.25
17	1	3	6	7	0	17	0.3	0.65	0.16	0.23
18	5	4	8	4	0	21	0.29	0.71	0.16	0.21
19	3	2	4	6	0	15	0.34	0.67	0.16	0.36
20	4	6	7	6	0	23	0.31	0.67	0.16	0.27
21	3	8	7	4	0	22	0.28	0.67	0.15	0.26
22	3	4	7	5	0	19	0.29	0.57	0.14	0.27
23	5	6	5	6	0	22	0.28	0.67	0.15	0.26
24	4	6	6	4	0	20	0.29	0.56	0.15	0.28
25	4	6	7	6	0	23	0.27	0.51	0.14	0.24
26	5	5	6	5	0	21	0.32	0.59	0.14	0.32
27	3	8	7	5	0	23	0.29	0.63	0.15	0.24
28	4	3	7	4	0	18	0.27	0.67	0.15	0.22
29	5	5	7	3	0	20	0.27	0.56	0.14	0.22
30	3	4	8	5	0	20	0.3	0.62	0.18	0.24
31	3	5	9	5	0	22	0.3	0.66	0.17	0.27
32	4	6	8	4	0	22	0.3	0.59	0.15	0.28
33	4	4	7	4	0	19	0.3	0.6	0.16	0.21
34	2	2	8	4	0	16	0.32	0.62	0.18	0.32
35	5	4	6	6	0	21	0.34	0.71	0.19	0.31
36	4	7	7	4	0	22	0.33	0.72	0.15	0.34
37	5	4	9	3	0	21	0.32	0.75	0.16	0.33
38	3	8	8	5	0	24	0.28	0.63	0.14	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, 114(IR:34, SQ:46, MR:19, LR:15, 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	1	1	3	0	6	1	2.6
0	1	1	1	0	3	2	5.3
2	2	1	1	0	6	3	7.9
0	0	1	1	0	2	4	10.5
1	0	2	0	0	3	5	13.2
0	0	0	0	0	0	6	15.8

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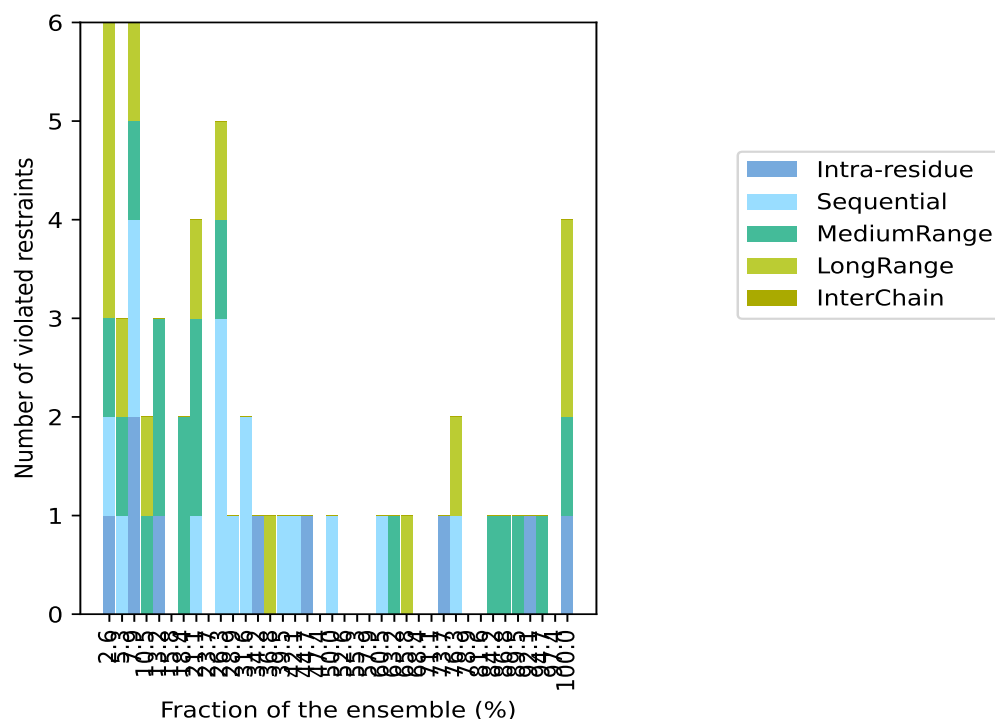
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	2	0	0	2	7	18.4
0	1	2	1	0	4	8	21.1
0	0	0	0	0	0	9	23.7
0	3	1	1	0	5	10	26.3
0	1	0	0	0	1	11	28.9
0	2	0	0	0	2	12	31.6
1	0	0	0	0	1	13	34.2
0	0	0	1	0	1	14	36.8
0	1	0	0	0	1	15	39.5
0	1	0	0	0	1	16	42.1
1	0	0	0	0	1	17	44.7
0	0	0	0	0	0	18	47.4
0	1	0	0	0	1	19	50.0
0	0	0	0	0	0	20	52.6
0	0	0	0	0	0	21	55.3
0	0	0	0	0	0	22	57.9
0	1	0	0	0	1	23	60.5
0	0	1	0	0	1	24	63.2
0	0	0	1	0	1	25	65.8
0	0	0	0	0	0	26	68.4
0	0	0	0	0	0	27	71.1
1	0	0	0	0	1	28	73.7
0	1	0	1	0	2	29	76.3
0	0	0	0	0	0	30	78.9
0	0	0	0	0	0	31	81.6
0	0	1	0	0	1	32	84.2
0	0	1	0	0	1	33	86.8
0	0	1	0	0	1	34	89.5
1	0	0	0	0	1	35	92.1
0	0	1	0	0	1	36	94.7
0	0	0	0	0	0	37	97.4
1	0	1	2	0	4	38	100.0

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

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

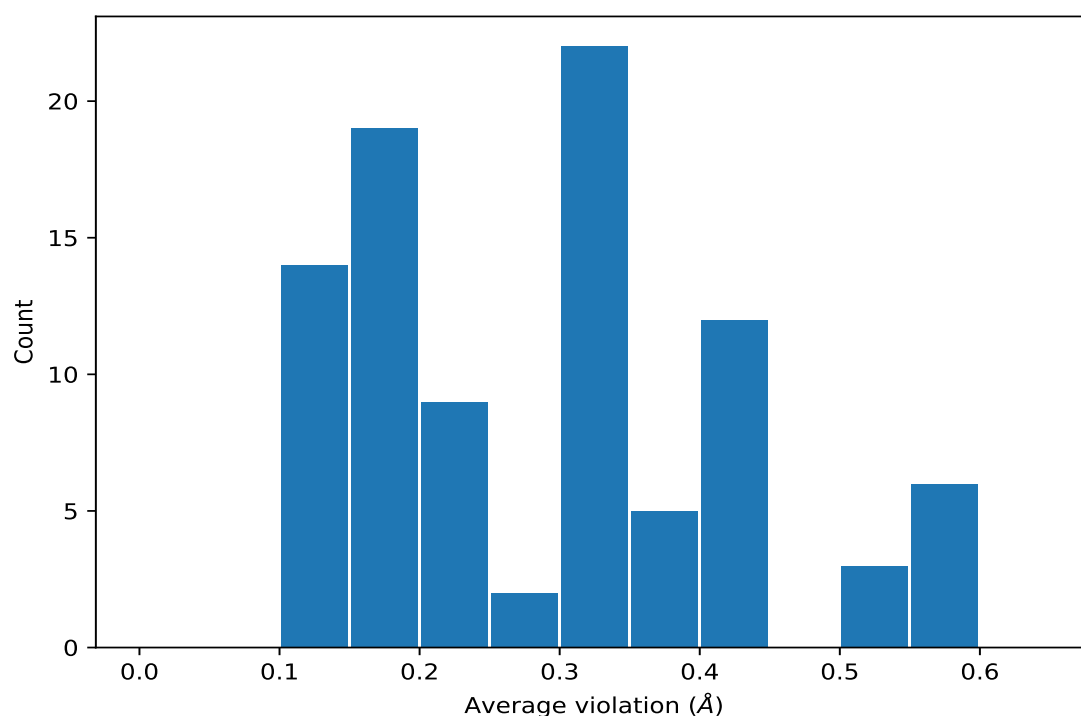
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	38	0.51	0.03	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	38	0.51	0.03	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	38	0.51	0.03	0.52
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	38	0.41	0.04	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	38	0.41	0.04	0.4
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	38	0.4	0.1	0.42
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	38	0.4	0.1	0.42
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	38	0.35	0.1	0.35
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	38	0.35	0.1	0.35
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	38	0.35	0.1	0.35
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	36	0.6	0.1	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	36	0.6	0.1	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	36	0.6	0.1	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	36	0.6	0.1	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	36	0.6	0.1	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	36	0.6	0.1	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	35	0.11	0.01	0.11
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	34	0.4	0.11	0.41
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	34	0.4	0.11	0.41
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	33	0.44	0.15	0.46
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	33	0.44	0.15	0.46
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	33	0.44	0.15	0.46
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	33	0.44	0.15	0.46
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	33	0.44	0.15	0.46
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	33	0.44	0.15	0.46
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	32	0.34	0.11	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	32	0.34	0.11	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	32	0.34	0.11	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	32	0.34	0.11	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	32	0.34	0.11	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	32	0.34	0.11	0.33
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	29	0.37	0.13	0.4
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	29	0.37	0.13	0.4
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	29	0.24	0.08	0.25
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	28	0.14	0.03	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	28	0.14	0.03	0.14
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	25	0.16	0.05	0.16
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	24	0.32	0.08	0.32
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	24	0.32	0.08	0.32
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	23	0.15	0.02	0.15
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	19	0.21	0.07	0.2
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	19	0.21	0.07	0.2
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	17	0.18	0.06	0.15
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	17	0.18	0.06	0.15
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	16	0.35	0.17	0.34
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	16	0.35	0.17	0.34
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	15	0.34	0.05	0.35
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	14	0.34	0.12	0.36
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	14	0.34	0.12	0.36
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	13	0.22	0.08	0.22
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	12	0.18	0.06	0.16
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	12	0.14	0.02	0.14
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	11	0.14	0.03	0.13
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	10	0.33	0.13	0.32
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	10	0.33	0.13	0.32
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	10	0.22	0.07	0.23
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	10	0.17	0.07	0.15
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	10	0.17	0.07	0.15

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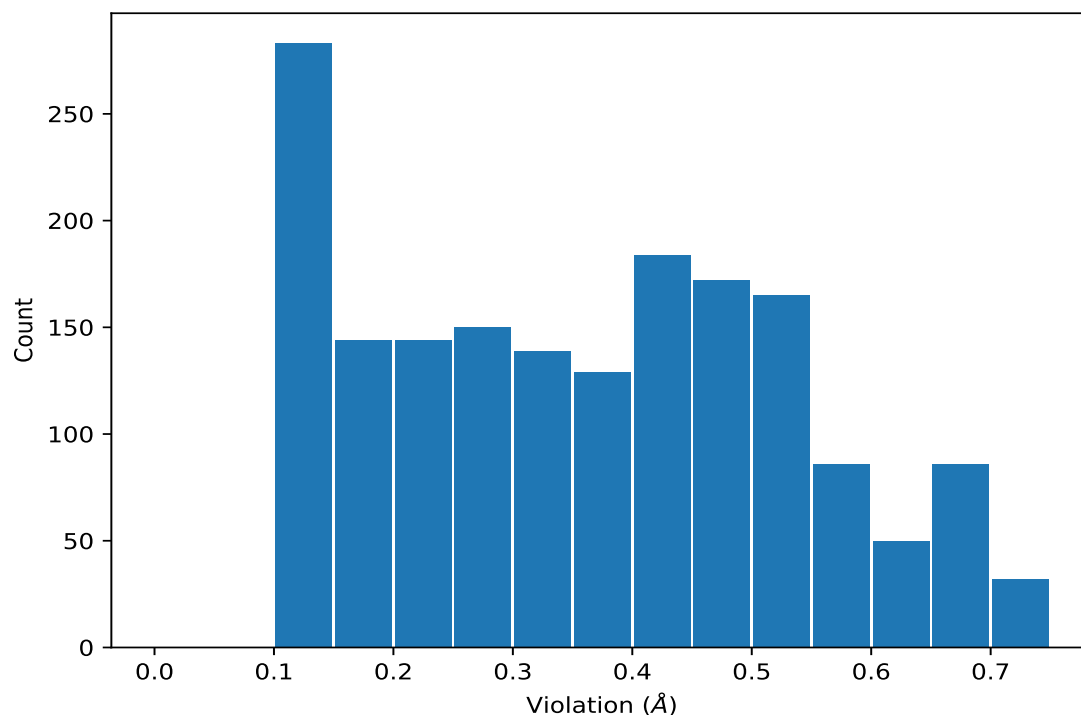
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	10	0.14	0.02	0.14
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	10	0.13	0.02	0.12
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	8	0.31	0.19	0.32
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	8	0.31	0.19	0.32
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	8	0.31	0.19	0.32
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	8	0.27	0.07	0.25
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	8	0.27	0.07	0.25
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	8	0.17	0.06	0.16
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	8	0.17	0.06	0.16
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	8	0.17	0.06	0.16
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	8	0.16	0.04	0.16
(1,7)	1:2:A:LEU:H	1:4:A:ILE:H	7	0.22	0.08	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD11	7	0.2	0.06	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD12	7	0.2	0.06	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD13	7	0.2	0.06	0.17
(1,142)	1:14:A:SER:HB3	1:14:A:SER:H	5	0.34	0.08	0.31
(1,8)	1:2:A:LEU:HA	1:5:A:GLN:H	5	0.17	0.05	0.17
(1,105)	1:7:A:LEU:HA	1:11:A:GLY:HA2	5	0.15	0.03	0.13
(1,82)	1:6:A:TRP:HH2	1:18:A:PRO:HB3	4	0.19	0.03	0.18
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB2	4	0.17	0.02	0.18
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB3	4	0.17	0.02	0.18
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD11	3	0.36	0.09	0.41
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD12	3	0.36	0.09	0.41
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD13	3	0.36	0.09	0.41
(1,4)	1:2:A:LEU:H	1:3:A:TYR:H	3	0.17	0.07	0.12
(1,73)	1:6:A:TRP:HE1	1:16:A:ARG:HB2	3	0.16	0.05	0.13
(1,73)	1:6:A:TRP:HE1	1:16:A:ARG:HB3	3	0.16	0.05	0.13
(1,12)	1:3:A:TYR:HD1	1:3:A:TYR:HB3	3	0.15	0.02	0.16
(1,12)	1:3:A:TYR:HD2	1:3:A:TYR:HB3	3	0.15	0.02	0.16
(1,120)	1:10:A:GLY:H	1:11:A:GLY:H	3	0.12	0.0	0.12
(1,39)	1:5:A:GLN:HB3	1:5:A:GLN:H	3	0.11	0.0	0.11
(1,46)	1:5:A:GLN:HA	1:8:A:LYS:H	2	0.18	0.07	0.18
(1,86)	1:6:A:TRP:HD1	1:19:A:PRO:HD2	2	0.18	0.04	0.18
(1,166)	1:18:A:PRO:HB2	1:19:A:PRO:HD2	2	0.13	0.02	0.13

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)
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	37	0.75
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	37	0.75
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	37	0.75
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	37	0.75
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	37	0.75
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	37	0.75
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	11	0.74
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	11	0.74
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	11	0.74
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	11	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	11	0.74
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	11	0.74
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	36	0.72
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	36	0.72
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	36	0.72
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	36	0.72
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	36	0.72
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	36	0.72
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	3	0.71
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	3	0.71
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	3	0.71
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	3	0.71
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	3	0.71
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	3	0.71
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	18	0.71
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	18	0.71
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	18	0.71
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	18	0.71
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	18	0.71
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	18	0.71
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	35	0.71
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	35	0.71
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	6	0.7
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	6	0.7
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	6	0.7
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	6	0.7
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	6	0.7
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	6	0.7
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	2	0.69
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	2	0.69
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	2	0.69
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	2	0.69
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	2	0.69
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	2	0.69
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	14	0.68
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	14	0.68
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	14	0.68
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	14	0.68
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	14	0.68
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	14	0.68
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	19	0.67
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	19	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	19	0.67
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	19	0.67
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	19	0.67
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	19	0.67
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	23	0.67
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	23	0.67
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	23	0.67
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	23	0.67
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	23	0.67
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	23	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	13	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	13	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	13	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	13	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	13	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	13	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	20	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	20	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	20	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	20	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	20	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	20	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	21	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	21	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	21	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	21	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	21	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	21	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	28	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	28	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	28	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	28	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	28	0.67
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	28	0.67
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	31	0.66
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	31	0.66
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	31	0.66
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	31	0.66
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	31	0.66
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	31	0.66
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	31	0.65
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	31	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	17	0.65
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	17	0.65
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	17	0.65
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	17	0.65
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	17	0.65
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	17	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	4	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	4	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	4	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	4	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	4	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	4	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	10	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	10	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	10	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	10	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	10	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	10	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	15	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	15	0.65
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	15	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	15	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	15	0.65
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	15	0.65
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	35	0.64
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	35	0.64
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	35	0.64
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	35	0.64
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	35	0.64
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	35	0.64
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	27	0.63
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	27	0.63
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	27	0.63
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	27	0.63
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	27	0.63
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	27	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	7	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	7	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	7	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	7	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	7	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	9	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	9	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	9	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	9	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	9	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	9	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	38	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	38	0.63
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	38	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	38	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	38	0.63
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	38	0.63
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	2	0.62
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	2	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	30	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	30	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	30	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	30	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	30	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	30	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	34	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	34	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	34	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	34	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	34	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	34	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	35	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	35	0.62
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	35	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	35	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	35	0.62
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	35	0.62
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	33	0.6
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	33	0.6
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	33	0.6
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	33	0.6
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	33	0.6
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	33	0.6
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	3	0.59
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	3	0.59
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	3	0.59
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	6	0.59
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	33	0.59
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	33	0.59
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	33	0.59
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	33	0.59
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	33	0.59
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	33	0.59
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	26	0.59
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	26	0.59
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	26	0.59
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	26	0.59
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	26	0.59
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	26	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	1	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	1	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	1	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	1	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	1	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	1	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	8	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	8	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	8	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	8	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	8	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	8	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	32	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	32	0.59
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	32	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	32	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	32	0.59
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	32	0.59
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	12	0.57
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	12	0.57
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	12	0.57
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	26	0.57
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	26	0.57
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	22	0.57
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	22	0.57
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	22	0.57
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	22	0.57
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	22	0.57
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	22	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	29	0.56
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	29	0.56
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	29	0.56
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	27	0.56
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	27	0.56
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	27	0.56
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	13	0.56
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	13	0.56
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	13	0.56
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	13	0.56
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	13	0.56
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	13	0.56
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	24	0.56
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	24	0.56
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	24	0.56
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	24	0.56
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	24	0.56
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	24	0.56
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	16	0.55
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	16	0.55
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	16	0.55
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	19	0.55
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	19	0.55
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	19	0.55
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	8	0.55
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	8	0.55
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	7	0.55
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	7	0.55
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	7	0.55
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	7	0.55
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	7	0.55
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	7	0.55
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	36	0.55
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	36	0.55
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	23	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	23	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	23	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	24	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	24	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	24	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	26	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	26	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	26	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	33	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	33	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	33	0.54
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	9	0.54
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	9	0.54
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	35	0.54
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	35	0.54
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	30	0.54
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	30	0.54
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	30	0.54
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	30	0.54
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	30	0.54
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	30	0.54
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	13	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	13	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	13	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	17	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	17	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	17	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	20	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	20	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	20	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	35	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	35	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	35	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	38	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	38	0.53
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	38	0.53
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	34	0.53
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	34	0.53
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	34	0.53
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	34	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	1	0.53
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	1	0.53
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	1	0.53
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	1	0.53
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	1	0.53
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	1	0.53
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	27	0.53
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	27	0.53
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	27	0.53
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	27	0.53
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	27	0.53
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	27	0.53
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	30	0.52
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	30	0.52
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	30	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	14	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	14	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	14	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	30	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	30	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	30	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	34	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	34	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	34	0.52
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	14	0.52
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	14	0.52
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	32	0.52
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	32	0.52
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	6	0.52
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	6	0.52
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	32	0.52
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	32	0.52
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	14	0.52
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	14	0.52
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	18	0.52
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	18	0.52
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	20	0.52
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	20	0.52
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	29	0.52
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	29	0.52
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	29	0.52
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	29	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	29	0.52
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	29	0.52
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.51
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.51
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.51
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	25	0.51
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	25	0.51
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	25	0.51
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	14	0.51
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	14	0.51
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	20	0.51
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	20	0.51
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	10	0.51
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	10	0.51
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	32	0.51
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	32	0.51
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	32	0.51
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	32	0.51
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	32	0.51
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	32	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	10	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	10	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	10	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	10	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	10	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	10	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	20	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	20	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	20	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	20	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	20	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	20	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	34	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	34	0.51
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	34	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	34	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	34	0.51
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	34	0.51
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	33	0.51
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	33	0.51
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	33	0.51
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	33	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	33	0.51
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	33	0.51
(1,142)	1:14:A:SER:HB3	1:14:A:SER:H	25	0.5
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	37	0.5
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	37	0.5
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	37	0.5
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	31	0.5
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	31	0.5
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	31	0.5
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	8	0.5
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	8	0.5
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	10	0.5
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	10	0.5
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	25	0.5
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	25	0.5
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	1	0.5
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	1	0.5
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	36	0.5
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	36	0.5
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	36	0.5
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	36	0.5
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	36	0.5
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	36	0.5
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	25	0.5
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	25	0.5
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	25	0.5
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	25	0.5
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	25	0.5
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	25	0.5
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	26	0.5
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	26	0.5
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	14	0.49
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	14	0.49
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	14	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	11	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	11	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	11	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	22	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	22	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	22	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	28	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	28	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	28	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	29	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	29	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	29	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	32	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	32	0.49
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	32	0.49
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	2	0.49
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	2	0.49
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	13	0.49
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	13	0.49
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	15	0.49
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	15	0.49
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	18	0.49
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	18	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	6	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	6	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	6	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	6	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	6	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	6	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	18	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	18	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	18	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	18	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	18	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	18	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	35	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	35	0.49
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	35	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	35	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	35	0.49
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	35	0.49
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	3	0.49
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	3	0.49
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	3	0.49
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	3	0.49
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	3	0.49
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	23	0.49
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	23	0.49
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	23	0.49
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	23	0.49
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	23	0.49
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	23	0.49
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	7	0.48
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	7	0.48
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	7	0.48
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	9	0.48
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	9	0.48
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	9	0.48
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	15	0.48
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	15	0.48
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	15	0.48
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	31	0.48
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	31	0.48
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	31	0.48
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.48
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.48
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.48
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	36	0.48
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	36	0.48
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	36	0.48
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	6	0.48
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	6	0.48
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	19	0.48
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	19	0.48
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	5	0.48
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	5	0.48
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	12	0.48
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	12	0.48
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	27	0.48
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	27	0.48
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	23	0.48
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	23	0.48
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	30	0.48
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	30	0.48
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	21	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	21	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	21	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	37	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	37	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	37	0.47
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	9	0.47
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	9	0.47
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	34	0.47
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	34	0.47
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	2	0.47
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	2	0.47
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	19	0.47
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	19	0.47
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	36	0.47
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	36	0.47
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	36	0.47
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	36	0.47
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	36	0.47
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	36	0.47
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	15	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	15	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	15	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	18	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	18	0.46
(1,91)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	18	0.46
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	37	0.46
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	37	0.46
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	5	0.46
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	5	0.46
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	19	0.46
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	19	0.46
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	13	0.46
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	13	0.46
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	13	0.46
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	13	0.46
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	13	0.46
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	24	0.46
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	24	0.46
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	24	0.46
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	24	0.46
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	24	0.46
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	24	0.46
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	2	0.46
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	2	0.46
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	4	0.45
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	4	0.45
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	4	0.45
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	24	0.45
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	24	0.45
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	26	0.45
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	26	0.45
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	30	0.45
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	30	0.45
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	12	0.45
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	12	0.45
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	33	0.45
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	33	0.45
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	38	0.45
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	38	0.45
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	38	0.45
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	38	0.45
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	38	0.45
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	38	0.45
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	16	0.45
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	16	0.45
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	21	0.45
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	21	0.45
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	20	0.44
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	20	0.44
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	20	0.44
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	22	0.44
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	22	0.44
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	22	0.44
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	35	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	35	0.44
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	35	0.44
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	31	0.44
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	31	0.44
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	36	0.44
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	36	0.44
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	12	0.44
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	12	0.44
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	7	0.44
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	7	0.44
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	31	0.44
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	31	0.44
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	35	0.44
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	35	0.44
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	6	0.44
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	6	0.44
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	2	0.44
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	2	0.44
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	2	0.44
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	2	0.44
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	2	0.44
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	2	0.44
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	30	0.44
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	30	0.44
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	30	0.44
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	30	0.44
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	30	0.44
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	30	0.44
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	17	0.44
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	17	0.44
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	17	0.44
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	17	0.44
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	17	0.44
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	17	0.44
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	3	0.43
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	3	0.43
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	27	0.43
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	27	0.43
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	33	0.43
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	33	0.43
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	17	0.43
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	23	0.43
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	23	0.43
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	12	0.43
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	12	0.43
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	38	0.43
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	38	0.43
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	3	0.43
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	3	0.43
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	27	0.43
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	27	0.43
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	9	0.43
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	9	0.43
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	9	0.43
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	9	0.43
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	9	0.43
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	9	0.43
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	5	0.43
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	5	0.43
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	5	0.43
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	5	0.43
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	5	0.43
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	5	0.43
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	5	0.43
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	5	0.43
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD11	22	0.43
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD12	22	0.43
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD13	22	0.43
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	37	0.43
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	37	0.43
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	12	0.42
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	10	0.42
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	22	0.42
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	22	0.42
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	20	0.42
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	20	0.42
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	20	0.42
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	20	0.42
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	25	0.42
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	25	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	6	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	6	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	10	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	13	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	13	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	29	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	29	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	36	0.42
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	36	0.42
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	5	0.42
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	5	0.42
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	24	0.42
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	24	0.42
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	24	0.42
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	24	0.42
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	24	0.42
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	24	0.42
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	12	0.42
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	12	0.42
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	12	0.42
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	12	0.42
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	12	0.42
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	12	0.42
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	4	0.42
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	4	0.42
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	18	0.41
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	18	0.41
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	18	0.41
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	28	0.41
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	28	0.41
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	28	0.41
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	17	0.41
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	17	0.41
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	1	0.41
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	1	0.41
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	4	0.41
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	4	0.41
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	14	0.41
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	14	0.41
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	29	0.41
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	29	0.41
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	4	0.41
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	4	0.41
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	5	0.41
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	15	0.41
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	15	0.41
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	28	0.41
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	28	0.41
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	16	0.41
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	16	0.41
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	21	0.41
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	21	0.41
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	31	0.41
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	31	0.41
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	37	0.41
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	37	0.41
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD11	16	0.41
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD12	16	0.41
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD13	16	0.41
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	24	0.4
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	14	0.4
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	12	0.4
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	12	0.4
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	12	0.4
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	7	0.4
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	7	0.4
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	15	0.4
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	15	0.4
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	16	0.4
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	16	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	1	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	1	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	28	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	28	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	32	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	32	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	37	0.4
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	37	0.4
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	21	0.4
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	21	0.4
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	8	0.4
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	8	0.4
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	8	0.4
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	8	0.4
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	8	0.4
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	37	0.4
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	37	0.4
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	37	0.4
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	37	0.4
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	37	0.4
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	37	0.4
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	22	0.4
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	22	0.4
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	7	0.39
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	7	0.39
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	7	0.39
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	10	0.39
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	10	0.39
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	10	0.39
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	36	0.39
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	36	0.39
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	36	0.39
(1,71)	1:6:A:TRP:HD1	1:16:A:ARG:HB2	38	0.39
(1,71)	1:6:A:TRP:HD1	1:16:A:ARG:HB3	38	0.39
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	17	0.39
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	17	0.39
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	21	0.39
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	21	0.39
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	22	0.39
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	22	0.39
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	3	0.39
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	3	0.39
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	21	0.39
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	21	0.39
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	2	0.38
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	6	0.38
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	9	0.38
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	16	0.38
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	6	0.38
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	6	0.38
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	6	0.38
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	33	0.38
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	33	0.38
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	33	0.38
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	24	0.38
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	24	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	23	0.38
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	23	0.38
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	29	0.38
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	29	0.38
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	36	0.38
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	36	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	8	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	8	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	9	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	9	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	11	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	11	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	19	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	19	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	30	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	30	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	34	0.38
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	34	0.38
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	31	0.38
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	31	0.38
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	14	0.38
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	14	0.38
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	29	0.38
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	29	0.38
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	26	0.37
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	6	0.37
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	16	0.37
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	16	0.37
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	16	0.37
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	12	0.37
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	12	0.37
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	12	0.37
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	12	0.37
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	11	0.37
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	11	0.37
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	21	0.37
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	21	0.37
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	37	0.37
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	37	0.37
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	16	0.37
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	16	0.37
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	17	0.37
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	1	0.37
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	1	0.37
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	1	0.37
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	1	0.37
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	1	0.37
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	1	0.37
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	6	0.37
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	6	0.37
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	6	0.37
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	6	0.37
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	6	0.37
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	6	0.37
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	11	0.37
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	11	0.37
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	11	0.37
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	11	0.37
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	11	0.37
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	11	0.37
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	19	0.37
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	19	0.37
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	19	0.37
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	19	0.37
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	19	0.37
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	19	0.37
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	12	0.37
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	12	0.37
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	32	0.37
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	32	0.37
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	35	0.36
(1,119)	1:9:A:ASP:HB3	1:14:A:SER:HB2	25	0.36
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	19	0.36
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	19	0.36
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	38	0.36
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	38	0.36
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	22	0.36
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	22	0.36
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	24	0.36
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	24	0.36
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	27	0.36
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	27	0.36
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	8	0.36
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	8	0.36
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	8	0.36
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	8	0.36
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	8	0.36
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	25	0.36
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	25	0.36
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	25	0.36
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	25	0.36
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	25	0.36
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	25	0.36
(1,7)	1:2:A:LEU:H	1:4:A:ILE:H	26	0.36
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	20	0.35
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	5	0.35
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	5	0.35
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	5	0.35
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	37	0.35
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	37	0.35
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	37	0.35
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	1	0.35
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	1	0.35
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	20	0.35
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	20	0.35
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	8	0.35
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	8	0.35
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	38	0.35
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	38	0.35
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	38	0.35
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	38	0.35
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	38	0.35
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	38	0.35
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	11	0.35
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	11	0.35
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	13	0.34
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	32	0.34
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	36	0.34
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	13	0.34
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	13	0.34
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	13	0.34
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	32	0.34
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	32	0.34
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	32	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	38	0.34
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	38	0.34
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	26	0.34
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	26	0.34
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	36	0.34
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	36	0.34
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	3	0.34
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	3	0.34
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	3	0.34
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	3	0.34
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	3	0.34
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	3	0.34
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	28	0.34
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	28	0.34
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	28	0.34
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	28	0.34
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	28	0.34
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	28	0.34
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD11	26	0.34
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD12	26	0.34
(1,22)	1:3:A:TYR:HD1	1:7:A:LEU:HD13	26	0.34
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD11	26	0.34
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD12	26	0.34
(1,22)	1:3:A:TYR:HD2	1:7:A:LEU:HD13	26	0.34
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	3	0.33
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	36	0.33
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	4	0.33
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	4	0.33
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	11	0.33
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	11	0.33
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	13	0.33
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	13	0.33
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	30	0.33
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	30	0.33
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	32	0.33
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	32	0.33
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	25	0.33
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG2	33	0.33
(1,28)	1:3:A:TYR:HA	1:19:A:PRO:HG3	33	0.33
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	26	0.33
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	26	0.33
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	35	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	35	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	15	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	15	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	15	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	15	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	15	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	15	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	20	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	20	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	20	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	20	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	20	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	20	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	34	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	34	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	34	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	34	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	34	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	34	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	37	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	37	0.33
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	37	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	37	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	37	0.33
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	37	0.33
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	28	0.33
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	28	0.33
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	31	0.32
(1,142)	1:14:A:SER:HB3	1:14:A:SER:H	27	0.32
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	18	0.32
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	18	0.32
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	24	0.32
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	38	0.32
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	38	0.32
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	22	0.32
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	22	0.32
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	38	0.32
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	26	0.32
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	26	0.32
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	18	0.32
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	18	0.32
(1,7)	1:2:A:LEU:H	1:4:A:ILE:H	37	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	1	0.32
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	1	0.32
(1,142)	1:14:A:SER:HB3	1:14:A:SER:H	1	0.31
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	38	0.31
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	14	0.31
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	14	0.31
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	25	0.31
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	25	0.31
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	25	0.31
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	25	0.31
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	25	0.31
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	35	0.31
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	6	0.31
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	6	0.31
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	36	0.31
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	17	0.31
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	17	0.31
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	9	0.31
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	9	0.31
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	9	0.31
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	9	0.31
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	9	0.31
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	9	0.31
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	15	0.31
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	15	0.31
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	5	0.3
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	8	0.3
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	8	0.3
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	8	0.3
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	21	0.3
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	21	0.3
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	21	0.3
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	34	0.3
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	34	0.3
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	34	0.3
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	18	0.3
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	18	0.3
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	27	0.3
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	27	0.3
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	27	0.3
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	27	0.3
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	27	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	27	0.3
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	30	0.3
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	30	0.3
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	23	0.3
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	23	0.3
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	23	0.29
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	37	0.29
(1,142)	1:14:A:SER:HB3	1:14:A:SER:H	24	0.29
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	14	0.29
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	7	0.29
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	26	0.29
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	26	0.29
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	26	0.29
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	3	0.29
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	3	0.29
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD11	8	0.29
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD12	8	0.29
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD13	8	0.29
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	14	0.29
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	14	0.29
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	14	0.29
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	14	0.29
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	14	0.29
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	14	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	15	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	15	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	15	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	15	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	15	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	15	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	18	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	18	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	18	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	18	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	18	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	18	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	21	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	21	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	21	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	21	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	21	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	21	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	32	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	32	0.29
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	32	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	32	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	32	0.29
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	32	0.29
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	27	0.29
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	27	0.29
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	2	0.28
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	2	0.28
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	26	0.28
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	26	0.28
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	26	0.28
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	38	0.28
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	38	0.28
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	38	0.28
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	10	0.28
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	10	0.28
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	35	0.28
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	35	0.28
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	31	0.28
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD11	26	0.28
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD12	26	0.28
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD13	26	0.28
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	23	0.28
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	23	0.28
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	36	0.28
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	36	0.28
(1,142)	1:14:A:SER:HB3	1:14:A:SER:H	36	0.27
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	25	0.27
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	31	0.27
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	4	0.27
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	22	0.27
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	22	0.27
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	1	0.27
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	1	0.27
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	1	0.27
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	19	0.27
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	19	0.27
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	19	0.27
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	28	0.27
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	24	0.27
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	24	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	21	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	21	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	21	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	21	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	21	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	21	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	23	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	23	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	23	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	23	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	23	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	23	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	31	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	31	0.27
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	31	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	31	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	31	0.27
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	31	0.27
(1,4)	1:2:A:LEU:H	1:3:A:TYR:H	14	0.27
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	23	0.26
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	23	0.26
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	7	0.26
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	15	0.26
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	26	0.26
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	37	0.26
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	24	0.26
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	24	0.26
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	24	0.26
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	1	0.26
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	1	0.26
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	21	0.26
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	16	0.26
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	16	0.26
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	23	0.26
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	23	0.26
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	32	0.26
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	32	0.26
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	26	0.25
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	27	0.25
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	19	0.25
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	16	0.25
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	16	0.25
(1,46)	1:5:A:GLN:HA	1:8:A:LYS:H	10	0.25
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	1	0.25
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	1	0.25
(1,8)	1:2:A:LEU:HA	1:5:A:GLN:H	16	0.25
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	28	0.24
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	11	0.24
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	11	0.24
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	23	0.24
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	23	0.24
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	23	0.24
(1,82)	1:6:A:TRP:HH2	1:18:A:PRO:HB3	38	0.24
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	21	0.24
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	21	0.24
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	25	0.24
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	25	0.24
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	10	0.24
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	29	0.24
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	10	0.24
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	10	0.24
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	4	0.24
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	4	0.24
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	4	0.24
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	4	0.24
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	4	0.24
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	4	0.24
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	10	0.24
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	10	0.24
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	10	0.24
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	10	0.24
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	10	0.24
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	10	0.24
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	2	0.24
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	2	0.24
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	6	0.24
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	6	0.24
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	20	0.24
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	20	0.24
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	25	0.24
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	25	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD11	27	0.24
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD12	27	0.24
(1,3)	1:1:A:ASN:HA	1:4:A:ILE:HD13	27	0.24
(1,152)	1:15:A:GLY:H	1:16:A:ARG:H	11	0.23
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	20	0.23
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	20	0.23
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	33	0.23
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	33	0.23
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	20	0.23
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	29	0.23
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	32	0.23
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	32	0.23
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	11	0.23
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	11	0.23
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	11	0.23
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	22	0.23
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	22	0.23
(1,73)	1:6:A:TRP:HE1	1:16:A:ARG:HB2	38	0.23
(1,73)	1:6:A:TRP:HE1	1:16:A:ARG:HB3	38	0.23
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	4	0.23
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	17	0.23
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	17	0.23
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	7	0.23
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	7	0.23
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	7	0.23
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	7	0.23
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	7	0.23
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	7	0.23
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	38	0.23
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	38	0.23
(1,7)	1:2:A:LEU:H	1:4:A:ILE:H	38	0.23
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	17	0.23
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	17	0.23
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	38	0.22
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	1	0.22
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	35	0.22
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	19	0.22
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	2	0.22
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	2	0.22
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	2	0.22
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	29	0.22
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	29	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	29	0.22
(1,86)	1:6:A:TRP:HD1	1:19:A:PRO:HD2	20	0.22
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	3	0.22
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	35	0.22
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	35	0.22
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	32	0.22
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	32	0.22
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	37	0.22
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	37	0.22
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	29	0.21
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	29	0.21
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	4	0.21
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	18	0.21
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	17	0.21
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	17	0.21
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	17	0.21
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	19	0.21
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	23	0.21
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	23	0.21
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	12	0.21
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	12	0.21
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	12	0.21
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	33	0.21
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	33	0.21
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	33	0.21
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	27	0.21
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD11	18	0.21
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD12	18	0.21
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD13	18	0.21
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	16	0.21
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	16	0.21
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	16	0.21
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	16	0.21
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	16	0.21
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	16	0.21
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	36	0.21
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	36	0.21
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	10	0.21
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	10	0.21
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	3	0.2
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	28	0.2
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	28	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	29	0.2
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	29	0.2
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	33	0.2
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	33	0.2
(1,105)	1:7:A:LEU:HA	1:11:A:GLY:HA2	29	0.2
(1,82)	1:6:A:TRP:HH2	1:18:A:PRO:HB3	31	0.2
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	18	0.2
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	28	0.2
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	28	0.2
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	5	0.2
(1,30)	1:3:A:TYR:HD1	1:19:A:PRO:HD2	27	0.2
(1,30)	1:3:A:TYR:HD2	1:19:A:PRO:HD2	27	0.2
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	9	0.2
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	9	0.2
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	2	0.2
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	2	0.2
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	2	0.2
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	2	0.2
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	2	0.2
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	2	0.2
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	22	0.2
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	22	0.2
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	9	0.2
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	9	0.2
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	10	0.2
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	9	0.19
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	9	0.19
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	9	0.19
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	20	0.19
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	23	0.19
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	33	0.19
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	18	0.19
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	18	0.19
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	2	0.19
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	2	0.19
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	33	0.19
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	33	0.19
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	5	0.19
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	8	0.19
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	8	0.19
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	22	0.19
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	22	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	11	0.19
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	11	0.19
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	11	0.19
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	11	0.19
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	11	0.19
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	11	0.19
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	31	0.19
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	31	0.19
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	31	0.19
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	31	0.19
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	31	0.19
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	31	0.19
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB2	17	0.19
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB3	17	0.19
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB2	33	0.19
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB3	33	0.19
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	4	0.19
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	4	0.19
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	18	0.19
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	18	0.19
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	1	0.18
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	8	0.18
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	2	0.18
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	21	0.18
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	21	0.18
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	23	0.18
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	23	0.18
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	14	0.18
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	9	0.18
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	9	0.18
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	30	0.18
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	30	0.18
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	4	0.18
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	4	0.18
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG2	14	0.18
(1,68)	1:6:A:TRP:HH2	1:12:A:PRO:HG3	14	0.18
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	22	0.18
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	15	0.18
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	15	0.18
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	7	0.18
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	7	0.18
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	35	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	35	0.18
(1,8)	1:2:A:LEU:HA	1:5:A:GLN:H	31	0.18
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	4	0.18
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	28	0.17
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	27	0.17
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	10	0.17
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	10	0.17
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	27	0.17
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	33	0.17
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	16	0.17
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	16	0.17
(1,105)	1:7:A:LEU:HA	1:11:A:GLY:HA2	9	0.17
(1,82)	1:6:A:TRP:HH2	1:18:A:PRO:HB3	25	0.17
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	2	0.17
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	7	0.17
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	26	0.17
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD2	27	0.17
(1,76)	1:6:A:TRP:HD1	1:16:A:ARG:HD3	27	0.17
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	36	0.17
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB2	28	0.17
(1,47)	1:5:A:GLN:HA	1:8:A:LYS:HB3	28	0.17
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	13	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD11	32	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD12	32	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD13	32	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD11	33	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD12	33	0.17
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD13	33	0.17
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	14	0.17
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	35	0.17
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	22	0.17
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	22	0.17
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	22	0.17
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	22	0.17
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	22	0.17
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	22	0.17
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	25	0.17
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	25	0.17
(1,12)	1:3:A:TYR:HD1	1:3:A:TYR:HB3	16	0.17
(1,12)	1:3:A:TYR:HD2	1:3:A:TYR:HB3	16	0.17
(1,8)	1:2:A:LEU:HA	1:5:A:GLN:H	18	0.17
(1,7)	1:2:A:LEU:H	1:4:A:ILE:H	24	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:2:A:LEU:H	1:4:A:ILE:H	31	0.17
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	26	0.17
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	27	0.17
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	32	0.17
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	36	0.17
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	13	0.16
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	12	0.16
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	34	0.16
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	7	0.16
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	7	0.16
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	9	0.16
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	19	0.16
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	19	0.16
(1,104)	1:7:A:LEU:HD21	1:11:A:GLY:HA3	27	0.16
(1,104)	1:7:A:LEU:HD22	1:11:A:GLY:HA3	27	0.16
(1,104)	1:7:A:LEU:HD23	1:11:A:GLY:HA3	27	0.16
(1,82)	1:6:A:TRP:HH2	1:18:A:PRO:HB3	14	0.16
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	4	0.16
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	29	0.16
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	1	0.16
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	16	0.16
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	16	0.16
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	16	0.16
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	22	0.16
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	22	0.16
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	22	0.16
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	18	0.16
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	32	0.16
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	4	0.16
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	4	0.16
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	15	0.16
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	15	0.16
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	29	0.16
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	29	0.16
(1,12)	1:3:A:TYR:HD1	1:3:A:TYR:HB3	12	0.16
(1,12)	1:3:A:TYR:HD2	1:3:A:TYR:HB3	12	0.16
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB2	7	0.16
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB3	7	0.16
(1,7)	1:2:A:LEU:H	1:4:A:ILE:H	30	0.16
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	1	0.16
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	2	0.16
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	37	0.16
(1,166)	1:18:A:PRO:HB2	1:19:A:PRO:HD2	38	0.15
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	30	0.15
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	6	0.15
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	6	0.15
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	20	0.15
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	29	0.15
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	35	0.15
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	2	0.15
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	2	0.15
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	12	0.15
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	12	0.15
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	12	0.15
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	6	0.15
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	36	0.15
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	37	0.15
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	21	0.15
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	15	0.15
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD11	27	0.15
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD12	27	0.15
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD13	27	0.15
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD11	28	0.15
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD12	28	0.15
(1,38)	1:4:A:ILE:HA	1:7:A:LEU:HD13	28	0.15
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	12	0.15
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	25	0.15
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	29	0.15
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	29	0.15
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	29	0.15
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	29	0.15
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	29	0.15
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	29	0.15
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	18	0.15
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	18	0.15
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB2	16	0.15
(1,9)	1:2:A:LEU:HA	1:5:A:GLN:HB3	16	0.15
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	5	0.15
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	5	0.15
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	25	0.15
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	25	0.15
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	8	0.15
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	16	0.15
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	30	0.15
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	33	0.15
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	38	0.15
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	19	0.14
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	24	0.14
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	32	0.14
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	5	0.14
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	5	0.14
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	32	0.14
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	32	0.14
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	21	0.14
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	38	0.14
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	18	0.14
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	21	0.14
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	15	0.14
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	15	0.14
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	20	0.14
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	20	0.14
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	1	0.14
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	16	0.14
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	23	0.14
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	4	0.14
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	4	0.14
(1,25)	1:3:A:TYR:HE1	1:18:A:PRO:HB2	34	0.14
(1,25)	1:3:A:TYR:HE2	1:18:A:PRO:HB2	34	0.14
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	5	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	5	0.14
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	6	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	6	0.14
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	9	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	9	0.14
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	21	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	21	0.14
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	28	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	28	0.14
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	30	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	30	0.14
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	32	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	32	0.14
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	34	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	34	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	36	0.14
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	36	0.14
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	4	0.14
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	4	0.14
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	29	0.14
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	29	0.14
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	5	0.14
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	21	0.14
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	24	0.14
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	31	0.14
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	35	0.14
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	1	0.13
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	31	0.13
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	1	0.13
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	10	0.13
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	1	0.13
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	1	0.13
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	11	0.13
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	11	0.13
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	25	0.13
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	27	0.13
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	27	0.13
(1,105)	1:7:A:LEU:HA	1:11:A:GLY:HA2	8	0.13
(1,86)	1:6:A:TRP:HD1	1:19:A:PRO:HD2	7	0.13
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	9	0.13
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG2	17	0.13
(1,77)	1:6:A:TRP:HD1	1:16:A:ARG:HG3	17	0.13
(1,73)	1:6:A:TRP:HE1	1:16:A:ARG:HB2	15	0.13
(1,73)	1:6:A:TRP:HE1	1:16:A:ARG:HB3	15	0.13
(1,73)	1:6:A:TRP:HE1	1:16:A:ARG:HB2	25	0.13
(1,73)	1:6:A:TRP:HE1	1:16:A:ARG:HB3	25	0.13
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	17	0.13
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	24	0.13
(1,66)	1:6:A:TRP:HA	1:9:A:ASP:HB2	34	0.13
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	30	0.13
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	20	0.13
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	8	0.13
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	8	0.13
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	11	0.13
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	11	0.13
(1,12)	1:3:A:TYR:HD1	1:3:A:TYR:HB3	26	0.13
(1,12)	1:3:A:TYR:HD2	1:3:A:TYR:HB3	26	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	20	0.13
(1,1)	1:1:A:ASN:HA	1:2:A:LEU:H	22	0.13
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	9	0.12
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	18	0.12
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	8	0.12
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	21	0.12
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	8	0.12
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	8	0.12
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	28	0.12
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	28	0.12
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	36	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	4	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	7	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	14	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	19	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	20	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	23	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	24	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	25	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	28	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	33	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	35	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	36	0.12
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	38	0.12
(1,120)	1:10:A:GLY:H	1:11:A:GLY:H	9	0.12
(1,120)	1:10:A:GLY:H	1:11:A:GLY:H	29	0.12
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	23	0.12
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	5	0.12
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	5	0.12
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	5	0.12
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	30	0.12
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	30	0.12
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	30	0.12
(1,105)	1:7:A:LEU:HA	1:11:A:GLY:HA2	7	0.12
(1,105)	1:7:A:LEU:HA	1:11:A:GLY:HA2	37	0.12
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	5	0.12
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	12	0.12
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	15	0.12
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	17	0.12
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	31	0.12
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	38	0.12
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	38	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	38	0.12
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	8	0.12
(1,44)	1:5:A:GLN:HB2	1:6:A:TRP:H	34	0.12
(1,39)	1:5:A:GLN:HB3	1:5:A:GLN:H	8	0.12
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	4	0.12
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	34	0.12
(1,29)	1:3:A:TYR:HB2	1:19:A:PRO:HG2	35	0.12
(1,29)	1:3:A:TYR:HB2	1:19:A:PRO:HG3	35	0.12
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD21	25	0.12
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD22	25	0.12
(1,24)	1:3:A:TYR:HE1	1:7:A:LEU:HD23	25	0.12
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD21	25	0.12
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD22	25	0.12
(1,24)	1:3:A:TYR:HE2	1:7:A:LEU:HD23	25	0.12
(1,21)	1:3:A:TYR:HE1	1:6:A:TRP:HZ3	3	0.12
(1,21)	1:3:A:TYR:HE2	1:6:A:TRP:HZ3	3	0.12
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	3	0.12
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	3	0.12
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	20	0.12
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	20	0.12
(1,8)	1:2:A:LEU:HA	1:5:A:GLN:H	1	0.12
(1,7)	1:2:A:LEU:H	1:4:A:ILE:H	10	0.12
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	6	0.12
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	6	0.12
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	13	0.12
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	13	0.12
(1,4)	1:2:A:LEU:H	1:3:A:TYR:H	15	0.12
(1,4)	1:2:A:LEU:H	1:3:A:TYR:H	23	0.12
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	8	0.12
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	8	0.12
(1,166)	1:18:A:PRO:HB2	1:19:A:PRO:HD2	3	0.11
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	4	0.11
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	14	0.11
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	5	0.11
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	35	0.11
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	35	0.11
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	17	0.11
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	24	0.11
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	9	0.11
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	30	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	1	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	5	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	6	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	8	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	9	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	10	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	11	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	12	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	13	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	15	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	16	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	18	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	26	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	27	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	29	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	31	0.11
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	32	0.11
(1,120)	1:10:A:GLY:H	1:11:A:GLY:H	7	0.11
(1,114)	1:9:A:ASP:HB3	1:9:A:ASP:H	22	0.11
(1,111)	1:8:A:LYS:HB2	1:9:A:ASP:H	37	0.11
(1,111)	1:8:A:LYS:HB3	1:9:A:ASP:H	37	0.11
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	30	0.11
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	23	0.11
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	23	0.11
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	23	0.11
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD21	27	0.11
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD22	27	0.11
(1,60)	1:6:A:TRP:HE3	1:7:A:LEU:HD23	27	0.11
(1,46)	1:5:A:GLN:HA	1:8:A:LYS:H	16	0.11
(1,43)	1:5:A:GLN:HB3	1:6:A:TRP:H	24	0.11
(1,39)	1:5:A:GLN:HB3	1:5:A:GLN:H	15	0.11
(1,39)	1:5:A:GLN:HB3	1:5:A:GLN:H	37	0.11
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	22	0.11
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	31	0.11
(1,37)	1:4:A:ILE:HA	1:7:A:LEU:H	38	0.11
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD11	28	0.11
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD12	28	0.11
(1,23)	1:3:A:TYR:HE1	1:7:A:LEU:HD13	28	0.11
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD11	28	0.11
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD12	28	0.11
(1,23)	1:3:A:TYR:HE2	1:7:A:LEU:HD13	28	0.11
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	1	0.11
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	2	0.11
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	2	0.11
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	24	0.11
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	24	0.11
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	31	0.11
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	31	0.11
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	33	0.11
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	33	0.11
(1,8)	1:2:A:LEU:HA	1:5:A:GLN:H	8	0.11
(1,2)	1:1:A:ASN:HB2	1:2:A:LEU:H	12	0.11
(1,2)	1:1:A:ASN:HB3	1:2:A:LEU:H	12	0.11
(1,169)	1:19:A:PRO:HB2	1:20:A:SER:H	5	0.1
(1,164)	1:18:A:PRO:HA	1:19:A:PRO:HD2	25	0.1
(1,157)	1:17:A:PRO:HB3	1:18:A:PRO:HD2	6	0.1
(1,138)	1:13:A:SER:HB2	1:13:A:SER:H	38	0.1
(1,138)	1:13:A:SER:HB3	1:13:A:SER:H	38	0.1
(1,137)	1:12:A:PRO:HA	1:15:A:GLY:H	34	0.1
(1,135)	1:12:A:PRO:HD2	1:13:A:SER:H	16	0.1
(1,133)	1:12:A:PRO:HB2	1:13:A:SER:H	12	0.1
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	3	0.1
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	21	0.1
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	30	0.1
(1,129)	1:12:A:PRO:HB3	1:12:A:PRO:HD3	37	0.1
(1,106)	1:7:A:LEU:HD21	1:11:A:GLY:HA2	32	0.1
(1,106)	1:7:A:LEU:HD22	1:11:A:GLY:HA2	32	0.1
(1,106)	1:7:A:LEU:HD23	1:11:A:GLY:HA2	32	0.1
(1,93)	1:7:A:LEU:HG	1:7:A:LEU:H	26	0.1
(1,78)	1:6:A:TRP:HZ2	1:18:A:PRO:HD3	25	0.1
(1,13)	1:3:A:TYR:HD1	1:3:A:TYR:HB2	23	0.1
(1,13)	1:3:A:TYR:HD2	1:3:A:TYR:HB2	23	0.1
(1,6)	1:2:A:LEU:HB2	1:3:A:TYR:H	21	0.1
(1,6)	1:2:A:LEU:HB3	1:3:A:TYR:H	21	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found