



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 2L71 / pdb_00002l71
BMRB ID : 17331
Title : NMR solution structure of GIP in Bicellular media
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Deposited on : 2010-12-01

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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

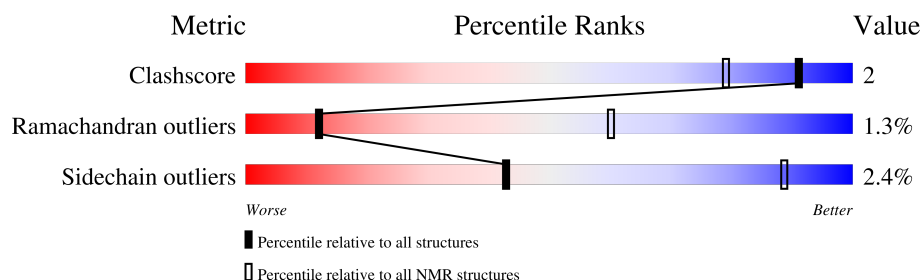
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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	42	40% 7% 52%

2 Ensemble composition and analysis

This entry contains 15 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:13-A:32 (20)	0.95	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 2 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 688 atoms, of which 336 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gastric inhibitory polypeptide.

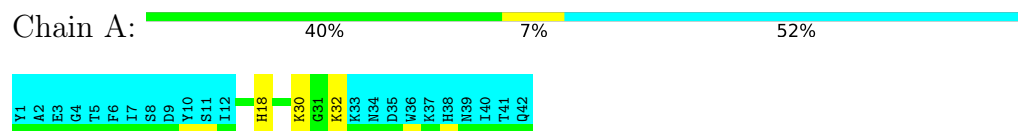
Mol	Chain	Residues	Atoms						Trace
1	A	42	Total	C	H	N	O	S	0
			688	226	336	60	65	1	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Gastric inhibitory polypeptide

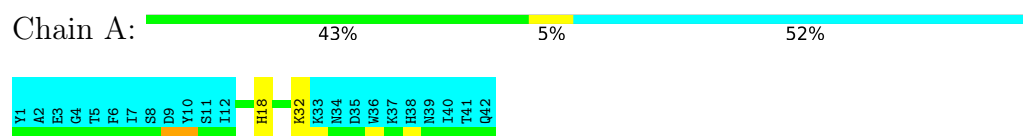


4.2 Scores per residue for each member of the ensemble

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

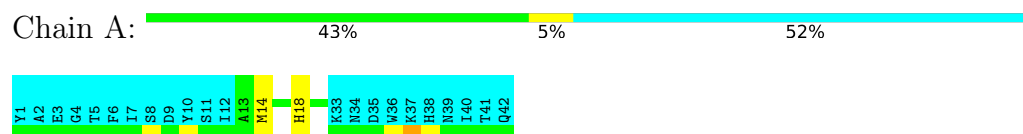
4.2.1 Score per residue for model 1

- Molecule 1: Gastric inhibitory polypeptide



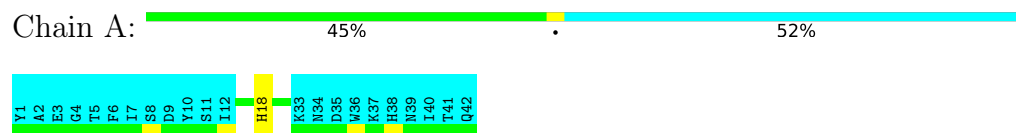
4.2.2 Score per residue for model 2

- Molecule 1: Gastric inhibitory polypeptide



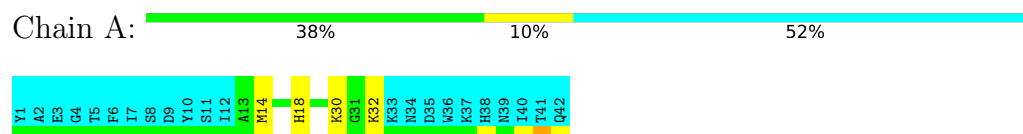
4.2.3 Score per residue for model 3

- Molecule 1: Gastric inhibitory polypeptide



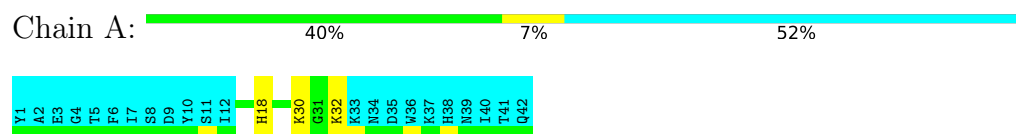
4.2.4 Score per residue for model 4

- Molecule 1: Gastric inhibitory polypeptide



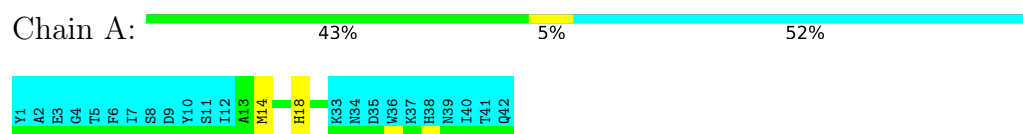
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Gastric inhibitory polypeptide



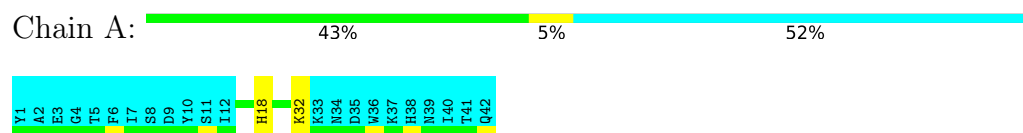
4.2.6 Score per residue for model 6

- Molecule 1: Gastric inhibitory polypeptide



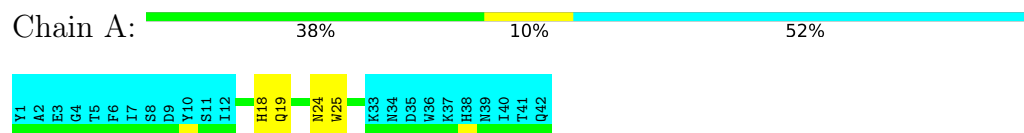
4.2.7 Score per residue for model 7

- Molecule 1: Gastric inhibitory polypeptide



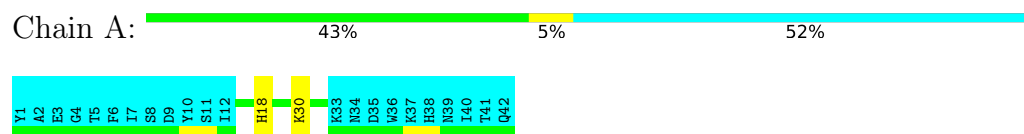
4.2.8 Score per residue for model 8

- Molecule 1: Gastric inhibitory polypeptide



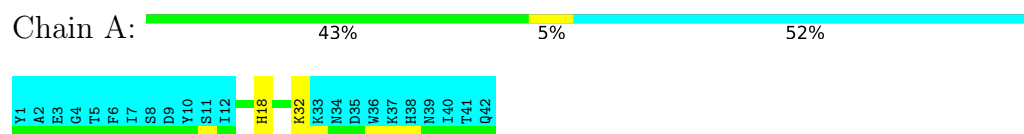
4.2.9 Score per residue for model 9

- Molecule 1: Gastric inhibitory polypeptide



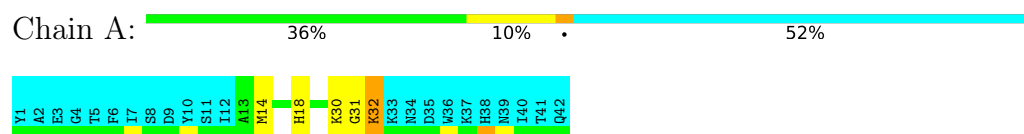
4.2.10 Score per residue for model 10

- Molecule 1: Gastric inhibitory polypeptide



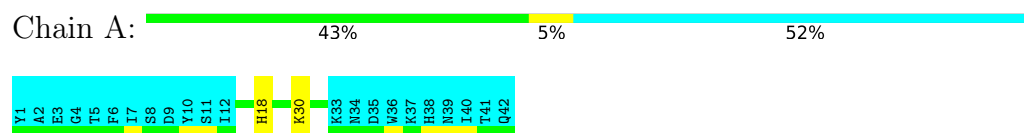
4.2.11 Score per residue for model 11

- Molecule 1: Gastric inhibitory polypeptide



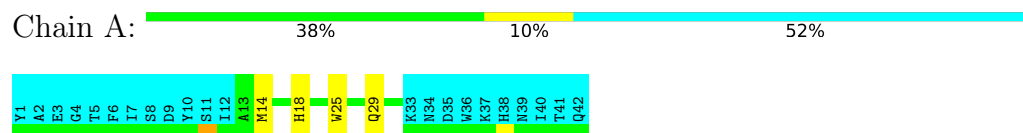
4.2.12 Score per residue for model 12

- Molecule 1: Gastric inhibitory polypeptide



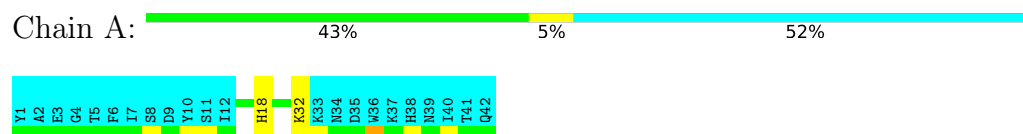
4.2.13 Score per residue for model 13

- Molecule 1: Gastric inhibitory polypeptide



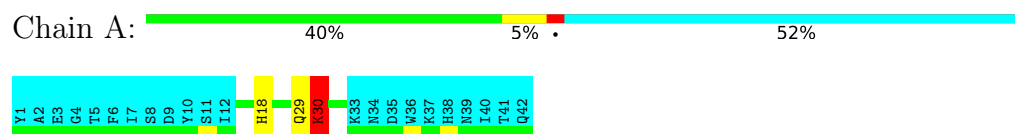
4.2.14 Score per residue for model 14

- Molecule 1: Gastric inhibitory polypeptide



4.2.15 Score per residue for model 15

- Molecule 1: Gastric inhibitory polypeptide



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0
CYANA	refinement	2.0

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	294
Number of shifts mapped to atoms	294
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.44±0.01	3±0/170 (1.8± 0.0%)	1.33±0.05	1±0/228 (0.5± 0.1%)
All	All	1.44	45/2550 (1.8%)	1.33	16/3420 (0.5%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	18	HIS	CE1-NE2	-6.76	1.25	1.32	4	15
1	A	18	HIS	CG-ND1	-5.93	1.31	1.38	9	15
1	A	18	HIS	CD2-NE2	5.92	1.44	1.37	12	15

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	18	HIS	CG-CD2-NE2	-6.41	100.79	107.20	9	15
1	A	30	LYS	N-CA-C	-5.85	104.81	111.07	4	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
1	A	166	167	167	1±1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	2490	2505	2505	8

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:MET:SD	1:A:14:MET:C	0.46	2.99	4	3
1:A:29:GLN:O	1:A:30:LYS:C	0.45	2.59	15	1
1:A:25:TRP:CE2	1:A:29:GLN:NE2	0.44	2.85	13	1
1:A:24:ASN:OD1	1:A:25:TRP:N	0.43	2.50	8	1
1:A:19:GLN:CD	1:A:19:GLN:C	0.43	2.85	8	1
1:A:31:GLY:O	1:A:32:LYS:C	0.42	2.63	11	1

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	20/42 (48%)	18±1 (90±7%)	2±1 (9±6%)	0±0 (1±2%)	12	60
All	All	300/630 (48%)	270 (90%)	26 (9%)	4 (1%)	12	60

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	14	MET	2
1	A	30	LYS	2

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	17/37 (46%)	17±1 (98±4%)	0±1 (2±4%)	43 89
All	All	255/555 (46%)	249 (98%)	6 (2%)	43 89

All 2 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	30	LYS	4
1	A	32	LYS	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 50% 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 [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	294
Number of shifts mapped to atoms	294
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 147 atoms were assigned a chemical shift out of a possible 290. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	41/101 (41%)	41/41 (100%)	0/40 (0%)	0/20 (0%)
Sidechain	95/160 (59%)	95/103 (92%)	0/50 (0%)	0/7 (0%)
Aromatic	11/29 (38%)	11/15 (73%)	0/12 (0%)	0/2 (0%)
Overall	147/290 (51%)	147/159 (92%)	0/102 (0%)	0/29 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 294 atoms were assigned a chemical shift out of a possible 589. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	85/212 (40%)	85/86 (99%)	0/84 (0%)	0/42 (0%)
Sidechain	179/301 (59%)	179/193 (93%)	0/96 (0%)	0/12 (0%)
Aromatic	30/76 (39%)	30/38 (79%)	0/34 (0%)	0/4 (0%)
Overall	294/589 (50%)	294/317 (93%)	0/214 (0%)	0/58 (0%)

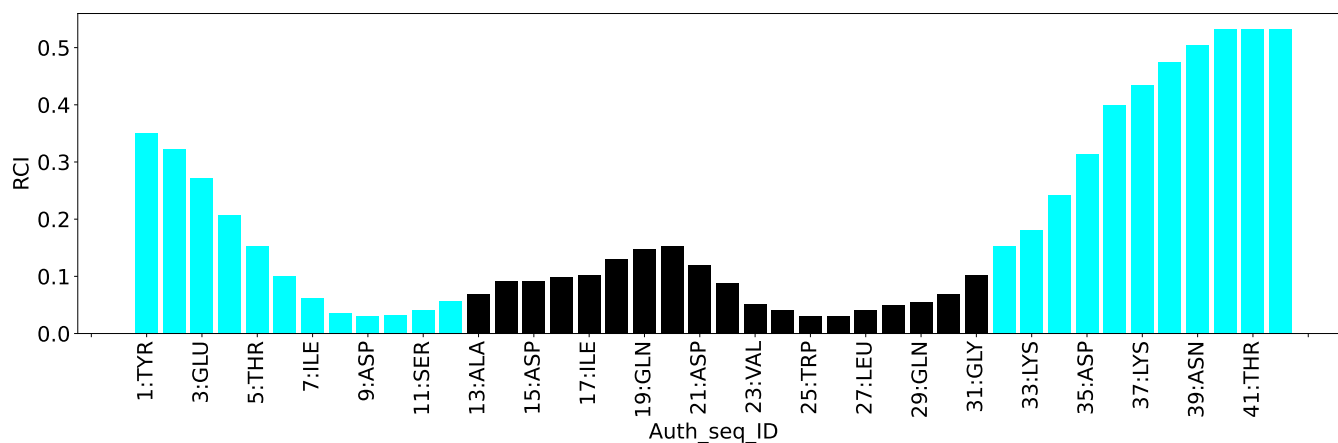
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	529
Intra-residue ($ i-j =0$)	226
Sequential ($ i-j =1$)	181
Medium range ($ i-j >1$ and $ i-j <5$)	120
Long range ($ i-j \geq 5$)	2
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	12.6
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	26.0	0.2
0.2-0.5 (Medium)	53.4	0.5
>0.5 (Large)	115.5	6.71

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 ⓘ

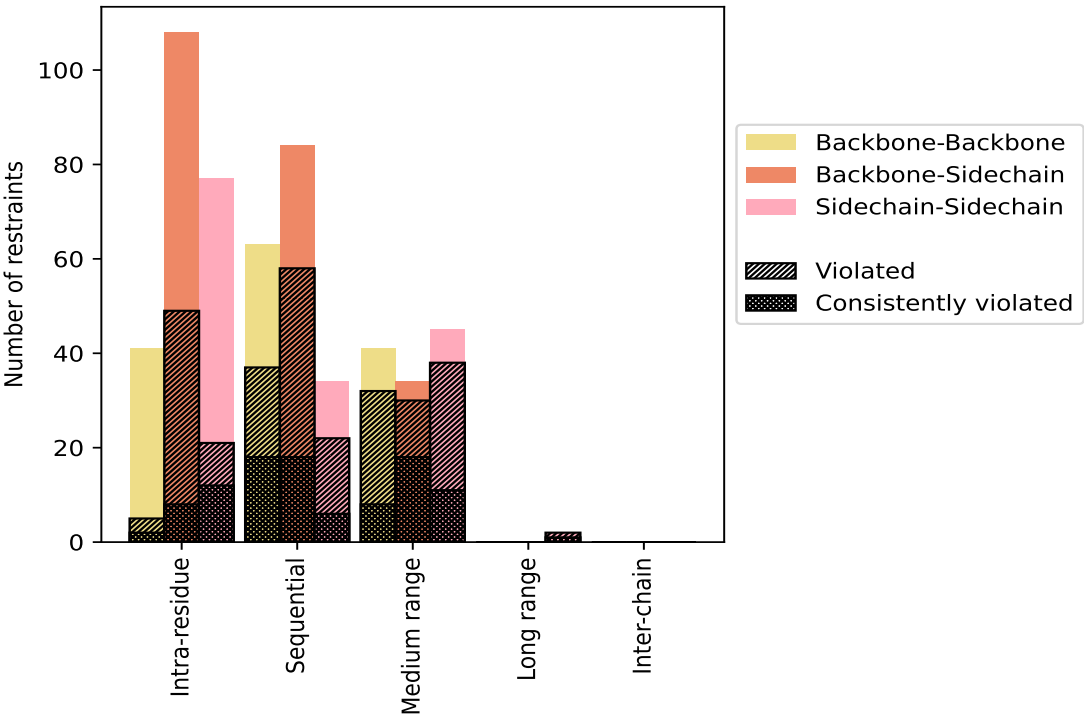
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	226	42.7	75	33.2	14.2	22	9.7	4.2
Backbone-Backbone	41	7.8	5	12.2	0.9	2	4.9	0.4
Backbone-Sidechain	108	20.4	49	45.4	9.3	8	7.4	1.5
Sidechain-Sidechain	77	14.6	21	27.3	4.0	12	15.6	2.3
Sequential ($i-j =1$)	181	34.2	117	64.6	22.1	42	23.2	7.9
Backbone-Backbone	63	11.9	37	58.7	7.0	18	28.6	3.4
Backbone-Sidechain	84	15.9	58	69.0	11.0	18	21.4	3.4
Sidechain-Sidechain	34	6.4	22	64.7	4.2	6	17.6	1.1
Medium range ($i-j >1$ & $i-j <5$)	120	22.7	100	83.3	18.9	37	30.8	7.0
Backbone-Backbone	41	7.8	32	78.0	6.0	8	19.5	1.5
Backbone-Sidechain	34	6.4	30	88.2	5.7	18	52.9	3.4
Sidechain-Sidechain	45	8.5	38	84.4	7.2	11	24.4	2.1
Long range ($i-j \geq 5$)	2	0.4	2	100.0	0.4	1	50.0	0.2
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	2	0.4	2	100.0	0.4	1	50.0	0.2
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	529	100.0	294	55.6	55.6	102	19.3	19.3
Backbone-Backbone	145	27.4	74	51.0	14.0	28	19.3	5.3
Backbone-Sidechain	226	42.7	137	60.6	25.9	44	19.5	8.3
Sidechain-Sidechain	158	29.9	83	52.5	15.7	30	19.0	5.7

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	56	85	67	2	0	210	0.99	5.06	0.91	0.7
2	49	84	64	2	0	199	0.95	5.52	0.96	0.59
3	53	79	67	2	0	201	1.02	5.66	0.96	0.73
4	47	78	61	2	0	188	0.98	5.61	0.93	0.65
5	50	76	61	2	0	189	0.98	5.52	0.91	0.64
6	48	80	62	2	0	192	0.98	5.27	0.9	0.7
7	50	80	63	2	0	195	1.01	5.1	1.03	0.63
8	53	81	71	2	0	207	0.99	6.07	0.97	0.66
9	54	84	68	2	0	208	0.95	4.92	0.96	0.56
10	55	80	65	2	0	202	1.0	5.32	0.97	0.7

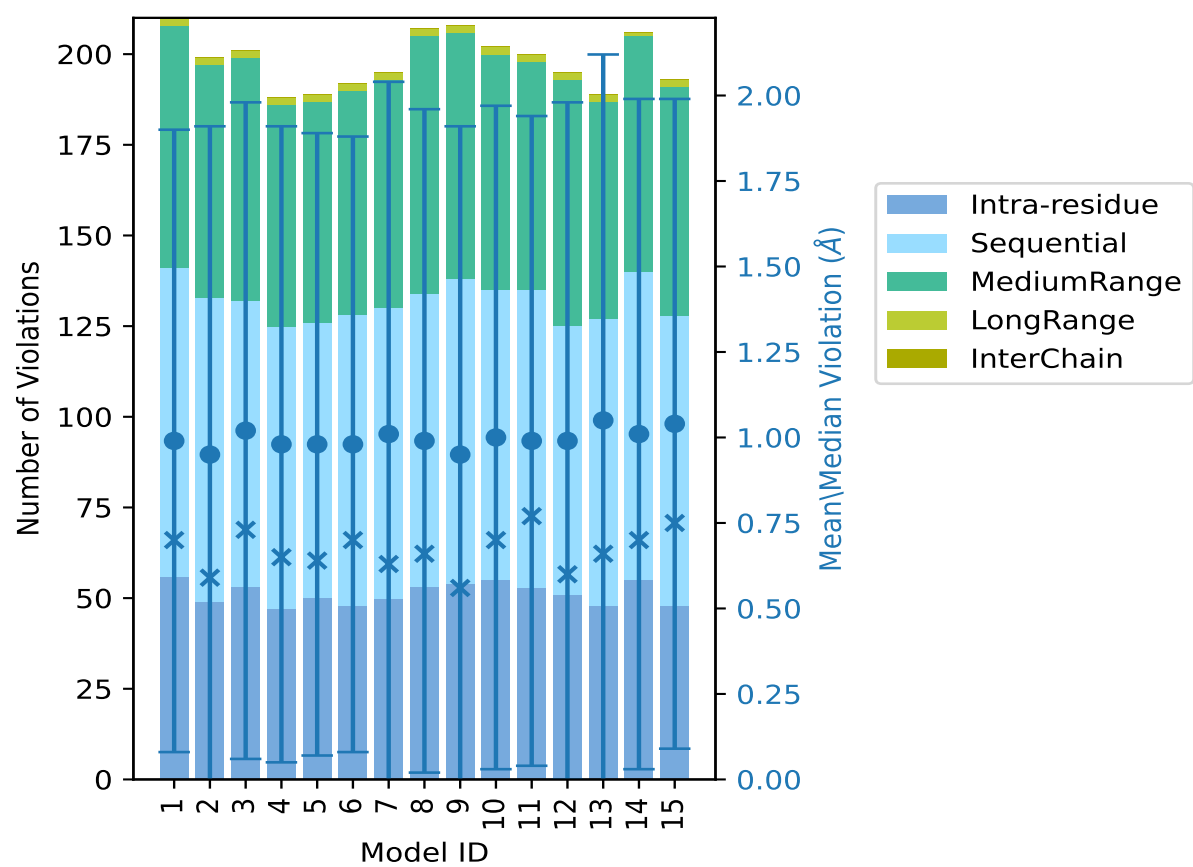
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	53	82	63	2	0	200	0.99	5.38	0.95	0.77
12	51	74	68	2	0	195	0.99	5.44	0.99	0.6
13	48	79	60	2	0	189	1.05	6.71	1.07	0.66
14	55	85	65	1	0	206	1.01	5.69	0.98	0.7
15	48	80	63	2	0	193	1.04	5.61	0.95	0.75

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

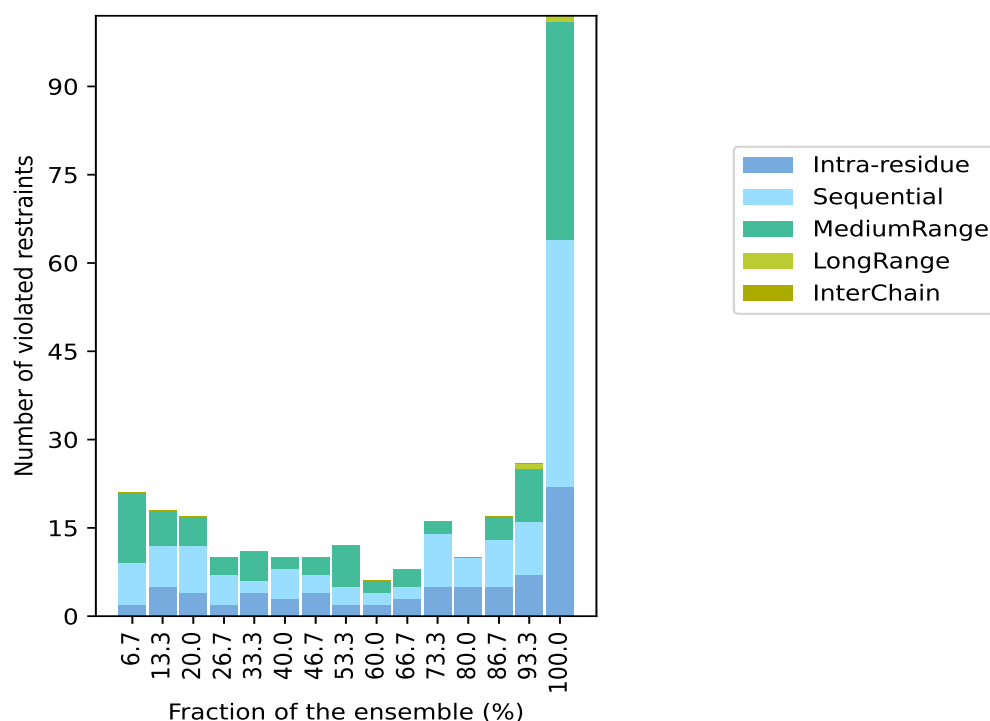
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 235(IR:151, SQ:64, MR:20, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	7	12	0	0	21	1	6.7
5	7	6	0	0	18	2	13.3
4	8	5	0	0	17	3	20.0
2	5	3	0	0	10	4	26.7
4	2	5	0	0	11	5	33.3
3	5	2	0	0	10	6	40.0
4	3	3	0	0	10	7	46.7
2	3	7	0	0	12	8	53.3
2	2	2	0	0	6	9	60.0
3	2	3	0	0	8	10	66.7
5	9	2	0	0	16	11	73.3
5	5	0	0	0	10	12	80.0
5	8	4	0	0	17	13	86.7
7	9	9	1	0	26	14	93.3
22	42	37	1	0	102	15	100.0

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

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

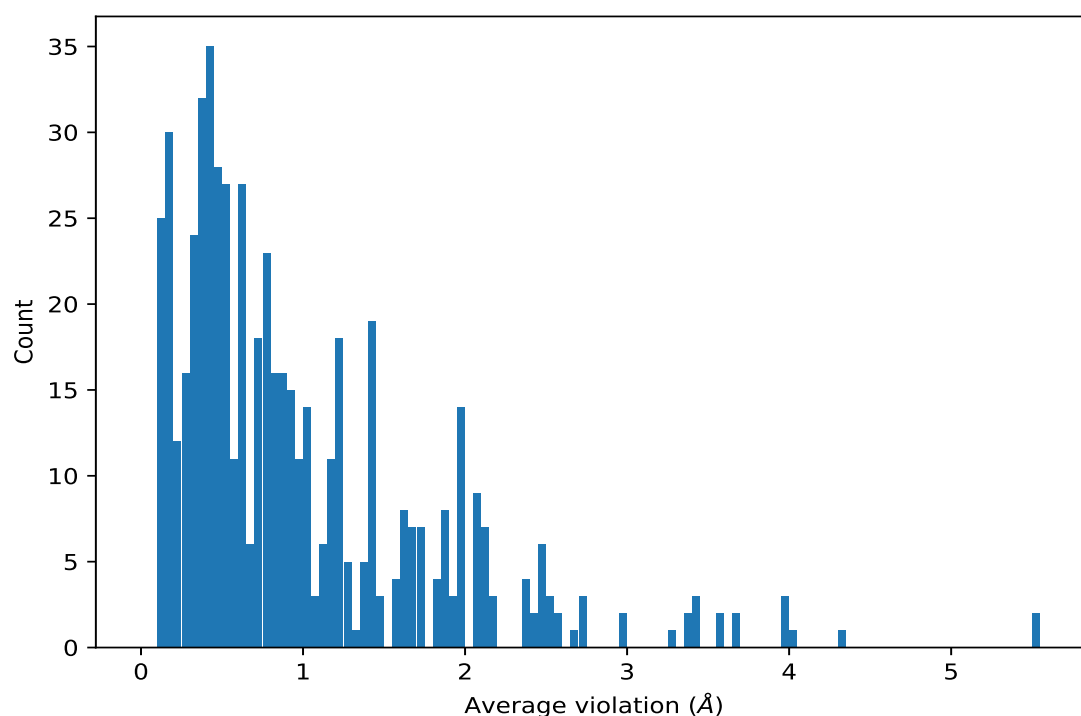
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	15	5.53	0.42	5.52
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	15	5.53	0.42	5.52
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	15	4.31	0.0	4.31
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	15	4.03	0.0	4.03
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	15	3.67	0.36	3.61
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	15	3.67	0.36	3.61
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	15	3.57	0.46	3.53
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	15	3.57	0.46	3.53
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	15	3.36	0.5	3.38
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	15	3.36	0.5	3.38
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	15	3.28	1.01	3.42
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	15	2.72	0.06	2.72
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	15	2.72	0.06	2.72
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	15	2.72	0.06	2.72
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	15	2.65	0.74	3.14
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	15	2.56	0.87	2.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	15	2.56	0.87	2.61
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	15	2.41	0.01	2.41
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	15	2.4	0.46	2.22
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	15	2.39	0.87	2.23
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	15	2.39	0.87	2.23
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	15	2.39	0.87	2.23
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	15	2.39	0.87	2.23
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	15	2.18	0.01	2.18
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	15	2.1	0.1	2.08
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	15	2.1	0.1	2.08
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	15	2.1	0.1	2.08
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	15	2.1	0.67	1.86
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	15	2.1	0.67	1.86
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	15	2.1	0.67	1.86
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	15	2.1	0.67	1.86
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	15	2.06	0.1	2.05
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	15	2.06	0.1	2.05
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	15	2.06	0.1	2.05
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	15	2.06	0.1	2.05
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	15	2.06	0.1	2.05
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	15	2.06	0.1	2.05
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	15	2.06	0.1	2.05
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	15	2.06	0.1	2.05
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	15	2.06	0.1	2.05
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	15	1.97	1.16	1.81
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	15	1.97	1.16	1.81
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	15	1.97	1.16	1.81
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	15	1.97	1.16	1.81
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	15	1.96	0.76	2.01
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	15	1.96	0.76	2.01
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	15	1.96	0.76	2.01
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	15	1.96	0.76	2.01
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	15	1.93	0.4	2.18
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	15	1.92	0.0	1.92
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	15	1.92	0.01	1.91
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	15	1.89	0.0	1.89
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	15	1.86	0.32	1.9
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	15	1.84	0.4	1.81
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	15	1.84	0.4	1.81
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	15	1.7	0.25	1.77
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	15	1.7	0.25	1.77
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	15	1.66	0.01	1.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	15	1.62	0.28	1.66
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	15	1.62	0.28	1.66
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	15	1.62	0.07	1.62
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	15	1.62	0.07	1.62
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	15	1.61	0.19	1.59
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	15	1.61	0.19	1.59
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	15	1.61	0.19	1.59
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	15	1.58	0.0	1.58
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	15	1.57	0.25	1.64
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	15	1.57	0.25	1.64
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	15	1.57	0.25	1.64
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	15	1.45	0.38	1.37
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	15	1.45	0.38	1.37
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	15	1.45	0.38	1.37
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	15	1.44	0.13	1.48
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	15	1.44	0.13	1.48
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	15	1.44	0.13	1.48
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	15	1.43	0.48	1.47
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	15	1.43	0.48	1.47
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	15	1.41	0.36	1.46
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	15	1.41	0.36	1.46
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	15	1.37	0.52	1.08
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	15	1.37	0.52	1.08
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	15	1.35	0.04	1.34
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	15	1.35	0.04	1.34
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	15	1.28	0.15	1.28
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	15	1.28	0.15	1.28
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	15	1.28	0.15	1.28
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	15	1.27	0.01	1.27
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	15	1.26	0.09	1.27
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	15	1.24	0.09	1.25
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	15	1.2	0.14	1.2
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	15	1.2	0.14	1.2
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	15	1.2	0.09	1.16
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	15	1.19	0.31	1.35
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	15	1.1	0.17	1.06
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	15	1.1	0.17	1.06
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	15	1.1	0.17	1.06
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	15	1.1	0.23	1.07
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	15	1.05	0.09	1.05
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	15	1.04	0.04	1.04
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	15	1.04	0.04	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	15	1.01	0.12	1.02
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	15	1.01	0.12	1.02
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	15	1.01	0.12	1.02
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	15	1.0	0.3	1.09
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	15	1.0	0.3	1.09
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	15	1.0	0.3	1.09
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	15	0.95	0.36	0.96
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	15	0.92	0.24	0.92
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	15	0.92	0.24	0.92
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	15	0.91	0.18	0.88
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	15	0.91	0.18	0.88
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	15	0.91	0.18	0.88
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	15	0.91	0.18	0.88
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	15	0.91	0.18	0.88
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	15	0.91	0.18	0.88
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	15	0.9	0.18	0.97
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	15	0.87	0.16	0.83
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	15	0.87	0.26	0.84
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	15	0.87	0.26	0.84
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	15	0.87	0.26	0.84
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	15	0.84	0.45	0.57
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	15	0.78	0.29	0.89
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	15	0.76	0.52	0.6
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	15	0.76	0.52	0.6
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	15	0.74	0.2	0.7
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	15	0.74	0.14	0.77
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	15	0.72	0.43	0.73
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	15	0.72	0.43	0.73
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	15	0.72	0.43	0.73
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	15	0.7	0.41	0.55
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	15	0.7	0.08	0.73
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	15	0.7	0.08	0.73
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	15	0.7	0.08	0.73
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	15	0.7	0.15	0.72
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	15	0.7	0.15	0.72
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	15	0.62	0.35	0.49
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	15	0.6	0.29	0.52
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	15	0.6	0.29	0.52
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	15	0.6	0.29	0.52
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	15	0.6	0.18	0.6
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	15	0.6	0.28	0.54
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	15	0.58	0.22	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	15	0.54	0.15	0.56
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	15	0.53	0.36	0.43
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	15	0.51	0.09	0.52
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	15	0.47	0.18	0.41
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	15	0.46	0.21	0.43
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	15	0.45	0.18	0.42
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	15	0.45	0.06	0.45
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	15	0.44	0.02	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	15	0.44	0.02	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	15	0.44	0.02	0.43
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	15	0.44	0.13	0.43
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	15	0.44	0.02	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	15	0.44	0.02	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	15	0.44	0.02	0.45
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	15	0.43	0.04	0.42
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	15	0.43	0.04	0.42
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	15	0.41	0.14	0.44
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	15	0.4	0.11	0.4
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	15	0.39	0.18	0.38
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	15	0.35	0.19	0.28
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	15	0.34	0.01	0.34
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	15	0.33	0.07	0.33
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	15	0.31	0.01	0.3
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	15	0.3	0.27	0.24
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	15	0.25	0.06	0.23
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	15	0.25	0.06	0.23
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	15	0.25	0.06	0.23
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	15	0.25	0.01	0.25
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	15	0.25	0.07	0.26
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	15	0.24	0.03	0.25
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	15	0.22	0.05	0.21
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	15	0.22	0.07	0.23
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	15	0.19	0.05	0.19
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	15	0.18	0.01	0.18
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	15	0.16	0.04	0.16
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	15	0.15	0.02	0.15
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	15	0.12	0.01	0.12
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	15	0.1	0.0	0.1
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	14	3.97	0.39	4.04
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	14	3.97	0.39	4.04
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	14	3.97	0.39	4.04
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	14	3.41	0.46	3.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	14	3.41	0.46	3.49
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	14	3.41	0.46	3.49
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	14	1.98	1.06	1.66
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	14	1.98	1.06	1.66
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	14	1.98	1.06	1.66
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	14	1.98	1.06	1.66
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	14	1.98	1.06	1.66
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	14	1.98	1.06	1.66
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	14	1.72	0.96	1.78
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	14	1.72	0.96	1.78
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	14	1.72	0.96	1.78
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	14	1.72	0.96	1.78
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	14	1.15	0.73	0.85
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	14	1.15	0.73	0.85
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	14	1.15	0.73	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	14	1.15	0.73	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	14	1.15	0.73	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	14	1.15	0.73	0.85
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	14	1.05	0.34	0.9
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	14	1.05	0.34	0.9
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	14	1.0	0.32	0.88
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	14	1.0	0.32	0.88
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	14	1.0	0.32	0.88
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	14	1.0	0.32	0.88
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	14	1.0	0.32	0.88
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	14	1.0	0.32	0.88
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	14	0.96	0.33	0.78
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	14	0.89	0.1	0.85
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	14	0.89	0.1	0.85
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	14	0.81	0.34	0.79
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	14	0.81	0.34	0.79
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	14	0.81	0.34	0.79
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	14	0.81	0.34	0.79
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	14	0.81	0.34	0.79
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	14	0.81	0.34	0.79
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	14	0.79	0.35	0.7
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	14	0.79	0.35	0.7
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	14	0.78	0.38	0.67
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	14	0.78	0.38	0.67
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	14	0.6	0.38	0.46
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	14	0.56	0.16	0.55
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	14	0.56	0.16	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	14	0.56	0.16	0.55
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	14	0.52	0.27	0.55
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	14	0.43	0.19	0.41
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	14	0.36	0.04	0.37
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	14	0.31	0.06	0.32
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	14	0.31	0.06	0.32
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	14	0.31	0.06	0.32
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	14	0.29	0.08	0.3
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	14	0.2	0.03	0.2
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	14	0.19	0.08	0.16
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	14	0.17	0.03	0.18
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	14	0.17	0.03	0.18
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	14	0.14	0.04	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	14	0.13	0.01	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	14	0.13	0.01	0.14
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	14	0.12	0.01	0.12
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	14	0.12	0.01	0.12
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	13	2.5	0.72	2.71
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	13	2.5	0.72	2.71
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	13	2.5	0.72	2.71
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	13	2.17	1.11	2.6
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	13	2.17	1.11	2.6
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	13	1.81	0.71	1.71
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	13	1.67	0.54	1.53
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	13	1.67	0.54	1.53
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	13	1.67	0.54	1.53
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	13	1.67	0.54	1.53
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	13	1.67	0.54	1.53
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	13	1.67	0.54	1.53
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	13	1.24	0.71	1.65
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	13	1.22	0.48	1.09
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	13	1.2	0.28	1.11
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	13	1.2	0.28	1.11
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	13	1.2	0.28	1.11
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	13	1.17	0.42	1.0
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	13	0.97	0.31	1.07
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	13	0.82	0.34	0.81
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	13	0.82	0.34	0.81
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	13	0.78	0.13	0.81
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	13	0.78	0.13	0.81
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	13	0.77	0.28	0.83
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	13	0.73	0.32	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	13	0.73	0.32	0.68
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	13	0.73	0.32	0.68
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	13	0.73	0.32	0.68
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	13	0.54	0.18	0.5
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	13	0.54	0.18	0.5
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	13	0.54	0.18	0.5
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	13	0.35	0.1	0.33
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	13	0.35	0.1	0.33
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	13	0.33	0.4	0.23
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	13	0.31	0.05	0.28
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	13	0.31	0.05	0.28
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	12	1.74	0.99	1.5
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	12	1.31	0.73	1.1
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	12	1.15	0.67	0.76
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	12	1.15	0.67	0.76
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	12	1.15	0.67	0.76
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	12	0.75	0.55	0.53
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	12	0.72	0.39	0.84
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	12	0.61	0.1	0.61
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	12	0.61	0.1	0.61
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	12	0.4	0.17	0.34
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	12	0.37	0.25	0.26
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	12	0.33	0.15	0.3
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	12	0.33	0.15	0.3
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	12	0.1	0.0	0.1
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	11	1.89	0.84	1.76
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	11	1.89	0.84	1.76
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	11	1.89	0.84	1.76
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	11	1.89	0.84	1.76
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	11	1.89	0.84	1.76
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	11	1.89	0.84	1.76
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	11	1.2	0.33	1.06
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	11	1.2	0.33	1.06
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	11	1.2	0.33	1.06
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	11	0.83	0.35	0.74
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	11	0.83	0.35	0.74
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	11	0.83	0.35	0.74
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	11	0.82	0.47	0.8
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	11	0.82	0.47	0.8
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	11	0.76	0.01	0.76
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	11	0.76	0.01	0.76
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	11	0.69	0.34	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	11	0.69	0.34	0.76
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	11	0.69	0.34	0.76
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	11	0.64	0.02	0.64
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	11	0.63	0.1	0.62
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	11	0.63	0.1	0.62
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	11	0.57	0.45	0.44
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	11	0.51	0.15	0.51
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	11	0.44	0.23	0.4
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	11	0.4	0.33	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	11	0.4	0.33	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	11	0.4	0.33	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	11	0.4	0.33	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	11	0.4	0.33	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	11	0.4	0.33	0.25
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	11	0.34	0.03	0.33
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	11	0.34	0.03	0.33
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	11	0.32	0.07	0.34
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	11	0.23	0.09	0.22
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	11	0.19	0.06	0.21
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	10	0.88	0.51	0.82
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	10	0.88	0.51	0.82
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	10	0.79	0.28	0.92
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	10	0.79	0.28	0.92
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	10	0.59	0.42	0.48
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	10	0.41	0.19	0.4
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	10	0.41	0.19	0.4
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	10	0.18	0.06	0.18
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	10	0.18	0.06	0.18
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	10	0.16	0.08	0.15
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	10	0.12	0.01	0.12
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	10	0.12	0.02	0.12
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	9	2.47	0.51	2.52
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	9	2.47	0.51	2.52
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	9	2.47	0.51	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	9	2.47	0.51	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	9	2.47	0.51	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	9	2.47	0.51	2.52
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	9	1.6	0.57	1.86
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	9	0.68	0.01	0.68
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	9	0.41	0.32	0.26
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	9	0.37	0.08	0.4
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	9	0.37	0.08	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	9	0.37	0.08	0.4
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	9	0.23	0.1	0.22
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	8	1.2	0.79	1.06
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	8	1.2	0.79	1.06
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	8	1.2	0.79	1.06
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	8	1.2	0.79	1.06
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	8	1.2	0.79	1.06
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	8	1.2	0.79	1.06
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	8	0.61	0.43	0.47
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	8	0.61	0.43	0.47
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	8	0.58	0.44	0.35
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	8	0.58	0.44	0.35
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	8	0.45	0.39	0.29
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	8	0.39	0.13	0.37
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	8	0.39	0.13	0.37
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	8	0.39	0.16	0.34
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	8	0.39	0.16	0.34
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	8	0.37	0.07	0.4
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	8	0.37	0.07	0.4
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	8	0.37	0.07	0.4
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	8	0.36	0.25	0.26
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	8	0.34	0.22	0.29
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	8	0.28	0.03	0.28
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	8	0.28	0.03	0.28
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	8	0.23	0.05	0.24
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	8	0.1	0.0	0.1
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD1	7	1.4	0.53	1.34
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD2	7	1.4	0.53	1.34
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD1	7	1.4	0.53	1.34
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD2	7	1.4	0.53	1.34
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD1	7	1.4	0.53	1.34
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD2	7	1.4	0.53	1.34
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD2	7	1.12	0.17	1.1
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD3	7	1.12	0.17	1.1
(1,235)	1:14:A:MET:HG2	1:15:A:ASP:H	7	0.77	0.36	0.85
(1,235)	1:14:A:MET:HG3	1:15:A:ASP:H	7	0.77	0.36	0.85
(1,247)	1:30:A:LYS:HG2	1:31:A:GLY:H	7	0.76	0.16	0.73
(1,247)	1:30:A:LYS:HG3	1:31:A:GLY:H	7	0.76	0.16	0.73
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE22	7	0.72	0.52	0.33
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE21	7	0.72	0.52	0.33
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD11	7	0.63	0.34	0.65
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD12	7	0.63	0.34	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD13	7	0.63	0.34	0.65
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG21	7	0.61	0.37	0.49
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG22	7	0.61	0.37	0.49
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG23	7	0.61	0.37	0.49
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG21	7	0.61	0.37	0.49
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG22	7	0.61	0.37	0.49
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG23	7	0.61	0.37	0.49
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG2	7	0.35	0.01	0.35
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG3	7	0.35	0.01	0.35
(1,203)	1:11:A:SER:H	1:12:A:ILE:HB	7	0.3	0.12	0.27
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG2	7	0.2	0.04	0.19
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG3	7	0.2	0.04	0.19
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG12	6	0.61	0.35	0.58
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG13	6	0.61	0.35	0.58
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG12	6	0.61	0.35	0.58
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG13	6	0.61	0.35	0.58
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD21	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD22	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD23	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD22	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD23	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD22	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD23	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD11	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD12	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD13	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD11	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD12	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD13	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD11	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD12	6	0.54	0.42	0.43
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD13	6	0.54	0.42	0.43
(1,80)	1:16:A:LYS:HA	1:19:A:GLN:H	6	0.45	0.15	0.5
(1,435)	1:41:A:THR:H	1:41:A:THR:HG21	6	0.41	0.03	0.4
(1,435)	1:41:A:THR:H	1:41:A:THR:HG22	6	0.41	0.03	0.4
(1,435)	1:41:A:THR:H	1:41:A:THR:HG23	6	0.41	0.03	0.4
(1,198)	1:11:A:SER:H	1:12:A:ILE:H	6	0.4	0.28	0.33
(1,1)	1:2:A:ALA:HA	1:3:A:GLU:H	6	0.34	0.01	0.34
(1,115)	1:13:A:ALA:HA	1:14:A:MET:H	6	0.27	0.06	0.28
(1,17)	1:15:A:ASP:H	1:15:A:ASP:HB3	6	0.21	0.02	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB1	6	0.19	0.06	0.18
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB2	6	0.19	0.06	0.18
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB3	6	0.19	0.06	0.18
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB1	6	0.19	0.06	0.18
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB2	6	0.19	0.06	0.18
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB3	6	0.19	0.06	0.18
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB1	6	0.19	0.06	0.18
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB2	6	0.19	0.06	0.18
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB3	6	0.19	0.06	0.18
(1,228)	1:5:A:THR:H	1:5:A:THR:HA	6	0.15	0.04	0.14
(1,212)	1:6:A:PHE:HA	1:10:A:TYR:H	5	0.82	0.41	0.83
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB2	5	0.75	0.46	0.62
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB3	5	0.75	0.46	0.62
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB2	5	0.75	0.46	0.62
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB3	5	0.75	0.46	0.62
(1,314)	1:39:A:ASN:HB3	1:39:A:ASN:HD22	5	0.45	0.02	0.45
(1,314)	1:39:A:ASN:HB2	1:39:A:ASN:HD22	5	0.45	0.02	0.45
(1,254)	1:33:A:LYS:HG2	1:34:A:ASN:H	5	0.43	0.12	0.4
(1,254)	1:33:A:LYS:HG3	1:34:A:ASN:H	5	0.43	0.12	0.4
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB1	5	0.38	0.21	0.31
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB2	5	0.38	0.21	0.31
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB3	5	0.38	0.21	0.31
(1,219)	1:30:A:LYS:HA	1:32:A:LYS:H	5	0.35	0.18	0.39
(1,84)	1:34:A:ASN:HA	1:37:A:LYS:H	5	0.32	0.11	0.34
(1,110)	1:5:A:THR:HB	1:6:A:PHE:H	5	0.29	0.26	0.17
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	5	0.15	0.06	0.14
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD3	5	0.15	0.06	0.14
(1,41)	1:25:A:TRP:H	1:25:A:TRP:HB3	5	0.15	0.01	0.15
(1,346)	1:36:A:TRP:H	1:36:A:TRP:HD1	5	0.15	0.03	0.15
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD21	4	0.85	0.44	0.86
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD22	4	0.85	0.44	0.86
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD23	4	0.85	0.44	0.86
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD11	4	0.85	0.44	0.86
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD12	4	0.85	0.44	0.86
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD13	4	0.85	0.44	0.86
(1,51)	1:30:A:LYS:HB2	1:31:A:GLY:H	4	0.55	0.19	0.56
(1,51)	1:30:A:LYS:HB3	1:31:A:GLY:H	4	0.55	0.19	0.56
(1,239)	1:16:A:LYS:HG2	1:17:A:ILE:H	4	0.35	0.01	0.34
(1,239)	1:16:A:LYS:HG3	1:17:A:ILE:H	4	0.35	0.01	0.34
(1,218)	1:29:A:GLN:HA	1:31:A:GLY:H	4	0.32	0.13	0.35
(1,119)	1:11:A:SER:HA	1:14:A:MET:H	4	0.32	0.15	0.31
(1,437)	1:17:A:ILE:HG21	1:18:A:HIS:H	4	0.25	0.05	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,437)	1:17:A:ILE:HG22	1:18:A:HIS:H	4	0.25	0.05	0.26
(1,437)	1:17:A:ILE:HG23	1:18:A:HIS:H	4	0.25	0.05	0.26
(1,230)	1:15:A:ASP:HA	1:18:A:HIS:H	4	0.23	0.07	0.26
(1,36)	1:21:A:ASP:HB2	1:22:A:PHE:H	4	0.16	0.02	0.15
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.13	0.02	0.14
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.13	0.02	0.14
(1,356)	1:36:A:TRP:HZ3	1:36:A:TRP:HE3	4	0.11	0.0	0.11
(1,322)	1:6:A:PHE:HE1	1:7:A:ILE:HG12	3	2.97	0.34	2.74
(1,322)	1:6:A:PHE:HE2	1:7:A:ILE:HG12	3	2.97	0.34	2.74
(1,277)	1:36:A:TRP:HE3	1:37:A:LYS:HA	3	1.81	0.97	2.43
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG21	3	1.4	0.26	1.29
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG22	3	1.4	0.26	1.29
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG23	3	1.4	0.26	1.29
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG21	3	1.4	0.26	1.29
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG22	3	1.4	0.26	1.29
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG23	3	1.4	0.26	1.29
(1,406)	1:6:A:PHE:HD1	1:7:A:ILE:HB	3	0.95	0.27	0.88
(1,406)	1:6:A:PHE:HD2	1:7:A:ILE:HB	3	0.95	0.27	0.88
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD11	3	0.91	0.59	0.74
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD12	3	0.91	0.59	0.74
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD13	3	0.91	0.59	0.74
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD11	3	0.91	0.59	0.74
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD12	3	0.91	0.59	0.74
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD13	3	0.91	0.59	0.74
(1,321)	1:6:A:PHE:HD1	1:7:A:ILE:HG12	3	0.85	0.39	0.58
(1,321)	1:6:A:PHE:HD2	1:7:A:ILE:HG12	3	0.85	0.39	0.58
(1,345)	1:6:A:PHE:HD1	1:8:A:SER:H	3	0.67	0.09	0.63
(1,345)	1:6:A:PHE:HD2	1:8:A:SER:H	3	0.67	0.09	0.63
(1,213)	1:8:A:SER:H	1:10:A:TYR:H	3	0.52	0.17	0.44
(2,11)	1:10:A:TYR:HD1	1:14:A:MET:HG2	3	0.41	0.33	0.24
(2,11)	1:10:A:TYR:HD1	1:14:A:MET:HG3	3	0.41	0.33	0.24
(2,11)	1:10:A:TYR:HD2	1:14:A:MET:HG2	3	0.41	0.33	0.24
(2,11)	1:10:A:TYR:HD2	1:14:A:MET:HG3	3	0.41	0.33	0.24
(1,325)	1:14:A:MET:HB2	1:18:A:HIS:HD2	3	0.39	0.18	0.39
(1,325)	1:14:A:MET:HB3	1:18:A:HIS:HD2	3	0.39	0.18	0.39
(1,428)	1:28:A:ALA:HB1	1:29:A:GLN:H	3	0.37	0.04	0.37
(1,428)	1:28:A:ALA:HB2	1:29:A:GLN:H	3	0.37	0.04	0.37
(1,428)	1:28:A:ALA:HB3	1:29:A:GLN:H	3	0.37	0.04	0.37
(1,251)	1:40:A:ILE:H	1:40:A:ILE:HG12	3	0.37	0.07	0.33
(1,251)	1:40:A:ILE:H	1:40:A:ILE:HG13	3	0.37	0.07	0.33
(1,150)	1:42:A:GLN:H	1:42:A:GLN:HB2	3	0.34	0.15	0.44
(1,234)	1:14:A:MET:H	1:14:A:MET:HG2	3	0.33	0.07	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,234)	1:14:A:MET:H	1:14:A:MET:HG3	3	0.33	0.07	0.32
(1,108)	1:3:A:GLU:HA	1:6:A:PHE:H	3	0.23	0.08	0.2
(1,12)	1:12:A:ILE:H	1:12:A:ILE:HB	3	0.11	0.0	0.11
(2,7)	1:1:A:TYR:HD1	1:2:A:ALA:HA	3	0.1	0.0	0.1
(2,7)	1:1:A:TYR:HD2	1:2:A:ALA:HA	3	0.1	0.0	0.1
(1,127)	1:29:A:GLN:HA	1:32:A:LYS:H	2	1.37	0.61	1.37
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD11	2	0.99	0.71	0.99
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD12	2	0.99	0.71	0.99
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD13	2	0.99	0.71	0.99
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD11	2	0.99	0.71	0.99
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD12	2	0.99	0.71	0.99
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD13	2	0.99	0.71	0.99
(1,287)	1:25:A:TRP:HD1	1:26:A:LEU:HA	2	0.83	0.19	0.83
(1,124)	1:28:A:ALA:HA	1:31:A:GLY:H	2	0.58	0.13	0.58
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD21	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD22	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD23	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD21	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD22	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD23	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD21	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD22	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD23	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD11	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD12	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD13	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD11	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD12	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD13	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD11	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD12	2	0.49	0.38	0.49
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD13	2	0.49	0.38	0.49
(1,71)	1:37:A:LYS:HB2	1:38:A:HIS:H	2	0.47	0.0	0.47
(1,71)	1:37:A:LYS:HB3	1:38:A:HIS:H	2	0.47	0.0	0.47
(1,148)	1:20:A:GLN:HB2	1:21:A:ASP:H	2	0.43	0.02	0.43
(1,148)	1:20:A:GLN:HB3	1:21:A:ASP:H	2	0.43	0.02	0.43
(1,216)	1:37:A:LYS:H	1:39:A:ASN:H	2	0.29	0.01	0.29
(1,140)	1:41:A:THR:H	1:41:A:THR:HB	2	0.29	0.12	0.29
(1,66)	1:35:A:ASP:HA	1:36:A:TRP:H	2	0.26	0.09	0.26
(1,5)	1:8:A:SER:H	1:8:A:SER:HB2	2	0.18	0.03	0.18
(1,5)	1:8:A:SER:H	1:8:A:SER:HB3	2	0.18	0.03	0.18
(1,166)	1:10:A:TYR:HB2	1:11:A:SER:H	2	0.18	0.02	0.18

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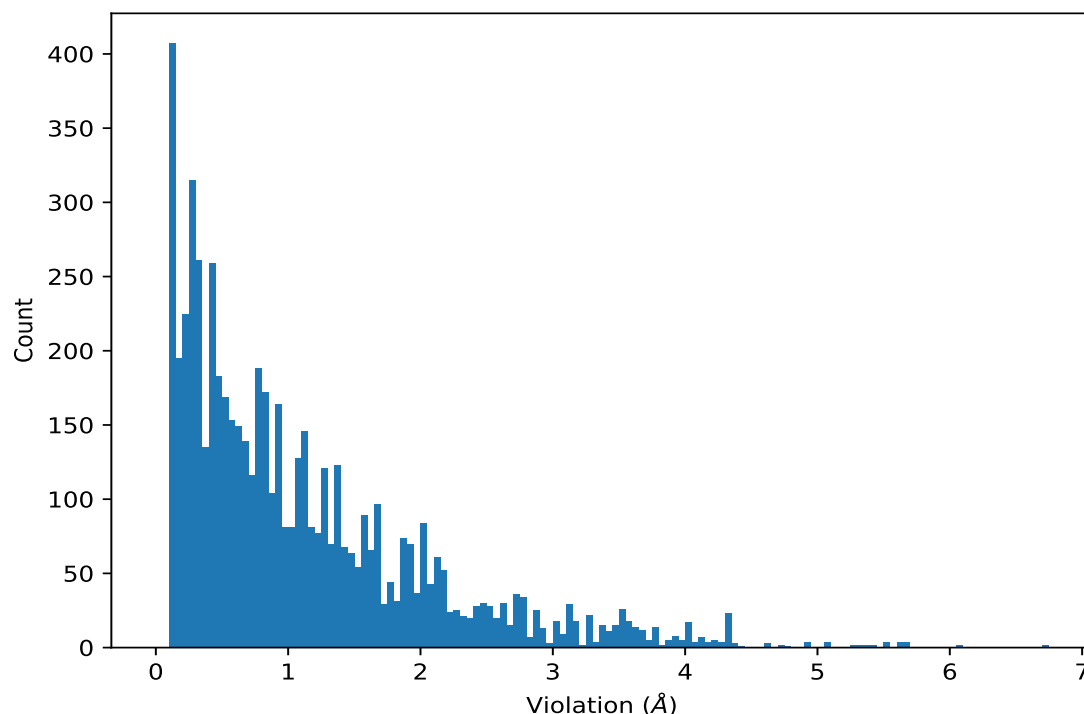
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,111)	1:32:A:LYS:HA	1:34:A:ASN:H	2	0.16	0.04	0.16
(1,253)	1:33:A:LYS:H	1:33:A:LYS:HG2	2	0.14	0.02	0.14
(1,253)	1:33:A:LYS:H	1:33:A:LYS:HG3	2	0.14	0.02	0.14
(1,45)	1:29:A:GLN:H	1:29:A:GLN:HB2	2	0.14	0.02	0.14
(1,45)	1:29:A:GLN:H	1:29:A:GLN:HB3	2	0.14	0.02	0.14
(1,92)	1:9:A:ASP:HB2	1:10:A:TYR:H	2	0.14	0.01	0.14
(1,92)	1:9:A:ASP:HB3	1:10:A:TYR:H	2	0.14	0.01	0.14
(1,338)	1:36:A:TRP:HE3	1:37:A:LYS:H	2	0.12	0.02	0.12
(1,72)	1:38:A:HIS:H	1:38:A:HIS:HA	2	0.11	0.0	0.11

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)
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	13	6.71
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	13	6.71
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	8	6.07
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	8	6.07
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	14	5.69
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	14	5.69
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	3	5.66
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	3	5.66
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	4	5.61
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	4	5.61
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	15	5.61
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	15	5.61
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	2	5.52
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	2	5.52
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	5	5.52
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	5	5.52
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	12	5.44
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	12	5.44
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	11	5.38
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	11	5.38
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	10	5.32
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	10	5.32
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	6	5.27
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	6	5.27
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	7	5.1
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	7	5.1
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	1	5.06
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	1	5.06
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	13	4.93
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	13	4.93
(1,369)	1:22:A:PHE:HE1	1:25:A:TRP:HH2	9	4.92
(1,369)	1:22:A:PHE:HE2	1:25:A:TRP:HH2	9	4.92
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	7	4.75
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	13	4.74
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	13	4.74
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	7	4.63
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	7	4.63
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	7	4.63
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	10	4.4
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	3	4.37
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	3	4.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	3	4.37
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	11	4.34
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	11	4.34
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	11	4.34
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	14	4.34
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	14	4.34
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	7	4.32
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	7	4.32
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	7	4.32
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	7	4.32
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	10	4.32
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	14	4.32
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	1	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	2	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	3	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	4	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	5	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	6	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	8	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	9	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	11	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	12	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	13	4.31
(1,363)	1:25:A:TRP:HZ3	1:25:A:TRP:HD1	15	4.31
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	10	4.29
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	10	4.29
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	10	4.29
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	10	4.29
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	11	4.23
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	14	4.21
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	14	4.21
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	14	4.21
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	14	4.2
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	8	4.18
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	8	4.18
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	8	4.18
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	2	4.16
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	1	4.14
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	1	4.14
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	1	4.14
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	12	4.13
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	12	4.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	8	4.11
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	8	4.11
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	12	4.09
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	12	4.09
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	12	4.09
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	9	4.06
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	8	4.03
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	8	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	1	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	3	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	4	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	5	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	6	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	7	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	9	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	13	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	14	4.03
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	2	4.02
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	8	4.02
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	10	4.02
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	11	4.02
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	12	4.02
(1,362)	1:25:A:TRP:HH2	1:25:A:TRP:HD1	15	4.02
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	13	3.98
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	13	3.98
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	13	3.98
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	7	3.98
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	7	3.98
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	2	3.94
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	2	3.94
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	3	3.92
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	3	3.92
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	3	3.92
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	15	3.91
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	15	3.91
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	15	3.91
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	4	3.9
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	4	3.9
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	9	3.88
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	9	3.88
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	9	3.88
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	3	3.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	3	3.81
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	15	3.79
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	15	3.79
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	8	3.79
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	8	3.79
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	2	3.78
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	2	3.78
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	2	3.78
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	4	3.77
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	4	3.77
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	10	3.75
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	10	3.75
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	10	3.75
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	14	3.75
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	14	3.75
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	11	3.72
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	11	3.72
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	11	3.72
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	11	3.72
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	11	3.72
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	14	3.69
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	14	3.69
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	7	3.68
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	7	3.68
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	7	3.68
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	7	3.68
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	7	3.68
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	7	3.68
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	2	3.66
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	2	3.66
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	4	3.66
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	4	3.66
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	15	3.65
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	15	3.65
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	3	3.64
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	3	3.64
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	14	3.62
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	14	3.62
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	14	3.62
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	5	3.61
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	5	3.61
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	12	3.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	12	3.61
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	5	3.61
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	12	3.6
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	12	3.6
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	7	3.59
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	7	3.59
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	7	3.59
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	7	3.59
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	8	3.59
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	8	3.59
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	9	3.58
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	9	3.58
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	9	3.58
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	9	3.58
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	9	3.58
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	9	3.58
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	10	3.57
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	10	3.57
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	10	3.57
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	10	3.57
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	11	3.56
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	11	3.56
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	4	3.54
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	4	3.54
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	1	3.53
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	1	3.53
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	1	3.53
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	1	3.53
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	1	3.53
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	1	3.53
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	8	3.53
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	8	3.53
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	8	3.53
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	2	3.53
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	2	3.53
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	5	3.53
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	5	3.53
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	6	3.51
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	6	3.51
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	12	3.5
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	12	3.5
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	12	3.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	12	3.5
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	12	3.5
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	12	3.5
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	12	3.5
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	12	3.5
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	12	3.5
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	3	3.49
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	3	3.49
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	13	3.48
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	13	3.48
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	10	3.48
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	10	3.48
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	1	3.47
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	1	3.47
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	1	3.47
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	12	3.46
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	12	3.46
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	12	3.46
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	12	3.46
(1,322)	1:6:A:PHE:HE1	1:7:A:ILE:HG12	1	3.45
(1,322)	1:6:A:PHE:HE2	1:7:A:ILE:HG12	1	3.45
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	4	3.42
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	4	3.42
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	4	3.42
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	13	3.42
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	13	3.42
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	13	3.42
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	3	3.42
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	7	3.41
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	7	3.41
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	7	3.41
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	7	3.41
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	13	3.4
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	15	3.4
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	11	3.4
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	11	3.4
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	11	3.4
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	11	3.4
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	9	3.38
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	9	3.38
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	6	3.37
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	6	3.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	6	3.37
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	11	3.36
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	11	3.36
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	10	3.35
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	10	3.35
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	12	3.31
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	12	3.31
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	12	3.31
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	12	3.31
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	6	3.3
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	6	3.3
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	11	3.29
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	11	3.29
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	11	3.29
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	7	3.29
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	7	3.29
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	6	3.29
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	6	3.29
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG21	2	3.28
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG22	2	3.28
(1,488)	1:20:A:GLN:HE22	1:23:A:VAL:HG23	2	3.28
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	1	3.28
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	1	3.28
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	5	3.27
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	3	3.26
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	3	3.26
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	3	3.26
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	12	3.26
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	12	3.26
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	12	3.26
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	12	3.26
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	13	3.24
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	13	3.24
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	13	3.19
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	13	3.19
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	13	3.19
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	13	3.19
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	1	3.19
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	1	3.19
(1,368)	1:22:A:PHE:HD1	1:25:A:TRP:HH2	9	3.19
(1,368)	1:22:A:PHE:HD2	1:25:A:TRP:HH2	9	3.19
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	15	3.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	7	3.18
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	9	3.18
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	9	3.18
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	9	3.18
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	9	3.18
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	1	3.17
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	15	3.17
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	2	3.16
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	5	3.16
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	14	3.15
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	14	3.15
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	14	3.15
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	14	3.15
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	6	3.15
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	6	3.15
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	3	3.15
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	14	3.15
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	9	3.14
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	10	3.13
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	11	3.13
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	10	3.13
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	10	3.13
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	2	3.13
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	2	3.13
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	2	3.13
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	2	3.13
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	3	3.13
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	3	3.13
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	3	3.13
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	3	3.13
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	9	3.13
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	15	3.11
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	15	3.11
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	15	3.11
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	7	3.1
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	7	3.1
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	13	3.1
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	13	3.1
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	9	3.09
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	9	3.09
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	9	3.09
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	8	3.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	6	3.07
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	4	3.06
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	4	3.06
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	1	3.06
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	1	3.06
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	9	3.04
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	9	3.04
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	2	3.03
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	2	3.03
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	10	3.01
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	10	3.01
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	10	3.01
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	15	3.01
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	15	3.01
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	13	3.01
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	13	3.01
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	13	3.01
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	13	3.01
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	10	3.0
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	10	3.0
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	15	3.0
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	15	3.0
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	15	3.0
(1,367)	1:22:A:PHE:HE1	1:25:A:TRP:HZ3	9	2.96
(1,367)	1:22:A:PHE:HE2	1:25:A:TRP:HZ3	9	2.96
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	12	2.95
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	10	2.93
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	10	2.93
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	10	2.93
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	10	2.93
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	10	2.93
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	10	2.93
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	13	2.93
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	8	2.92
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	8	2.92
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	8	2.92
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	8	2.92
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	8	2.92
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	8	2.92
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	15	2.9
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	15	2.9
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	7	2.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	7	2.89
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	7	2.89
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	7	2.89
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	7	2.89
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	7	2.89
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	12	2.88
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	12	2.88
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	12	2.88
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	12	2.88
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	12	2.88
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	12	2.88
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	9	2.86
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	9	2.86
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	9	2.86
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	9	2.86
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	7	2.86
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	7	2.86
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	7	2.85
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	7	2.85
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	7	2.85
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	7	2.85
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	1	2.85
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	11	2.84
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	11	2.84
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	11	2.84
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	11	2.84
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	8	2.84
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	8	2.84
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	8	2.84
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	5	2.79
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	5	2.79
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	5	2.79
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	4	2.79
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	4	2.79
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	4	2.79
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	4	2.79
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	13	2.78
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	13	2.78
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	13	2.78
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	13	2.78
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	11	2.77
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	11	2.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	11	2.77
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	13	2.77
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	13	2.77
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	13	2.77
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	1	2.76
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	1	2.76
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	1	2.76
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	12	2.76
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	12	2.76
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	12	2.76
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	14	2.76
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	14	2.76
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	14	2.76
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	1	2.76
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	1	2.76
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	8	2.75
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	8	2.75
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	8	2.75
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	8	2.75
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	8	2.75
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	8	2.75
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	12	2.74
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	12	2.74
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	12	2.74
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	12	2.74
(1,322)	1:6:A:PHE:HE1	1:7:A:ILE:HG12	8	2.74
(1,322)	1:6:A:PHE:HE2	1:7:A:ILE:HG12	8	2.74
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	7	2.73
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	7	2.73
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	7	2.73
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	9	2.73
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	9	2.73
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	9	2.73
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	3	2.72
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	3	2.72
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	3	2.72
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	14	2.72
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	14	2.72
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	14	2.72
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	4	2.71
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	4	2.71
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	4	2.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	10	2.71
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	10	2.71
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	10	2.71
(1,322)	1:6:A:PHE:HE1	1:7:A:ILE:HG12	9	2.71
(1,322)	1:6:A:PHE:HE2	1:7:A:ILE:HG12	9	2.71
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	9	2.7
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	9	2.7
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	9	2.7
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	10	2.7
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	10	2.7
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	10	2.7
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	6	2.7
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	6	2.7
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	6	2.7
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	6	2.7
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	5	2.69
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	5	2.69
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	5	2.69
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	2	2.67
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	2	2.67
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	2	2.67
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	5	2.66
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	5	2.66
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	5	2.66
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	5	2.66
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	5	2.66
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	5	2.66
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	7	2.66
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	7	2.66
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	7	2.66
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	4	2.64
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	4	2.64
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	4	2.64
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG21	6	2.63
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG22	6	2.63
(1,485)	1:20:A:GLN:HE21	1:23:A:VAL:HG23	6	2.63
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	15	2.63
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	15	2.63
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	15	2.63
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	4	2.63
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	8	2.63
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	8	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	8	2.63
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	8	2.63
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	10	2.63
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	10	2.63
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG11	6	2.62
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG12	6	2.62
(1,484)	1:22:A:PHE:H	1:23:A:VAL:HG13	6	2.62
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	5	2.61
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	5	2.61
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	1	2.6
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	1	2.6
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	3	2.6
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	3	2.6
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	3	2.6
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	3	2.6
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	2	2.6
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	2	2.6
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	2	2.6
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	15	2.59
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	15	2.59
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	15	2.59
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	15	2.59
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	15	2.59
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	15	2.59
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	2	2.58
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	2	2.58
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	2	2.58
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	2	2.58
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	6	2.56
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	6	2.56
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	6	2.56
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	6	2.56
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	6	2.56
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	6	2.56
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	1	2.56
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	1	2.56
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	1	2.56
(1,277)	1:36:A:TRP:HE3	1:37:A:LYS:HA	13	2.56
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	13	2.55
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	13	2.55
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	13	2.55
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	13	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	13	2.55
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	13	2.55
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	11	2.54
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	3	2.53
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	8	2.53
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	5	2.53
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	5	2.53
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	14	2.53
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	10	2.52
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	10	2.52
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	10	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	10	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	10	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	10	2.52
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	15	2.52
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	15	2.52
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	15	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	15	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	15	2.52
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	15	2.52
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	8	2.5
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	8	2.5
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	8	2.5
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	8	2.5
(1,312)	1:1:A:TYR:HE1	1:3:A:GLU:HA	14	2.49
(1,312)	1:1:A:TYR:HE2	1:3:A:GLU:HA	14	2.49
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	1	2.49
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	1	2.49
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	10	2.47
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	10	2.47
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	10	2.47
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	10	2.47
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	10	2.47
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	10	2.47
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	12	2.47
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	12	2.47
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	12	2.47
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	12	2.47
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	13	2.47
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	13	2.47
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	13	2.47
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	13	2.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	6	2.47
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	6	2.47
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	6	2.47
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	6	2.47
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	6	2.47
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	6	2.47
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	14	2.45
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	14	2.45
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	14	2.45
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	14	2.45
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	14	2.45
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	14	2.45
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	10	2.44
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	10	2.44
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	10	2.44
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	10	2.44
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	10	2.44
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	10	2.44
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	4	2.44
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	6	2.43
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	6	2.43
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	6	2.43
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	6	2.43
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	6	2.43
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	6	2.43
(1,277)	1:36:A:TRP:HE3	1:37:A:LYS:HA	4	2.43
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	8	2.42
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	8	2.42
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	8	2.42
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	1	2.42
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	3	2.42
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	5	2.42
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	6	2.42
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	13	2.42
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	14	2.42
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	2	2.41
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	7	2.41
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	9	2.41
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	10	2.41
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	11	2.41
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	1	2.4
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	8	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	12	2.4
(1,372)	1:25:A:TRP:HD1	1:25:A:TRP:HZ2	15	2.4
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	14	2.39
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	14	2.39
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	14	2.39
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	14	2.39
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	14	2.39
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	14	2.39
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	7	2.39
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	7	2.39
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	7	2.39
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	7	2.39
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	2	2.37
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	2	2.37
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	2	2.37
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	2	2.37
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	2	2.37
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	2	2.37
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	5	2.33
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	15	2.33
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	15	2.32
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	15	2.32
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	15	2.32
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	15	2.32
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	15	2.32
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	15	2.32
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	15	2.32
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	15	2.32
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	15	2.32
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	9	2.31
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	9	2.31
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	9	2.31
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	9	2.31
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	6	2.31
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	6	2.31
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	6	2.31
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	9	2.31
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	10	2.31
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	12	2.31
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	13	2.29
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	13	2.29
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	13	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	13	2.29
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	13	2.29
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	13	2.29
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	13	2.29
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	13	2.29
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	13	2.29
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	13	2.29
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	13	2.29
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	13	2.29
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	11	2.28
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	11	2.28
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	11	2.28
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	7	2.28
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	14	2.27
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	14	2.27
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	7	2.27
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	14	2.26
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	14	2.26
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	14	2.26
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	14	2.26
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	14	2.26
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	14	2.26
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	7	2.24
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	7	2.24
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	7	2.24
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	7	2.24
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	7	2.24
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	7	2.24
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	5	2.24
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	5	2.24
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	5	2.24
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	15	2.23
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	10	2.23
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	10	2.23
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	10	2.23
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	10	2.23
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	14	2.23
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	14	2.22
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	2	2.22
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	15	2.22
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	6	2.21
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	6	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	6	2.21
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	5	2.2
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	5	2.2
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	6	2.2
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	14	2.19
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	14	2.19
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	14	2.19
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	4	2.19
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	14	2.18
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	14	2.18
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	14	2.18
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	14	2.18
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	4	2.18
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	4	2.18
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	4	2.18
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	4	2.18
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	4	2.18
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	4	2.18
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	7	2.18
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	7	2.18
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	7	2.18
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	12	2.18
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	12	2.18
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	12	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	1	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	2	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	5	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	6	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	7	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	8	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	10	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	13	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	14	2.18
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	8	2.18
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	8	2.18
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	1	2.18
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	6	2.18
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	13	2.18
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	3	2.17
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	9	2.17
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	11	2.17
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	12	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:25:A:TRP:HH2	1:25:A:TRP:HE1	15	2.17
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	11	2.17
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	4	2.17
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	6	2.17
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	7	2.15
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	7	2.15
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	7	2.15
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	7	2.15
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	7	2.15
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	7	2.15
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	7	2.15
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	7	2.15
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	7	2.15
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	5	2.15
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	9	2.14
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	9	2.14
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	9	2.14
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	9	2.14
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	9	2.14
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	9	2.14
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	9	2.14
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	9	2.14
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	9	2.14
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	14	2.13
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	14	2.13
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	14	2.13
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	14	2.13
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	14	2.13
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	14	2.13
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	3	2.13
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	3	2.13
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	3	2.13
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	3	2.13
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	3	2.13
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	3	2.13
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	3	2.13
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	3	2.13
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	3	2.13
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	6	2.13
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	6	2.13
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	6	2.13
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	6	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	6	2.13
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	6	2.13
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	6	2.13
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	6	2.13
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	6	2.13
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	12	2.13
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	14	2.13
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	6	2.13
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	5	2.11
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	5	2.11
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	5	2.11
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	5	2.11
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	5	2.11
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	5	2.11
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	5	2.11
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	5	2.11
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	5	2.11
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	4	2.11
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	4	2.11
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	4	2.11
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	6	2.11
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	6	2.11
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	6	2.11
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	6	2.11
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	9	2.1
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	9	2.1
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	9	2.1
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	3	2.1
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	3	2.1
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	3	2.1
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	1	2.1
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	7	2.1
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	7	2.1
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD1	5	2.09
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD2	5	2.09
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD1	5	2.09
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD2	5	2.09
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD1	5	2.09
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD2	5	2.09
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	1	2.09
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	1	2.09
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	1	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	9	2.09
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	9	2.08
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	9	2.08
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	9	2.08
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	9	2.08
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	9	2.08
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	9	2.08
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	12	2.08
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	12	2.08
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	12	2.08
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	12	2.08
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	12	2.08
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	12	2.08
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	2	2.08
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	2	2.08
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	2	2.08
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	2	2.08
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	2	2.08
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	2	2.08
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	2	2.08
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	2	2.08
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	2	2.08
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	1	2.08
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	1	2.08
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	1	2.08
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	2	2.08
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	2	2.07
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	2	2.07
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	2	2.07
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	14	2.07
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	8	2.06
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	8	2.06
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	5	2.06
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	7	2.06
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	2	2.05
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	2	2.05
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	2	2.05
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	2	2.05
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	8	2.05
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	8	2.05
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	8	2.05
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	8	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	8	2.05
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	8	2.05
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	8	2.05
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	8	2.05
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	8	2.05
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	8	2.05
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	8	2.05
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	8	2.05
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	5	2.05
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	5	2.05
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	10	2.04
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	10	2.04
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	10	2.04
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	15	2.04
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	15	2.04
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	15	2.04
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	5	2.03
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	5	2.03
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	5	2.03
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	5	2.03
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	4	2.03
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	4	2.03
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	4	2.03
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	4	2.03
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	4	2.03
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	4	2.03
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	4	2.03
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	4	2.03
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	4	2.03
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	13	2.03
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	13	2.03
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	3	2.02
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	3	2.02
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	3	2.02
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	1	2.02
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	1	2.02
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	1	2.02
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	1	2.02
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	1	2.02
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	1	2.02
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	1	2.02
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	1	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	1	2.02
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	8	2.02
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	8	2.02
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	8	2.02
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	8	2.02
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	4	2.02
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	1	2.01
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	1	2.01
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	1	2.01
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	1	2.01
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	3	2.01
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	3	2.01
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	3	2.01
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	3	2.01
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	11	2.01
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	11	2.01
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	11	2.01
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	3	2.01
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	13	2.0
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	13	2.0
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	13	2.0
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	13	2.0
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	13	2.0
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	13	2.0
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	13	2.0
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	13	2.0
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	13	2.0
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	5	2.0
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	5	2.0
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	5	2.0
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	5	2.0
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	9	2.0
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	9	2.0
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	2	2.0
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	13	1.99
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	13	1.99
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	13	1.99
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	5	1.98
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	5	1.98
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	5	1.98
(1,127)	1:29:A:GLN:HA	1:32:A:LYS:H	11	1.98
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	7	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	8	1.97
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	10	1.96
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	10	1.96
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	10	1.96
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	10	1.96
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	10	1.96
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	10	1.96
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	10	1.96
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	10	1.96
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	10	1.96
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	11	1.96
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	11	1.96
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	11	1.96
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	11	1.96
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	11	1.96
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	11	1.96
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	11	1.96
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	11	1.96
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	11	1.96
(1,433)	1:27:A:LEU:HD21	1:29:A:GLN:H	9	1.96
(1,433)	1:27:A:LEU:HD22	1:29:A:GLN:H	9	1.96
(1,433)	1:27:A:LEU:HD23	1:29:A:GLN:H	9	1.96
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	10	1.96
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	12	1.96
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	12	1.96
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	4	1.96
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	4	1.96
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	15	1.96
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	15	1.96
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	12	1.94
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	12	1.94
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	12	1.94
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	12	1.94
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	12	1.94
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	12	1.94
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	12	1.94
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	12	1.94
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	12	1.94
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	14	1.94
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	14	1.94
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	10	1.94
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	10	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD1	13	1.93
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD2	13	1.93
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD1	13	1.93
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD2	13	1.93
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD1	13	1.93
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD2	13	1.93
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD11	14	1.93
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD12	14	1.93
(1,474)	1:23:A:VAL:HG21	1:27:A:LEU:HD13	14	1.93
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD11	14	1.93
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD12	14	1.93
(1,474)	1:23:A:VAL:HG22	1:27:A:LEU:HD13	14	1.93
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD11	14	1.93
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD12	14	1.93
(1,474)	1:23:A:VAL:HG23	1:27:A:LEU:HD13	14	1.93
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	3	1.93
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	3	1.93
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	4	1.93
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	4	1.93
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	13	1.93
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	15	1.93
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	15	1.93
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	1	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	2	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	3	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	5	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	6	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	7	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	8	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	9	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	10	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	11	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	12	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	13	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	14	1.92
(1,361)	1:25:A:TRP:HZ3	1:25:A:TRP:HZ2	15	1.92
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	3	1.92
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	5	1.92
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	6	1.92
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	9	1.92
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	14	1.92
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	6	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	6	1.92
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	11	1.92
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	11	1.92
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	15	1.92
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	1	1.91
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	7	1.91
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	8	1.91
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	10	1.91
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	11	1.91
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	12	1.91
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	15	1.91
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	8	1.91
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	8	1.91
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	8	1.91
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	8	1.91
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	15	1.9
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	15	1.9
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	15	1.9
(1,359)	1:36:A:TRP:HH2	1:36:A:TRP:HE3	2	1.9
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	9	1.9
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	7	1.9
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	7	1.9
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	12	1.9
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	14	1.89
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	14	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	1	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	2	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	3	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	4	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	5	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	6	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	7	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	8	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	9	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	10	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	11	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	12	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	13	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	14	1.89
(1,365)	1:25:A:TRP:HH2	1:25:A:TRP:HE3	15	1.89
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	10	1.89
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	10	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	13	1.89
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	13	1.89
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	1	1.89
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	1	1.89
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	1	1.89
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	1	1.89
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	5	1.89
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	3	1.89
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	3	1.89
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	15	1.88
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	15	1.88
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	13	1.88
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	13	1.88
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	4	1.88
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	4	1.88
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	13	1.88
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD1	1	1.87
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD2	1	1.87
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD1	1	1.87
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD2	1	1.87
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD1	1	1.87
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD2	1	1.87
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	8	1.87
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	8	1.87
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	8	1.87
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	12	1.87
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	15	1.87
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	15	1.87
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	12	1.86
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	12	1.86
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	12	1.86
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	9	1.86
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	9	1.86
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	9	1.86
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	9	1.86
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	1	1.86
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	8	1.86
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	4	1.85
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	4	1.85
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	4	1.85
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	13	1.85
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	13	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	13	1.85
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	3	1.85
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	3	1.85
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	12	1.85
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	12	1.85
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	12	1.84
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	12	1.84
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	2	1.84
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	13	1.83
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	13	1.83
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	13	1.83
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	6	1.83
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	6	1.83
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	4	1.82
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	14	1.82
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	4	1.81
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	4	1.81
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	4	1.81
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	4	1.81
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	4	1.81
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	4	1.81
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	1	1.81
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	1	1.81
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	1	1.81
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	1	1.81
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	2	1.81
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	2	1.81
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	8	1.81
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	12	1.8
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	12	1.8
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	12	1.8
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	10	1.8
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	10	1.8
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	3	1.8
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	15	1.8
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	15	1.8
(1,407)	1:25:A:TRP:HZ2	1:26:A:LEU:HG	9	1.79
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	11	1.79
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	11	1.79
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	3	1.79
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	3	1.79
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	3	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	3	1.78
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	3	1.78
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	3	1.77
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	3	1.77
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	3	1.77
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	5	1.77
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	5	1.77
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	5	1.77
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	6	1.77
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	2	1.77
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	2	1.77
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	11	1.77
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	11	1.77
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	2	1.77
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	11	1.76
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	11	1.76
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	11	1.76
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	4	1.76
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	4	1.76
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	4	1.76
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	4	1.76
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	4	1.76
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	4	1.76
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG21	1	1.76
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG22	1	1.76
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG23	1	1.76
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG21	1	1.76
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG22	1	1.76
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG23	1	1.76
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	9	1.76
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	9	1.76
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	3	1.76
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	3	1.76
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	10	1.76
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	12	1.75
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	12	1.75
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	1	1.75
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	1	1.75
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	5	1.74
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	5	1.74
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	2	1.73
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	2	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	2	1.73
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	8	1.73
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	8	1.73
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	8	1.73
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	10	1.73
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	3	1.72
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	3	1.72
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	3	1.72
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	6	1.72
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	6	1.72
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	13	1.72
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	1	1.72
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	3	1.71
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	3	1.71
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	3	1.71
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	3	1.71
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	3	1.71
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	3	1.71
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	3	1.71
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	3	1.71
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	11	1.71
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	11	1.71
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	2	1.71
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	12	1.71
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	12	1.71
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD11	3	1.7
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD12	3	1.7
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD13	3	1.7
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD11	3	1.7
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD12	3	1.7
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD13	3	1.7
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD11	1	1.7
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD12	1	1.7
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD13	1	1.7
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD11	1	1.7
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD12	1	1.7
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD13	1	1.7
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	4	1.7
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	4	1.7
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	9	1.7
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	15	1.7
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	14	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	14	1.69
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	14	1.69
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	2	1.69
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	2	1.69
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	2	1.69
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	5	1.69
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	5	1.69
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	5	1.69
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	5	1.69
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	9	1.69
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	12	1.69
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	12	1.69
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	13	1.68
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	13	1.68
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	1	1.68
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	1	1.68
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	1	1.68
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	1	1.68
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	1	1.68
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	1	1.68
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	5	1.68
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	5	1.68
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	5	1.68
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	3	1.68
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	13	1.67
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	13	1.67
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	13	1.67
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	13	1.67
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	8	1.67
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	8	1.67
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	8	1.67
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	8	1.67
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	8	1.67
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	8	1.67
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	5	1.67
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	9	1.67
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	14	1.67
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	4	1.67
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	4	1.67
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	4	1.67
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	4	1.67
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG21	9	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG22	9	1.66
(2,38)	1:1:A:TYR:HE1	1:5:A:THR:HG23	9	1.66
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG21	9	1.66
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG22	9	1.66
(2,38)	1:1:A:TYR:HE2	1:5:A:THR:HG23	9	1.66
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	2	1.66
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	2	1.66
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	7	1.66
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	7	1.66
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	6	1.66
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	6	1.66
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	6	1.66
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	13	1.66
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	13	1.66
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	13	1.66
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	11	1.66
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	11	1.66
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	11	1.66
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	7	1.66
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	7	1.66
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	7	1.66
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	7	1.66
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	11	1.66
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	11	1.66
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	11	1.66
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	11	1.66
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	3	1.66
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	6	1.66
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	7	1.66
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	8	1.66
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	11	1.66
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	12	1.66
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	13	1.66
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	15	1.66
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	4	1.66
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	8	1.66
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	8	1.66
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	10	1.66
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	12	1.65
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	12	1.65
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	4	1.65
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	4	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	4	1.65
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	1	1.65
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	10	1.65
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	6	1.65
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	6	1.65
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	11	1.65
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	11	1.65
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	3	1.65
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	11	1.65
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	14	1.65
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	15	1.64
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	15	1.64
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	15	1.64
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	15	1.64
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	12	1.64
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	12	1.64
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	12	1.64
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	2	1.64
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	2	1.64
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	2	1.64
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	2	1.64
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	2	1.64
(1,373)	1:36:A:TRP:HD1	1:36:A:TRP:HZ2	4	1.64
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	10	1.64
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	10	1.64
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	13	1.64
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	4	1.64
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	5	1.64
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	5	1.63
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	5	1.63
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	5	1.63
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	6	1.63
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	6	1.63
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	6	1.63
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	1	1.63
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	1	1.63
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	4	1.63
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	15	1.62
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	15	1.62
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	15	1.62
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	15	1.62
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	15	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	15	1.62
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	5	1.62
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	5	1.62
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	15	1.62
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	15	1.62
(2,19)	1:6:A:PHE:HE1	1:10:A:TYR:HD1	8	1.61
(2,19)	1:6:A:PHE:HE1	1:10:A:TYR:HD2	8	1.61
(2,19)	1:6:A:PHE:HE2	1:10:A:TYR:HD1	8	1.61
(2,19)	1:6:A:PHE:HE2	1:10:A:TYR:HD2	8	1.61
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	6	1.61
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	6	1.61
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	2	1.61
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	2	1.61
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	9	1.6
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	9	1.6
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	10	1.6
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	10	1.6
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	14	1.6
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	14	1.6
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	6	1.6
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	15	1.59
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	15	1.59
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	15	1.59
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	3	1.59
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	5	1.59
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	9	1.59
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	5	1.59
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	5	1.59
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	12	1.59
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	12	1.59
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	14	1.59
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	7	1.59
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	11	1.58
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	11	1.58
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	11	1.58
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	11	1.58
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	11	1.58
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	11	1.58
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	4	1.58
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	4	1.58
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	4	1.58
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	15	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	15	1.58
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	15	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	1	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	2	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	4	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	6	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	7	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	8	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	10	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	11	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	12	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	13	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	14	1.58
(1,357)	1:36:A:TRP:HZ3	1:36:A:TRP:HZ2	15	1.58
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	2	1.58
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	2	1.58
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	9	1.58
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	13	1.58
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	14	1.57
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	14	1.57
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	14	1.57
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	9	1.57
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	9	1.57
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	9	1.57
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	15	1.57
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	15	1.57
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	15	1.57
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	14	1.57
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	14	1.57
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	11	1.56
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	11	1.56
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	11	1.56
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	11	1.56
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	11	1.56
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	11	1.56
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	8	1.56
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	8	1.56
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	15	1.56
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	15	1.56
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	15	1.56
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	12	1.56
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	12	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	12	1.56
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	6	1.56
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	6	1.56
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	6	1.56
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	5	1.56
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	13	1.56
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	13	1.56
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	7	1.55
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	7	1.55
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	7	1.55
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	10	1.55
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	10	1.55
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	10	1.55
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	14	1.55
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	14	1.55
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	14	1.55
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	14	1.55
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	8	1.55
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	8	1.55
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	8	1.55
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	14	1.55
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	14	1.55
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	5	1.55
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	3	1.55
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	3	1.55
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	15	1.54
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	15	1.54
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	15	1.54
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	10	1.54
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	10	1.54
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	10	1.54
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	15	1.54
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	15	1.54
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	15	1.54
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	14	1.54
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	14	1.54
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	9	1.53
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	9	1.53
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	9	1.53
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	9	1.53
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	9	1.53
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	9	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	7	1.53
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	7	1.53
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	7	1.53
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	5	1.53
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	5	1.53
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	13	1.53
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	11	1.53
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	3	1.53
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	3	1.53
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	3	1.52
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	3	1.52
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	3	1.52
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	14	1.52
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	14	1.52
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	14	1.52
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE22	3	1.52
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE21	3	1.52
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	6	1.52
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	3	1.52
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	2	1.51
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	2	1.51
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	2	1.51
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	8	1.51
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	8	1.51
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	8	1.51
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	2	1.51
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	2	1.51
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	2	1.51
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	6	1.51
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	1	1.5
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	1	1.5
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	3	1.5
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	3	1.5
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	3	1.5
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	2	1.5
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	3	1.5
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	15	1.5
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	3	1.49
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	3	1.49
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	3	1.49
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	2	1.49
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	2	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD2	9	1.49
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD3	9	1.49
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	15	1.49
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	5	1.48
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	5	1.48
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	5	1.48
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	13	1.48
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	13	1.48
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	13	1.48
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	3	1.48
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	3	1.48
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	10	1.48
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	10	1.48
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	14	1.48
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	14	1.48
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	6	1.47
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	6	1.47
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	6	1.47
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	6	1.47
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	7	1.47
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	7	1.47
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	7	1.47
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	7	1.47
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	7	1.47
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	7	1.47
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	14	1.47
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	14	1.47
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	14	1.47
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	14	1.47
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	14	1.47
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	14	1.47
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	10	1.47
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	10	1.47
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	10	1.47
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	3	1.47
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	3	1.47
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	3	1.47
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	3	1.47
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	11	1.47
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	11	1.47
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	6	1.47
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	6	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	9	1.47
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	9	1.47
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	12	1.47
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	9	1.46
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	9	1.46
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	9	1.46
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	4	1.46
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	4	1.46
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	4	1.46
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	1	1.46
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	1	1.46
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	1	1.46
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	1	1.46
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	7	1.46
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	7	1.46
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	10	1.46
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	10	1.46
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	6	1.45
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	6	1.45
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	6	1.45
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	6	1.45
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	6	1.45
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	6	1.45
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	11	1.45
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	11	1.45
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	11	1.45
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	11	1.45
(2,6)	1:1:A:TYR:HE1	1:2:A:ALA:HA	4	1.45
(2,6)	1:1:A:TYR:HE2	1:2:A:ALA:HA	4	1.45
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	3	1.45
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	3	1.45
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	4	1.45
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	4	1.45
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	1	1.45
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	7	1.45
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	14	1.45
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	4	1.45
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	10	1.45
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	11	1.45
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	12	1.45
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	1	1.44
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	1	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	1	1.44
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	1	1.44
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	1	1.44
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	1	1.44
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG21	1	1.44
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG22	1	1.44
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG23	1	1.44
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG21	1	1.44
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG22	1	1.44
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG23	1	1.44
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	5	1.44
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	5	1.44
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	11	1.44
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	3	1.44
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	3	1.44
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE21	11	1.43
(1,388)	1:26:A:LEU:HG	1:29:A:GLN:HE22	11	1.43
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	7	1.43
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	7	1.43
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	5	1.43
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	5	1.43
(1,212)	1:6:A:PHE:HA	1:10:A:TYR:H	1	1.43
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB2	10	1.42
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB3	10	1.42
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB2	10	1.42
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB3	10	1.42
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	1	1.42
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	1	1.42
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	1	1.42
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	1	1.42
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	1	1.42
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	2	1.42
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	2	1.42
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	4	1.42
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	4	1.42
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	4	1.42
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	9	1.42
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	9	1.42
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	13	1.42
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	3	1.42
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	14	1.42
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	6	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	8	1.41
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	4	1.4
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	4	1.4
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	8	1.4
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	8	1.4
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	8	1.4
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	8	1.4
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	8	1.4
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	8	1.4
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD21	8	1.4
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD22	8	1.4
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD23	8	1.4
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	8	1.4
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD22	8	1.4
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD23	8	1.4
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	8	1.4
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD22	8	1.4
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD23	8	1.4
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD11	8	1.4
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD12	8	1.4
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD13	8	1.4
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD11	8	1.4
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD12	8	1.4
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD13	8	1.4
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD11	8	1.4
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD12	8	1.4
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD13	8	1.4
(1,321)	1:6:A:PHE:HD1	1:7:A:ILE:HG12	1	1.4
(1,321)	1:6:A:PHE:HD2	1:7:A:ILE:HG12	1	1.4
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	15	1.4
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	15	1.4
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	3	1.4
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	7	1.4
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	7	1.39
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	7	1.39
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	7	1.39
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	1	1.39
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	1	1.39
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	1	1.39
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	1	1.39
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	1	1.39
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	1	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	3	1.39
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	3	1.39
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	3	1.39
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	3	1.39
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	3	1.39
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	3	1.39
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	6	1.39
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	6	1.39
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	4	1.39
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	9	1.38
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	9	1.38
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	11	1.38
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	11	1.38
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	11	1.38
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	1	1.38
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	1	1.38
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	1	1.38
(1,327)	1:34:A:ASN:HD22	1:38:A:HIS:HA	4	1.38
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	9	1.38
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	9	1.38
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	15	1.38
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	8	1.38
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	8	1.38
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	1	1.38
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	2	1.38
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	14	1.37
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	14	1.37
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	9	1.37
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	9	1.37
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	9	1.37
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	15	1.37
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	15	1.37
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	15	1.37
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	6	1.37
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	6	1.37
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	6	1.37
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	15	1.37
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	15	1.37
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	15	1.37
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	14	1.37
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	14	1.37
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	14	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	12	1.36
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	12	1.36
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	13	1.36
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	13	1.36
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	3	1.36
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	3	1.36
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	3	1.36
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	4	1.36
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	4	1.36
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	4	1.36
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	12	1.36
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	8	1.36
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	8	1.36
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	9	1.36
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	3	1.36
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	2	1.36
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	3	1.35
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	3	1.35
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	3	1.35
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	5	1.35
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	5	1.35
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	5	1.35
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	5	1.35
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	5	1.35
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	5	1.35
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD21	13	1.35
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD22	13	1.35
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD23	13	1.35
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD11	13	1.35
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD12	13	1.35
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD13	13	1.35
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	7	1.35
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	7	1.35
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	7	1.35
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	9	1.35
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	9	1.35
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	9	1.35
(1,366)	1:22:A:PHE:HD1	1:25:A:TRP:HZ3	9	1.35
(1,366)	1:22:A:PHE:HD2	1:25:A:TRP:HZ3	9	1.35
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	8	1.35
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD1	3	1.34
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD2	3	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD1	3	1.34
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD2	3	1.34
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD1	3	1.34
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD2	3	1.34
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	3	1.34
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	3	1.34
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	11	1.34
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	11	1.34
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	15	1.34
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	15	1.34
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	13	1.34
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	13	1.34
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	13	1.34
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	15	1.34
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	15	1.34
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	10	1.34
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	4	1.33
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	4	1.33
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	4	1.33
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	4	1.33
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	6	1.33
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	6	1.33
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	7	1.33
(1,263)	1:12:A:ILE:HG12	1:13:A:ALA:H	13	1.33
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	6	1.33
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	6	1.33
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	15	1.33
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	3	1.33
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	3	1.33
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	13	1.33
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	10	1.33
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	2	1.32
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	2	1.32
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	8	1.32
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	8	1.32
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	10	1.32
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	10	1.32
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	10	1.32
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	1	1.32
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	1	1.32
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	1	1.32
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	12	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	12	1.32
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	12	1.32
(1,406)	1:6:A:PHE:HD1	1:7:A:ILE:HB	1	1.32
(1,406)	1:6:A:PHE:HD2	1:7:A:ILE:HB	1	1.32
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	7	1.32
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	12	1.32
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	5	1.32
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	13	1.32
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	4	1.32
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	1	1.31
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	1	1.31
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	7	1.31
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	7	1.31
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	6	1.31
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	6	1.31
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	6	1.31
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	6	1.31
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	5	1.31
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	5	1.31
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	5	1.31
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	8	1.3
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	8	1.3
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	8	1.3
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	2	1.3
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	3	1.3
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	15	1.3
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG21	8	1.29
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG22	8	1.29
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG23	8	1.29
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG21	8	1.29
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG22	8	1.29
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG23	8	1.29
(1,439)	1:23:A:VAL:HG11	1:26:A:LEU:H	11	1.29
(1,439)	1:23:A:VAL:HG12	1:26:A:LEU:H	11	1.29
(1,439)	1:23:A:VAL:HG13	1:26:A:LEU:H	11	1.29
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	3	1.29
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	3	1.29
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	3	1.29
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	3	1.29
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	6	1.29
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	6	1.29
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	6	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	4	1.29
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	4	1.29
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	15	1.29
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	15	1.29
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	8	1.29
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	2	1.29
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	4	1.29
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	5	1.29
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	8	1.29
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	6	1.29
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	5	1.28
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	5	1.28
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	5	1.28
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	4	1.28
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	4	1.28
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	4	1.28
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	4	1.28
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	4	1.28
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	4	1.28
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	14	1.28
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	14	1.28
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	14	1.28
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	9	1.28
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	9	1.28
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	9	1.28
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	12	1.28
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	12	1.28
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	12	1.28
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	10	1.28
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	10	1.28
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	10	1.28
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	10	1.28
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	7	1.28
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	7	1.28
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	10	1.28
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	10	1.28
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	8	1.28
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	13	1.28
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	12	1.28
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	11	1.28
(2,3)	1:10:A:TYR:HE1	1:11:A:SER:HA	10	1.27
(2,3)	1:10:A:TYR:HE2	1:11:A:SER:HA	10	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	6	1.27
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	6	1.27
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	7	1.27
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	10	1.27
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	14	1.27
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	1	1.27
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	2	1.27
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	8	1.27
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	5	1.27
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	4	1.26
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	4	1.26
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	4	1.26
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	4	1.26
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	9	1.26
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	9	1.26
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	9	1.26
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	9	1.26
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	6	1.26
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	6	1.26
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	6	1.26
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	6	1.26
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	13	1.26
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	13	1.26
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	13	1.26
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	15	1.26
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	15	1.26
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	15	1.26
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	15	1.26
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	13	1.26
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	13	1.26
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	14	1.26
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	14	1.26
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	15	1.26
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	1	1.26
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	9	1.26
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	12	1.26
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	13	1.26
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	15	1.26
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	13	1.26
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	9	1.25
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	9	1.25
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	9	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	6	1.25
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	6	1.25
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	6	1.25
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	10	1.25
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	10	1.25
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	10	1.25
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE22	11	1.25
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE21	11	1.25
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	3	1.25
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	11	1.25
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	11	1.25
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	6	1.25
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	6	1.25
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	4	1.25
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	4	1.25
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	5	1.25
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	5	1.25
(1,27)	1:21:A:ASP:H	1:21:A:ASP:HB3	3	1.25
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	7	1.25
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	10	1.25
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	12	1.25
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	10	1.24
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	10	1.24
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	10	1.24
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	10	1.24
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	15	1.24
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	15	1.24
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	15	1.24
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	15	1.24
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	15	1.24
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	15	1.24
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	11	1.24
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	11	1.24
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	11	1.24
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	7	1.24
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	7	1.24
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	7	1.24
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	3	1.24
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	4	1.24
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	4	1.24
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	4	1.24
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	4	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	14	1.24
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	11	1.24
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	5	1.23
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	5	1.23
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	5	1.23
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	4	1.23
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	14	1.23
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	14	1.23
(1,235)	1:14:A:MET:HG2	1:15:A:ASP:H	1	1.23
(1,235)	1:14:A:MET:HG3	1:15:A:ASP:H	1	1.23
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	10	1.23
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	9	1.23
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	12	1.22
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	12	1.22
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	12	1.22
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	2	1.22
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	2	1.22
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	2	1.22
(1,438)	1:17:A:ILE:HD11	1:21:A:ASP:H	1	1.22
(1,438)	1:17:A:ILE:HD12	1:21:A:ASP:H	1	1.22
(1,438)	1:17:A:ILE:HD13	1:21:A:ASP:H	1	1.22
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	9	1.22
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	9	1.22
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	9	1.22
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	7	1.22
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	7	1.22
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	7	1.22
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	11	1.22
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	2	1.22
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	2	1.22
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	8	1.21
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	8	1.21
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	8	1.21
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	8	1.21
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	8	1.21
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	8	1.21
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	7	1.21
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	7	1.21
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	7	1.21
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	7	1.21
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	7	1.21
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	7	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD21	4	1.21
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD22	4	1.21
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD23	4	1.21
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD11	4	1.21
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD12	4	1.21
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD13	4	1.21
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	11	1.21
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	1	1.21
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	10	1.21
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	10	1.21
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	4	1.21
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	9	1.21
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	3	1.21
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	14	1.21
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	8	1.2
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	8	1.2
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	8	1.2
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	8	1.2
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	13	1.2
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	13	1.2
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	13	1.2
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	13	1.2
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	13	1.2
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	13	1.2
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	11	1.2
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	11	1.2
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	11	1.2
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	2	1.2
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	2	1.2
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	2	1.2
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	2	1.2
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	2	1.2
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	2	1.2
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	5	1.2
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	5	1.2
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	5	1.2
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	11	1.2
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	11	1.2
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	4	1.2
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	4	1.2
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	2	1.2
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	11	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	11	1.2
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	12	1.2
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	12	1.2
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	6	1.2
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	14	1.2
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	1	1.19
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	1	1.19
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	1	1.19
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	2	1.19
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	2	1.19
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	2	1.19
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	3	1.19
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	12	1.19
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	9	1.19
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	9	1.19
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	1	1.19
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	5	1.19
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	15	1.19
(1,210)	1:4:A:GLY:HA2	1:6:A:PHE:H	1	1.18
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	14	1.18
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	15	1.18
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	9	1.17
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	9	1.17
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	9	1.17
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	9	1.17
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	9	1.17
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	9	1.17
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	1	1.17
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	12	1.17
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG21	9	1.16
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG22	9	1.16
(2,27)	1:6:A:PHE:HE1	1:7:A:ILE:HG23	9	1.16
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG21	9	1.16
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG22	9	1.16
(2,27)	1:6:A:PHE:HE2	1:7:A:ILE:HG23	9	1.16
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG2	1	1.16
(1,400)	1:30:A:LYS:HD2	1:32:A:LYS:HG3	1	1.16
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG2	1	1.16
(1,400)	1:30:A:LYS:HD3	1:32:A:LYS:HG3	1	1.16
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	14	1.16
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	13	1.16
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	13	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	15	1.16
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	15	1.16
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD2	13	1.16
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD3	13	1.16
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	3	1.16
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	4	1.16
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	5	1.16
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	11	1.16
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	13	1.16
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	2	1.16
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	11	1.16
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB2	14	1.15
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB3	14	1.15
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB2	14	1.15
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB3	14	1.15
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	2	1.15
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	2	1.15
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	2	1.15
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	14	1.15
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	14	1.15
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	14	1.15
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	2	1.15
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	2	1.15
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	2	1.15
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	7	1.15
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	7	1.15
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	7	1.15
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	2	1.15
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	2	1.15
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	2	1.15
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	2	1.15
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	2	1.15
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	2	1.15
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	5	1.15
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	5	1.15
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	5	1.15
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	5	1.15
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	5	1.15
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	5	1.15
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	10	1.15
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	10	1.15
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	10	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	10	1.15
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	10	1.15
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	10	1.15
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	3	1.15
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	3	1.15
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	15	1.15
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	8	1.15
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	8	1.15
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	2	1.15
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	2	1.15
(1,235)	1:14:A:MET:HG2	1:15:A:ASP:H	5	1.15
(1,235)	1:14:A:MET:HG3	1:15:A:ASP:H	5	1.15
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	2	1.15
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	3	1.15
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	11	1.15
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	6	1.14
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	6	1.14
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	6	1.14
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	14	1.14
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	14	1.14
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	14	1.14
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	14	1.14
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	14	1.14
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	14	1.14
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE22	15	1.14
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE21	15	1.14
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	15	1.14
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	15	1.14
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	15	1.14
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	15	1.14
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	3	1.14
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	6	1.14
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	7	1.14
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	10	1.14
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	15	1.14
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	9	1.14
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	3	1.14
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	12	1.13
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	12	1.13
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	12	1.13
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	5	1.13
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	5	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	5	1.13
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	5	1.13
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	5	1.13
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	5	1.13
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	2	1.13
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	2	1.13
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	2	1.13
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	2	1.13
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	2	1.13
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	2	1.13
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	6	1.13
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	9	1.13
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD1	2	1.12
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD2	2	1.12
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD1	2	1.12
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD2	2	1.12
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD1	2	1.12
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD2	2	1.12
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	4	1.12
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	4	1.12
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	4	1.12
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	3	1.12
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	3	1.12
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	3	1.12
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	1	1.12
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	12	1.12
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	12	1.12
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	13	1.12
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	13	1.12
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	14	1.12
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	14	1.12
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	5	1.12
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	6	1.12
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	8	1.11
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	8	1.11
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	8	1.11
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	8	1.11
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	8	1.11
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	8	1.11
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	8	1.11
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	4	1.11
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	4	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	4	1.11
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	7	1.11
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	7	1.11
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	7	1.11
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	8	1.11
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	8	1.11
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	8	1.11
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	5	1.11
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	5	1.11
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	3	1.11
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	9	1.11
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	9	1.11
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	11	1.11
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	12	1.11
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	4	1.11
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	10	1.1
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	10	1.1
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	10	1.1
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	5	1.1
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	5	1.1
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	5	1.1
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	15	1.1
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD2	3	1.1
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD3	3	1.1
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD2	14	1.1
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD3	14	1.1
(1,247)	1:30:A:LYS:HG2	1:31:A:GLY:H	11	1.1
(1,247)	1:30:A:LYS:HG3	1:31:A:GLY:H	11	1.1
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	6	1.1
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	6	1.1
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	1	1.1
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	2	1.09
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	2	1.09
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	2	1.09
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	10	1.09
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	10	1.09
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	10	1.09
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	15	1.09
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	15	1.09
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	15	1.09
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	15	1.09
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	15	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	15	1.09
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	8	1.09
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	8	1.09
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	8	1.09
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	6	1.09
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	6	1.09
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	12	1.09
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	12	1.09
(1,232)	1:7:A:ILE:H	1:7:A:ILE:HG12	14	1.09
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	9	1.09
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	11	1.09
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	8	1.09
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	2	1.08
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	2	1.08
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	2	1.08
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	2	1.08
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	2	1.08
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	2	1.08
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	2	1.08
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	2	1.08
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	2	1.08
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	2	1.08
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG21	8	1.08
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG22	8	1.08
(1,478)	1:11:A:SER:H	1:12:A:ILE:HG23	8	1.08
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	1	1.08
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	1	1.08
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	1	1.08
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	6	1.08
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	6	1.08
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	9	1.08
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	9	1.08
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	8	1.08
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	8	1.08
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD2	5	1.08
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD3	5	1.08
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	7	1.08
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	7	1.08
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	11	1.08
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	11	1.08
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	7	1.08
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	3	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	11	1.07
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	11	1.07
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	11	1.07
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	11	1.07
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	11	1.07
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	11	1.07
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	10	1.07
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	10	1.07
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	10	1.07
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	1	1.07
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	1	1.07
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	1	1.07
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	1	1.07
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	4	1.07
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	4	1.07
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	13	1.07
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	13	1.07
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	14	1.07
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	14	1.07
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	7	1.07
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	7	1.07
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	14	1.07
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	14	1.07
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	1	1.07
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	1	1.07
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	10	1.07
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	15	1.07
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	6	1.07
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	7	1.07
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	15	1.07
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	9	1.07
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	5	1.07
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	10	1.06
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	10	1.06
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	10	1.06
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	3	1.06
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	3	1.06
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	3	1.06
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	10	1.06
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	10	1.06
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	10	1.06
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	13	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	13	1.06
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	13	1.06
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	7	1.06
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	7	1.06
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	7	1.06
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	7	1.06
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	7	1.06
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	7	1.06
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	10	1.06
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	10	1.06
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	10	1.06
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	12	1.06
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	10	1.06
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	10	1.06
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	12	1.06
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	12	1.06
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	2	1.06
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	3	1.06
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	5	1.06
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	14	1.06
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD11	1	1.05
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD12	1	1.05
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD13	1	1.05
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD11	3	1.05
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD12	3	1.05
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD13	3	1.05
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	6	1.05
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	6	1.05
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	15	1.05
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	15	1.05
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	15	1.05
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	10	1.05
(1,25)	1:18:A:HIS:HB3	1:19:A:GLN:H	11	1.05
(2,40)	1:10:A:TYR:HE1	1:12:A:ILE:HD11	3	1.04
(2,40)	1:10:A:TYR:HE1	1:12:A:ILE:HD12	3	1.04
(2,40)	1:10:A:TYR:HE1	1:12:A:ILE:HD13	3	1.04
(2,40)	1:10:A:TYR:HE2	1:12:A:ILE:HD11	3	1.04
(2,40)	1:10:A:TYR:HE2	1:12:A:ILE:HD12	3	1.04
(2,40)	1:10:A:TYR:HE2	1:12:A:ILE:HD13	3	1.04
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	15	1.04
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	15	1.04
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	15	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	15	1.04
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	5	1.04
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	5	1.04
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	5	1.04
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	9	1.04
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	9	1.04
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	9	1.04
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	7	1.04
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	7	1.04
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	8	1.04
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	8	1.04
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	11	1.04
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	11	1.04
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	3	1.04
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	14	1.04
(1,2)	1:1:A:TYR:HB2	1:2:A:ALA:H	7	1.04
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	14	1.03
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	14	1.03
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	14	1.03
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG12	6	1.03
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG13	6	1.03
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG12	6	1.03
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG13	6	1.03
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	10	1.03
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	10	1.03
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	12	1.03
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	12	1.03
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	8	1.03
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	3	1.03
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	7	1.03
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	10	1.03
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	5	1.03
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	2	1.03
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	15	1.02
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	15	1.02
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	15	1.02
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	4	1.02
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	4	1.02
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	15	1.02
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	15	1.02
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	3	1.02
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	3	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:25:A:TRP:HD1	1:26:A:LEU:HA	13	1.02
(1,212)	1:6:A:PHE:HA	1:10:A:TYR:H	8	1.02
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	14	1.02
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	14	1.02
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	13	1.02
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	12	1.01
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	2	1.01
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	2	1.01
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	11	1.01
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	11	1.01
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	15	1.01
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	15	1.01
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	10	1.01
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	2	1.01
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	15	1.0
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	15	1.0
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	15	1.0
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	12	1.0
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	12	1.0
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	13	1.0
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	13	1.0
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	7	1.0
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	7	1.0
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	15	1.0
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	15	1.0
(1,198)	1:11:A:SER:H	1:12:A:ILE:H	14	1.0
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	10	1.0
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	8	1.0
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	12	1.0
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	14	1.0
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	4	0.99
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	4	0.99
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	4	0.99
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	4	0.99
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	4	0.99
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	4	0.99
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	15	0.99
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	15	0.99
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	15	0.99
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	1	0.99
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	1	0.99
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	1	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	14	0.99
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	14	0.99
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	14	0.99
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	7	0.99
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	11	0.99
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	14	0.99
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	14	0.99
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB2	13	0.99
(1,207)	1:34:A:ASN:H	1:37:A:LYS:HB3	13	0.99
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	6	0.99
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	2	0.99
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	1	0.99
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	7	0.99
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	2	0.98
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	2	0.98
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	2	0.98
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	11	0.98
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	11	0.98
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	11	0.98
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG12	14	0.98
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG13	14	0.98
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG12	14	0.98
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG13	14	0.98
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE1	9	0.98
(1,333)	1:5:A:THR:HA	1:6:A:PHE:HE2	9	0.98
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	15	0.98
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	15	0.98
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	12	0.98
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	12	0.98
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD2	4	0.98
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD3	4	0.98
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	5	0.98
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	5	0.98
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	8	0.98
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	8	0.98
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	3	0.98
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	9	0.98
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	8	0.97
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	8	0.97
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	8	0.97
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	6	0.97
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	6	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	6	0.97
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	11	0.97
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	7	0.97
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	7	0.97
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	1	0.97
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB2	1	0.97
(1,208)	1:5:A:THR:H	1:6:A:PHE:HB3	1	0.97
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	1	0.97
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	4	0.97
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	6	0.97
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	2	0.97
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	8	0.97
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	5	0.96
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	5	0.96
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	5	0.96
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	4	0.96
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	4	0.96
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	4	0.96
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	13	0.96
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	13	0.96
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	13	0.96
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	11	0.96
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	11	0.96
(1,303)	1:10:A:TYR:HD1	1:11:A:SER:HA	1	0.96
(1,303)	1:10:A:TYR:HD2	1:11:A:SER:HA	1	0.96
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	11	0.96
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	13	0.96
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	14	0.95
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	14	0.95
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	14	0.95
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	6	0.95
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	6	0.95
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	6	0.95
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	6	0.95
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	6	0.95
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	6	0.95
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	7	0.95
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	7	0.95
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	13	0.95
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	13	0.95
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	13	0.95
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	13	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	13	0.95
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	13	0.95
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	9	0.95
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	9	0.95
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	9	0.95
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	9	0.95
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	9	0.95
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	9	0.95
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	9	0.95
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	9	0.95
(1,336)	1:24:A:ASN:H	1:24:A:ASN:HD22	12	0.95
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	6	0.95
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	6	0.95
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	8	0.95
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	15	0.95
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	15	0.95
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	3	0.95
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	3	0.95
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	2	0.95
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	2	0.95
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	1	0.94
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	1	0.94
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	1	0.94
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB2	11	0.94
(2,10)	1:10:A:TYR:HE1	1:14:A:MET:HB3	11	0.94
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB2	11	0.94
(2,10)	1:10:A:TYR:HE2	1:14:A:MET:HB3	11	0.94
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	5	0.94
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	5	0.94
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	5	0.94
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	5	0.94
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	5	0.94
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	5	0.94
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	11	0.94
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	11	0.94
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	11	0.94
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	10	0.94
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	10	0.94
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	10	0.94
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	10	0.94
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	6	0.94
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	8	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	10	0.94
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	7	0.93
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	7	0.93
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	7	0.93
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD1	14	0.93
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD2	14	0.93
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD1	14	0.93
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD2	14	0.93
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD1	14	0.93
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD2	14	0.93
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	10	0.93
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	10	0.93
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	10	0.93
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	11	0.93
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	11	0.93
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	11	0.93
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	11	0.93
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	11	0.93
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	11	0.93
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	12	0.93
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	12	0.93
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	12	0.93
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	12	0.93
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	12	0.93
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	12	0.93
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	15	0.93
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	15	0.93
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	12	0.93
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	12	0.93
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	1	0.93
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	1	0.93
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD2	6	0.93
(1,248)	1:37:A:LYS:H	1:37:A:LYS:HD3	6	0.93
(1,235)	1:14:A:MET:HG2	1:15:A:ASP:H	3	0.93
(1,235)	1:14:A:MET:HG3	1:15:A:ASP:H	3	0.93
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	4	0.92
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	4	0.92
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	4	0.92
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	1	0.92
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	1	0.92
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	1	0.92
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	8	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	6	0.92
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	9	0.92
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	9	0.92
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	11	0.92
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	9	0.92
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	11	0.92
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	10	0.91
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	10	0.91
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	10	0.91
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	10	0.91
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	10	0.91
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	10	0.91
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	1	0.91
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	1	0.91
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	1	0.91
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	7	0.91
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	7	0.91
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	7	0.91
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	10	0.91
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	10	0.91
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	10	0.91
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	15	0.91
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	15	0.91
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	15	0.91
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	4	0.91
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	4	0.91
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	4	0.91
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	4	0.91
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	4	0.91
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	4	0.91
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	3	0.91
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	3	0.91
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	3	0.91
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	2	0.91
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	2	0.91
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	2	0.91
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	6	0.91
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	6	0.91
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	6	0.91
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	10	0.91
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	10	0.91
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	6	0.91
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	10	0.91
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	10	0.91
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	6	0.91
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	14	0.91
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	12	0.91
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	15	0.9
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	15	0.9
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	15	0.9
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	15	0.9
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	15	0.9
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	15	0.9
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	13	0.9
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	13	0.9
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	13	0.9
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	12	0.9
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	11	0.9
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	11	0.9
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	15	0.9
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	15	0.9
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	7	0.9
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	9	0.9
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	9	0.9
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	4	0.89
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	4	0.89
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	4	0.89
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	4	0.89
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	4	0.89
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	4	0.89
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	4	0.89
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	4	0.89
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	4	0.89
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	4	0.89
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	4	0.89
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	4	0.89
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	14	0.89
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	14	0.89
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	14	0.89
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	15	0.89
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	8	0.89
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	6	0.89
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	6	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	11	0.89
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	11	0.89
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	7	0.89
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	5	0.89
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	7	0.88
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	7	0.88
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	7	0.88
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	11	0.88
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	11	0.88
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	11	0.88
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	1	0.88
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	1	0.88
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	1	0.88
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	1	0.88
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	1	0.88
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	1	0.88
(1,449)	1:28:A:ALA:HB1	1:29:A:GLN:HE21	6	0.88
(1,449)	1:28:A:ALA:HB2	1:29:A:GLN:HE21	6	0.88
(1,449)	1:28:A:ALA:HB3	1:29:A:GLN:HE21	6	0.88
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	13	0.88
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	13	0.88
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	13	0.88
(1,406)	1:6:A:PHE:HD1	1:7:A:ILE:HB	8	0.88
(1,406)	1:6:A:PHE:HD2	1:7:A:ILE:HB	8	0.88
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	8	0.88
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	8	0.88
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	8	0.88
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	8	0.88
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	14	0.88
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	14	0.88
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	10	0.88
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	10	0.88
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	11	0.88
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	11	0.88
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	6	0.88
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	6	0.88
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	3	0.88
(2,11)	1:10:A:TYR:HD1	1:14:A:MET:HG2	10	0.87
(2,11)	1:10:A:TYR:HD1	1:14:A:MET:HG3	10	0.87
(2,11)	1:10:A:TYR:HD2	1:14:A:MET:HG2	10	0.87
(2,11)	1:10:A:TYR:HD2	1:14:A:MET:HG3	10	0.87
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	14	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	14	0.87
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	14	0.87
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD21	8	0.87
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD22	8	0.87
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD23	8	0.87
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD21	8	0.87
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD22	8	0.87
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD23	8	0.87
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD21	8	0.87
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD22	8	0.87
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD23	8	0.87
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD11	8	0.87
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD12	8	0.87
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD13	8	0.87
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD11	8	0.87
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD12	8	0.87
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD13	8	0.87
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD11	8	0.87
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD12	8	0.87
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD13	8	0.87
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	7	0.87
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	14	0.87
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	14	0.87
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	9	0.86
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	9	0.86
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	9	0.86
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	9	0.86
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	9	0.86
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	9	0.86
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD11	10	0.86
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD12	10	0.86
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD13	10	0.86
(1,418)	1:12:A:ILE:HD11	1:13:A:ALA:H	11	0.86
(1,418)	1:12:A:ILE:HD12	1:13:A:ALA:H	11	0.86
(1,418)	1:12:A:ILE:HD13	1:13:A:ALA:H	11	0.86
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	5	0.86
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	14	0.86
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	13	0.86
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	11	0.86
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	11	0.86
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	11	0.86
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	15	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	11	0.86
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	12	0.85
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	12	0.85
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	12	0.85
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	10	0.85
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	10	0.85
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	10	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	10	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	10	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	10	0.85
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	13	0.85
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	13	0.85
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	13	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	13	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	13	0.85
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	13	0.85
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	3	0.85
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	3	0.85
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	3	0.85
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	3	0.85
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	3	0.85
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	3	0.85
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	11	0.85
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	11	0.85
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	11	0.85
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	11	0.85
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	11	0.85
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	11	0.85
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	8	0.85
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	8	0.85
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	5	0.85
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	5	0.85
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	12	0.85
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	12	0.85
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	13	0.85
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	13	0.85
(1,247)	1:30:A:LYS:HG2	1:31:A:GLY:H	14	0.85
(1,247)	1:30:A:LYS:HG3	1:31:A:GLY:H	14	0.85
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	2	0.85
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	2	0.85
(1,235)	1:14:A:MET:HG2	1:15:A:ASP:H	10	0.85
(1,235)	1:14:A:MET:HG3	1:15:A:ASP:H	10	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	11	0.85
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	14	0.85
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	14	0.85
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	9	0.85
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	11	0.85
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	3	0.85
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	6	0.84
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	6	0.84
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	6	0.84
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	13	0.84
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	13	0.84
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	13	0.84
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	5	0.84
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	5	0.84
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	2	0.84
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	3	0.84
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	3	0.84
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	8	0.83
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	8	0.83
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	8	0.83
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	15	0.83
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	15	0.83
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	15	0.83
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	12	0.83
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	12	0.83
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	12	0.83
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	12	0.83
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	12	0.83
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	12	0.83
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG12	2	0.83
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG13	2	0.83
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG12	2	0.83
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG13	2	0.83
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	14	0.83
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	9	0.83
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	14	0.83
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	14	0.83
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	7	0.83
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	7	0.83
(1,212)	1:6:A:PHE:HA	1:10:A:TYR:H	13	0.83
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	4	0.83
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	12	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	3	0.83
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	12	0.83
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	15	0.83
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	11	0.82
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	11	0.82
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	11	0.82
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	5	0.82
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	5	0.82
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	5	0.82
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	5	0.82
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	5	0.82
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	5	0.82
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	14	0.82
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	14	0.82
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	14	0.82
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	9	0.82
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	9	0.82
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	9	0.82
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	9	0.82
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	9	0.82
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	9	0.82
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	5	0.82
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	2	0.82
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	2	0.82
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	3	0.82
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	12	0.82
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	12	0.82
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	7	0.82
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	7	0.82
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	3	0.82
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	3	0.82
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	6	0.82
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	6	0.82
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	8	0.82
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	8	0.82
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	7	0.82
(1,192)	1:5:A:THR:H	1:7:A:ILE:H	1	0.82
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	5	0.82
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	1	0.82
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	4	0.82
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	6	0.82
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	7	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	7	0.81
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	7	0.81
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	7	0.81
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	7	0.81
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	7	0.81
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	8	0.81
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	8	0.81
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	8	0.81
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	11	0.81
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	11	0.81
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	5	0.81
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	11	0.81
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	11	0.81
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	1	0.81
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	1	0.81
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	10	0.81
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	10	0.81
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	1	0.81
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	1	0.81
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	3	0.81
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	3	0.81
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	13	0.81
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	13	0.81
(1,110)	1:5:A:THR:HB	1:6:A:PHE:H	1	0.81
(1,26)	1:21:A:ASP:HB3	1:22:A:PHE:H	8	0.81
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	12	0.8
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	12	0.8
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	12	0.8
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD11	14	0.8
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD12	14	0.8
(1,481)	1:24:A:ASN:H	1:27:A:LEU:HD13	14	0.8
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	2	0.8
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	2	0.8
(1,345)	1:6:A:PHE:HD1	1:8:A:SER:H	8	0.8
(1,345)	1:6:A:PHE:HD2	1:8:A:SER:H	8	0.8
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	2	0.8
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	13	0.8
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	13	0.8
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	11	0.8
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	11	0.8
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	9	0.8
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	9	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	11	0.8
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	11	0.8
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	13	0.8
(1,51)	1:30:A:LYS:HB2	1:31:A:GLY:H	11	0.8
(1,51)	1:30:A:LYS:HB3	1:31:A:GLY:H	11	0.8
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	1	0.79
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	1	0.79
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	1	0.79
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	1	0.79
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	2	0.79
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	2	0.79
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	2	0.79
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	9	0.79
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	9	0.79
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	9	0.79
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	15	0.79
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	15	0.79
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	15	0.79
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	11	0.79
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	11	0.79
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	11	0.79
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	13	0.79
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	13	0.79
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	13	0.79
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	13	0.79
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	13	0.79
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	13	0.79
(1,420)	1:14:A:MET:H	1:14:A:MET:HE1	3	0.79
(1,420)	1:14:A:MET:H	1:14:A:MET:HE2	3	0.79
(1,420)	1:14:A:MET:H	1:14:A:MET:HE3	3	0.79
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	1	0.79
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	14	0.79
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	1	0.79
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	2	0.79
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	12	0.79
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	11	0.79
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	11	0.79
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	4	0.79
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	4	0.79
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	14	0.79
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	14	0.79
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	14	0.79
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	4	0.79
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	13	0.79
(2,39)	1:28:A:ALA:HB1	1:29:A:GLN:HE22	8	0.78
(2,39)	1:28:A:ALA:HB2	1:29:A:GLN:HE22	8	0.78
(2,39)	1:28:A:ALA:HB3	1:29:A:GLN:HE22	8	0.78
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	7	0.78
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	7	0.78
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	7	0.78
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	10	0.78
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	10	0.78
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	10	0.78
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	5	0.78
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	5	0.78
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	5	0.78
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	1	0.78
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	1	0.78
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	1	0.78
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	12	0.78
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	12	0.78
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	9	0.78
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	9	0.78
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	3	0.78
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	3	0.78
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	8	0.78
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	8	0.78
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	7	0.78
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	7	0.78
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	10	0.78
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	10	0.78
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	1	0.78
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	4	0.78
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	15	0.78
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	2	0.78
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	8	0.77
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	8	0.77
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	8	0.77
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	8	0.77
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	8	0.77
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	8	0.77
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	13	0.77
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	13	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	13	0.77
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	14	0.77
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	14	0.77
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	14	0.77
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	11	0.77
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	11	0.77
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	11	0.77
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	7	0.77
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	7	0.77
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	7	0.77
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	7	0.77
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	7	0.77
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	7	0.77
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	8	0.77
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	8	0.77
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	8	0.77
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	8	0.77
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	8	0.77
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	8	0.77
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	15	0.77
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	15	0.77
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	15	0.77
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	15	0.77
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	15	0.77
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	15	0.77
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	4	0.77
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	4	0.77
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	4	0.77
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	11	0.77
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	1	0.77
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	1	0.77
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	8	0.77
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	8	0.77
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	15	0.77
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	15	0.77
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	12	0.77
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	12	0.77
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	8	0.77
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	8	0.77
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	10	0.77
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	10	0.77
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	4	0.77
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	1	0.77
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	3	0.76
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	3	0.76
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	3	0.76
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	5	0.76
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	5	0.76
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	5	0.76
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	2	0.76
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	2	0.76
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	2	0.76
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	2	0.76
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	2	0.76
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	2	0.76
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	10	0.76
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	10	0.76
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	10	0.76
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	10	0.76
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	10	0.76
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	10	0.76
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	14	0.76
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	14	0.76
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	14	0.76
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	2	0.76
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	2	0.76
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	2	0.76
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	7	0.76
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	9	0.76
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	9	0.76
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	2	0.76
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	2	0.76
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	7	0.76
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	7	0.76
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	10	0.76
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	10	0.76
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	6	0.76
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	8	0.76
(1,213)	1:8:A:SER:H	1:10:A:TYR:H	13	0.76
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	10	0.76
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	10	0.76
(1,127)	1:29:A:GLN:HA	1:32:A:LYS:H	12	0.76
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	13	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	1	0.75
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	1	0.75
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	1	0.75
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	5	0.75
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	5	0.75
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	5	0.75
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	1	0.75
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	1	0.75
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	4	0.75
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	4	0.75
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD1	4	0.75
(1,298)	1:5:A:THR:HA	1:6:A:PHE:HD2	4	0.75
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	15	0.75
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	5	0.75
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	5	0.75
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	9	0.75
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	9	0.75
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG2	14	0.75
(1,266)	1:29:A:GLN:H	1:29:A:GLN:HG3	14	0.75
(1,247)	1:30:A:LYS:HG2	1:31:A:GLY:H	7	0.75
(1,247)	1:30:A:LYS:HG3	1:31:A:GLY:H	7	0.75
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	13	0.75
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	4	0.75
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	1	0.75
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	9	0.75
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD11	8	0.74
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD12	8	0.74
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD13	8	0.74
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD11	8	0.74
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD12	8	0.74
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD13	8	0.74
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG21	12	0.74
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG22	12	0.74
(1,475)	1:40:A:ILE:HG12	1:41:A:THR:HG23	12	0.74
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG21	12	0.74
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG22	12	0.74
(1,475)	1:40:A:ILE:HG13	1:41:A:THR:HG23	12	0.74
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	12	0.74
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	12	0.74
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	12	0.74
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	4	0.74
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	4	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	4	0.74
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	4	0.74
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	9	0.74
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	2	0.74
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	2	0.74
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	7	0.74
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	7	0.74
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	12	0.74
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	10	0.74
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	1	0.74
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	2	0.74
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	6	0.73
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	6	0.73
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	6	0.73
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	15	0.73
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	15	0.73
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	15	0.73
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	6	0.73
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	6	0.73
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	6	0.73
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	6	0.73
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	6	0.73
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	6	0.73
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	6	0.73
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	6	0.73
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	6	0.73
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	3	0.73
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	3	0.73
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	3	0.73
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	3	0.73
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	3	0.73
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	3	0.73
(1,414)	1:5:A:THR:HG21	1:7:A:ILE:H	9	0.73
(1,414)	1:5:A:THR:HG22	1:7:A:ILE:H	9	0.73
(1,414)	1:5:A:THR:HG23	1:7:A:ILE:H	9	0.73
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	2	0.73
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	5	0.73
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	5	0.73
(1,247)	1:30:A:LYS:HG2	1:31:A:GLY:H	10	0.73
(1,247)	1:30:A:LYS:HG3	1:31:A:GLY:H	10	0.73
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	6	0.73
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	7	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	3	0.73
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	9	0.72
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	9	0.72
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	9	0.72
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	4	0.72
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	4	0.72
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	4	0.72
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	10	0.72
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	10	0.72
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	10	0.72
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	1	0.72
(1,124)	1:28:A:ALA:HA	1:31:A:GLY:H	11	0.72
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	12	0.72
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	1	0.72
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	11	0.71
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	11	0.71
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	4	0.71
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	4	0.71
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	4	0.71
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	10	0.71
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	10	0.71
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	10	0.71
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	10	0.71
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	10	0.71
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	10	0.71
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	1	0.71
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	1	0.71
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	1	0.71
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	1	0.71
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	1	0.71
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	1	0.71
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	6	0.71
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	6	0.71
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	6	0.71
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	6	0.71
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	6	0.71
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	6	0.71
(1,432)	1:26:A:LEU:HD21	1:29:A:GLN:H	8	0.71
(1,432)	1:26:A:LEU:HD22	1:29:A:GLN:H	8	0.71
(1,432)	1:26:A:LEU:HD23	1:29:A:GLN:H	8	0.71
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	4	0.71
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	4	0.71
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	11	0.71
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	11	0.71
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	14	0.71
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	14	0.71
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	1	0.71
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	1	0.71
(1,247)	1:30:A:LYS:HG2	1:31:A:GLY:H	4	0.71
(1,247)	1:30:A:LYS:HG3	1:31:A:GLY:H	4	0.71
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	1	0.71
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	15	0.71
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	7	0.71
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	11	0.71
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	13	0.71
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	8	0.71
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	13	0.7
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	13	0.7
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	13	0.7
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	13	0.7
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	13	0.7
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	13	0.7
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	6	0.7
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	6	0.7
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	6	0.7
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	1	0.7
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	1	0.7
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	1	0.7
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	8	0.7
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	8	0.7
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	2	0.7
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	2	0.7
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	14	0.7
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	14	0.7
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	7	0.7
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	7	0.7
(1,222)	1:20:A:GLN:HA	1:24:A:ASN:H	5	0.7
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	5	0.7
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	5	0.7
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	1	0.7
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	15	0.7
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	10	0.7
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	6	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	9	0.7
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	14	0.69
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	14	0.69
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	7	0.69
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	7	0.69
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	7	0.69
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	5	0.69
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	9	0.69
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	10	0.69
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	15	0.69
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	3	0.69
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	3	0.69
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	6	0.69
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	3	0.69
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	3	0.69
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	6	0.69
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	12	0.69
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	8	0.68
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	8	0.68
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	8	0.68
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	8	0.68
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	8	0.68
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	8	0.68
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	1	0.68
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	14	0.68
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	5	0.68
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	5	0.68
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	5	0.68
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	5	0.68
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	15	0.68
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	14	0.68
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	6	0.68
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	8	0.68
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	6	0.68
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	7	0.68
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	12	0.67
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	12	0.67
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	5	0.67
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	5	0.67
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	5	0.67
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	2	0.67
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	6	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:12:A:ILE:HB	1:12:A:ILE:HG12	11	0.67
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	15	0.67
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	15	0.67
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB2	13	0.67
(1,323)	1:25:A:TRP:HE3	1:26:A:LEU:HB3	13	0.67
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	11	0.67
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	11	0.67
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	3	0.67
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	14	0.67
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	14	0.67
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	13	0.67
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	15	0.67
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	9	0.67
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	4	0.67
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	13	0.67
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	15	0.67
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG21	8	0.66
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG22	8	0.66
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG23	8	0.66
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG21	8	0.66
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG22	8	0.66
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG23	8	0.66
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	10	0.66
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	10	0.66
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	10	0.66
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	6	0.66
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	6	0.66
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	6	0.66
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	6	0.66
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	6	0.66
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	6	0.66
(1,406)	1:6:A:PHE:HD1	1:7:A:ILE:HB	9	0.66
(1,406)	1:6:A:PHE:HD2	1:7:A:ILE:HB	9	0.66
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	9	0.66
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	13	0.66
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	14	0.66
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	14	0.66
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	4	0.66
(1,261)	1:32:A:LYS:HG2	1:36:A:TRP:H	13	0.66
(1,261)	1:32:A:LYS:HG3	1:36:A:TRP:H	13	0.66
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	5	0.66
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	8	0.66
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	8	0.66
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	10	0.66
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	3	0.66
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	2	0.66
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	10	0.66
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	1	0.66
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	1	0.66
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	1	0.66
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	8	0.65
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	8	0.65
(2,2)	1:32:A:LYS:HG2	1:34:A:ASN:H	15	0.65
(2,2)	1:32:A:LYS:HG3	1:34:A:ASN:H	15	0.65
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB2	12	0.65
(1,459)	1:23:A:VAL:HG21	1:27:A:LEU:HB3	12	0.65
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB2	12	0.65
(1,459)	1:23:A:VAL:HG22	1:27:A:LEU:HB3	12	0.65
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB2	12	0.65
(1,459)	1:23:A:VAL:HG23	1:27:A:LEU:HB3	12	0.65
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD11	12	0.65
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD12	12	0.65
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD13	12	0.65
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	7	0.65
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	7	0.65
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	5	0.65
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	5	0.65
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	5	0.65
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	8	0.65
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	11	0.64
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	11	0.64
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	11	0.64
(1,287)	1:25:A:TRP:HD1	1:26:A:LEU:HA	4	0.64
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	11	0.64
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	15	0.64
(1,212)	1:6:A:PHE:HA	1:10:A:TYR:H	5	0.64
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	3	0.64
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	8	0.64
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	15	0.64
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	13	0.64
(1,80)	1:16:A:LYS:HA	1:19:A:GLN:H	15	0.64
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	6	0.63
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	6	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	6	0.63
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	6	0.63
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	8	0.63
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	8	0.63
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	8	0.63
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	8	0.63
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	8	0.63
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	8	0.63
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	8	0.63
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	8	0.63
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	8	0.63
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB1	11	0.63
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB2	11	0.63
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB3	11	0.63
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	8	0.63
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	8	0.63
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	8	0.63
(1,345)	1:6:A:PHE:HD1	1:8:A:SER:H	9	0.63
(1,345)	1:6:A:PHE:HD2	1:8:A:SER:H	9	0.63
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD1	8	0.63
(1,310)	1:8:A:SER:HB3	1:10:A:TYR:HD2	8	0.63
(1,258)	1:30:A:LYS:HD2	1:32:A:LYS:H	9	0.63
(1,258)	1:30:A:LYS:HD3	1:32:A:LYS:H	9	0.63
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	4	0.63
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	4	0.63
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	10	0.63
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	10	0.63
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	7	0.63
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	7	0.63
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	5	0.63
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	5	0.63
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	11	0.63
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	11	0.63
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	3	0.63
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	6	0.63
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	15	0.63
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	1	0.63
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	15	0.63
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	8	0.63
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	9	0.63
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	1	0.63
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB1	2	0.62
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB2	2	0.62
(2,35)	1:10:A:TYR:HD1	1:13:A:ALA:HB3	2	0.62
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB1	2	0.62
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB2	2	0.62
(2,35)	1:10:A:TYR:HD2	1:13:A:ALA:HB3	2	0.62
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB2	13	0.62
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB3	13	0.62
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB2	13	0.62
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB3	13	0.62
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	12	0.62
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	12	0.62
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	12	0.62
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	3	0.62
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	3	0.62
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	3	0.62
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB1	13	0.62
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB2	13	0.62
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB3	13	0.62
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	10	0.62
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	10	0.62
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	10	0.62
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	3	0.62
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	3	0.62
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	3	0.62
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	1	0.62
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	1	0.62
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	11	0.62
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	4	0.62
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	5	0.62
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	5	0.62
(1,219)	1:30:A:LYS:HA	1:32:A:LYS:H	15	0.62
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	3	0.62
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	5	0.62
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	5	0.62
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	7	0.62
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	11	0.62
(1,107)	1:38:A:HIS:HA	1:39:A:ASN:H	14	0.62
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	5	0.61
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	5	0.61
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	5	0.61
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	5	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	5	0.61
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	5	0.61
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	1	0.61
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	1	0.61
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	1	0.61
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD21	12	0.61
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD22	12	0.61
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD23	12	0.61
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	12	0.61
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD22	12	0.61
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD23	12	0.61
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	12	0.61
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD22	12	0.61
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD23	12	0.61
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD11	12	0.61
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD12	12	0.61
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD13	12	0.61
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD11	12	0.61
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD12	12	0.61
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD13	12	0.61
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD11	12	0.61
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD12	12	0.61
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD13	12	0.61
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	10	0.61
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	10	0.61
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	10	0.61
(1,325)	1:14:A:MET:HB2	1:18:A:HIS:HD2	4	0.61
(1,325)	1:14:A:MET:HB3	1:18:A:HIS:HD2	4	0.61
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	1	0.61
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	1	0.61
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	2	0.61
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	2	0.61
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	14	0.61
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	14	0.61
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	1	0.61
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	1	0.61
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	7	0.61
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	7	0.61
(1,252)	1:32:A:LYS:HD2	1:33:A:LYS:H	10	0.61
(1,252)	1:32:A:LYS:HD3	1:33:A:LYS:H	10	0.61
(1,247)	1:30:A:LYS:HG2	1:31:A:GLY:H	1	0.61
(1,247)	1:30:A:LYS:HG3	1:31:A:GLY:H	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:14:A:MET:HG2	1:15:A:ASP:H	4	0.61
(1,235)	1:14:A:MET:HG3	1:15:A:ASP:H	4	0.61
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	4	0.61
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	5	0.61
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	2	0.61
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	12	0.61
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	9	0.61
(1,86)	1:23:A:VAL:HA	1:25:A:TRP:H	15	0.61
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	6	0.61
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	11	0.6
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	11	0.6
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	11	0.6
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	13	0.6
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	13	0.6
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	13	0.6
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	11	0.6
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	11	0.6
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	11	0.6
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	11	0.6
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	11	0.6
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	11	0.6
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	2	0.6
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	2	0.6
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	12	0.6
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	12	0.6
(1,254)	1:33:A:LYS:HG2	1:34:A:ASN:H	8	0.6
(1,254)	1:33:A:LYS:HG3	1:34:A:ASN:H	8	0.6
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	12	0.6
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	12	0.6
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	13	0.6
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	1	0.6
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	14	0.6
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	8	0.6
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	1	0.6
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	5	0.6
(1,85)	1:18:A:HIS:HA	1:22:A:PHE:H	13	0.6
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	5	0.6
(1,8)	1:10:A:TYR:H	1:10:A:TYR:HB2	13	0.6
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	14	0.59
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	14	0.59
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	14	0.59
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	2	0.59
(1,345)	1:6:A:PHE:HD1	1:8:A:SER:H	1	0.59
(1,345)	1:6:A:PHE:HD2	1:8:A:SER:H	1	0.59
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB2	14	0.59
(1,309)	1:1:A:TYR:HD1	1:6:A:PHE:HB3	14	0.59
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB2	14	0.59
(1,309)	1:1:A:TYR:HD2	1:6:A:PHE:HB3	14	0.59
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	1	0.59
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	2	0.59
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	7	0.59
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	10	0.59
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG21	5	0.58
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG22	5	0.58
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG23	5	0.58
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG21	5	0.58
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG22	5	0.58
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG23	5	0.58
(1,489)	1:23:A:VAL:HG11	1:25:A:TRP:H	4	0.58
(1,489)	1:23:A:VAL:HG12	1:25:A:TRP:H	4	0.58
(1,489)	1:23:A:VAL:HG13	1:25:A:TRP:H	4	0.58
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	12	0.58
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	12	0.58
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	12	0.58
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	3	0.58
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	3	0.58
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	3	0.58
(1,321)	1:6:A:PHE:HD1	1:7:A:ILE:HG12	8	0.58
(1,321)	1:6:A:PHE:HD2	1:7:A:ILE:HG12	8	0.58
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	2	0.58
(1,247)	1:30:A:LYS:HG2	1:31:A:GLY:H	2	0.58
(1,247)	1:30:A:LYS:HG3	1:31:A:GLY:H	2	0.58
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	7	0.58
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	7	0.58
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	13	0.58
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	13	0.58
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	6	0.58
(1,51)	1:30:A:LYS:HB2	1:31:A:GLY:H	9	0.58
(1,51)	1:30:A:LYS:HB3	1:31:A:GLY:H	9	0.58
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	3	0.57
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	3	0.57
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	2	0.57
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	2	0.57
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	11	0.57
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	11	0.57
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	11	0.57
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	12	0.57
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	12	0.57
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	12	0.57
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	10	0.57
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	10	0.57
(1,343)	1:35:A:ASP:H	1:36:A:TRP:HD1	15	0.57
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	5	0.57
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	5	0.57
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	14	0.57
(1,276)	1:36:A:TRP:HA	1:36:A:TRP:HE3	2	0.57
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	5	0.57
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	10	0.57
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	1	0.57
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	15	0.57
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	11	0.57
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	6	0.57
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	4	0.57
(1,168)	1:4:A:GLY:H	1:5:A:THR:H	14	0.57
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	5	0.56
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	5	0.56
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	5	0.56
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	5	0.56
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	15	0.56
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	15	0.56
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	15	0.56
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	15	0.56
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	15	0.56
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	15	0.56
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	5	0.56
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	5	0.56
(1,321)	1:6:A:PHE:HD1	1:7:A:ILE:HG12	9	0.56
(1,321)	1:6:A:PHE:HD2	1:7:A:ILE:HG12	9	0.56
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	5	0.56
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	13	0.56
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	9	0.56
(1,204)	1:29:A:GLN:HB2	1:31:A:GLY:H	12	0.56
(1,204)	1:29:A:GLN:HB3	1:31:A:GLY:H	12	0.56
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	6	0.56
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	1	0.56
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	14	0.56
(1,80)	1:16:A:LYS:HA	1:19:A:GLN:H	12	0.56
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	14	0.56
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD1	9	0.55
(2,37)	1:7:A:ILE:HG21	1:10:A:TYR:HD2	9	0.55
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD1	9	0.55
(2,37)	1:7:A:ILE:HG22	1:10:A:TYR:HD2	9	0.55
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD1	9	0.55
(2,37)	1:7:A:ILE:HG23	1:10:A:TYR:HD2	9	0.55
(1,468)	1:13:A:ALA:HB1	1:17:A:ILE:HG21	14	0.55
(1,468)	1:13:A:ALA:HB1	1:17:A:ILE:HG22	14	0.55
(1,468)	1:13:A:ALA:HB1	1:17:A:ILE:HG23	14	0.55
(1,468)	1:13:A:ALA:HB2	1:17:A:ILE:HG21	14	0.55
(1,468)	1:13:A:ALA:HB2	1:17:A:ILE:HG22	14	0.55
(1,468)	1:13:A:ALA:HB2	1:17:A:ILE:HG23	14	0.55
(1,468)	1:13:A:ALA:HB3	1:17:A:ILE:HG21	14	0.55
(1,468)	1:13:A:ALA:HB3	1:17:A:ILE:HG22	14	0.55
(1,468)	1:13:A:ALA:HB3	1:17:A:ILE:HG23	14	0.55
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	14	0.55
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	8	0.55
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	8	0.55
(1,254)	1:33:A:LYS:HG2	1:34:A:ASN:H	13	0.55
(1,254)	1:33:A:LYS:HG3	1:34:A:ASN:H	13	0.55
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	10	0.55
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	10	0.55
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	7	0.55
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	14	0.55
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	2	0.55
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	1	0.55
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	7	0.55
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	10	0.55
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	5	0.55
(1,51)	1:30:A:LYS:HB2	1:31:A:GLY:H	5	0.55
(1,51)	1:30:A:LYS:HB3	1:31:A:GLY:H	5	0.55
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	12	0.54
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	12	0.54
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	12	0.54
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	12	0.54
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	12	0.54
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	12	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	7	0.54
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	7	0.54
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	7	0.54
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	8	0.54
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	8	0.54
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	8	0.54
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	11	0.54
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	11	0.54
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	11	0.54
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	11	0.54
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	3	0.54
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	3	0.54
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	3	0.54
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	3	0.54
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	5	0.54
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	3	0.54
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	13	0.54
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	9	0.54
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	8	0.54
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	12	0.54
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	3	0.54
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	1	0.54
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	12	0.53
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	12	0.53
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	12	0.53
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	12	0.53
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	12	0.53
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	12	0.53
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	9	0.53
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	9	0.53
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	4	0.53
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	4	0.53
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	7	0.53
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	12	0.53
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	3	0.53
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	6	0.53
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	14	0.53
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	5	0.53
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	9	0.53
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	11	0.53
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	10	0.53
(1,80)	1:16:A:LYS:HA	1:19:A:GLN:H	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	4	0.52
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	4	0.52
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	4	0.52
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD21	5	0.52
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD22	5	0.52
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD23	5	0.52
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	5	0.52
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD22	5	0.52
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD23	5	0.52
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	5	0.52
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD22	5	0.52
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD23	5	0.52
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD11	5	0.52
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD12	5	0.52
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD13	5	0.52
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD11	5	0.52
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD12	5	0.52
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD13	5	0.52
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD11	5	0.52
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD12	5	0.52
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD13	5	0.52
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD21	11	0.52
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD22	11	0.52
(1,446)	1:22:A:PHE:HE1	1:26:A:LEU:HD23	11	0.52
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD21	11	0.52
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD22	11	0.52
(1,446)	1:22:A:PHE:HE2	1:26:A:LEU:HD23	11	0.52
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	1	0.52
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	1	0.52
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	1	0.52
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	5	0.52
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	5	0.52
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	5	0.52
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD21	3	0.52
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD22	3	0.52
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD23	3	0.52
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD11	3	0.52
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD12	3	0.52
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD13	3	0.52
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	10	0.52
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	10	0.52
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	7	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	7	0.52
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	3	0.52
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	3	0.52
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	13	0.52
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	13	0.52
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	2	0.52
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	5	0.52
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	7	0.52
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	4	0.52
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	12	0.52
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	8	0.52
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	8	0.52
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	3	0.52
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	3	0.51
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	3	0.51
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	3	0.51
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE1	14	0.51
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE2	14	0.51
(2,22)	1:10:A:TYR:HE1	1:14:A:MET:HE3	14	0.51
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE1	14	0.51
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE2	14	0.51
(2,22)	1:10:A:TYR:HE2	1:14:A:MET:HE3	14	0.51
(1,483)	1:3:A:GLU:H	1:5:A:THR:HG21	1	0.51
(1,483)	1:3:A:GLU:H	1:5:A:THR:HG22	1	0.51
(1,483)	1:3:A:GLU:H	1:5:A:THR:HG23	1	0.51
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	2	0.51
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	2	0.51
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	2	0.51
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	2	0.51
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	2	0.51
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	2	0.51
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	13	0.51
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	13	0.51
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	13	0.51
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	8	0.51
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	8	0.51
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	2	0.51
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	6	0.51
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	6	0.51
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	1	0.51
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	8	0.51
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	9	0.51
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	11	0.51
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	5	0.51
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	2	0.51
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	2	0.51
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	5	0.51
(1,119)	1:11:A:SER:HA	1:14:A:MET:H	7	0.51
(1,117)	1:11:A:SER:HB2	1:12:A:ILE:H	10	0.51
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	10	0.5
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	10	0.5
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	10	0.5
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	15	0.5
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	15	0.5
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	15	0.5
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	4	0.5
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	4	0.5
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	4	0.5
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	8	0.5
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	8	0.5
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	8	0.5
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	12	0.5
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	6	0.5
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	6	0.5
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	10	0.5
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	10	0.5
(1,235)	1:14:A:MET:HG2	1:15:A:ASP:H	11	0.5
(1,235)	1:14:A:MET:HG3	1:15:A:ASP:H	11	0.5
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	12	0.5
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	1	0.5
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	3	0.5
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	11	0.5
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	3	0.5
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	8	0.5
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	13	0.5
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	10	0.5
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	12	0.5
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	12	0.5
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG21	6	0.49
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG22	6	0.49
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG23	6	0.49
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG21	6	0.49
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG22	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG23	6	0.49
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	12	0.49
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	12	0.49
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	12	0.49
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG21	9	0.49
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG22	9	0.49
(1,461)	1:16:A:LYS:HG2	1:17:A:ILE:HG23	9	0.49
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG21	9	0.49
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG22	9	0.49
(1,461)	1:16:A:LYS:HG3	1:17:A:ILE:HG23	9	0.49
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	1	0.49
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	1	0.49
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	1	0.49
(1,314)	1:39:A:ASN:HB3	1:39:A:ASN:HD22	13	0.49
(1,314)	1:39:A:ASN:HB2	1:39:A:ASN:HD22	13	0.49
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD2	2	0.49
(1,257)	1:30:A:LYS:H	1:30:A:LYS:HD3	2	0.49
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	8	0.49
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	8	0.49
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	11	0.49
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	11	0.49
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	7	0.49
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	8	0.49
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	11	0.49
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	7	0.49
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	8	0.49
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	4	0.48
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	4	0.48
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	4	0.48
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	4	0.48
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD1	7	0.48
(1,326)	1:21:A:ASP:HB3	1:22:A:PHE:HD2	7	0.48
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	8	0.48
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	13	0.48
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	4	0.48
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	15	0.48
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	15	0.48
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	9	0.48
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	11	0.48
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	1	0.48
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD11	8	0.47
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD12	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:11:A:SER:H	1:12:A:ILE:HD13	8	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	8	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	8	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	8	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	11	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	11	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	11	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	12	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	12	0.47
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	12	0.47
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	12	0.47
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	12	0.47
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	12	0.47
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	12	0.47
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	13	0.47
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	13	0.47
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	13	0.47
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	13	0.47
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE22	8	0.47
(1,376)	1:29:A:GLN:H	1:29:A:GLN:HE21	8	0.47
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	4	0.47
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	8	0.47
(1,251)	1:40:A:ILE:H	1:40:A:ILE:HG12	12	0.47
(1,251)	1:40:A:ILE:H	1:40:A:ILE:HG13	12	0.47
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	1	0.47
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	1	0.47
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	10	0.47
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	7	0.47
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	12	0.47
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	9	0.47
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	3	0.47
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	2	0.47
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	3	0.47
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	12	0.47
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	14	0.47
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	4	0.47
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	2	0.47
(1,71)	1:37:A:LYS:HB2	1:38:A:HIS:H	3	0.47
(1,71)	1:37:A:LYS:HB3	1:38:A:HIS:H	3	0.47
(1,71)	1:37:A:LYS:HB2	1:38:A:HIS:H	6	0.47
(1,71)	1:37:A:LYS:HB3	1:38:A:HIS:H	6	0.47
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	2	0.46
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	2	0.46
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	14	0.46
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	14	0.46
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	14	0.46
(1,435)	1:41:A:THR:H	1:41:A:THR:HG21	12	0.46
(1,435)	1:41:A:THR:H	1:41:A:THR:HG22	12	0.46
(1,435)	1:41:A:THR:H	1:41:A:THR:HG23	12	0.46
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	10	0.46
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	10	0.46
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	10	0.46
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	13	0.46
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	13	0.46
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	13	0.46
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	7	0.46
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	7	0.46
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	7	0.46
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	6	0.46
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	6	0.46
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	6	0.46
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	6	0.46
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	6	0.46
(1,314)	1:39:A:ASN:HB3	1:39:A:ASN:HD22	14	0.46
(1,314)	1:39:A:ASN:HB2	1:39:A:ASN:HD22	14	0.46
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	5	0.46
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	5	0.46
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	1	0.46
(1,218)	1:29:A:GLN:HA	1:31:A:GLY:H	1	0.46
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	4	0.46
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	4	0.46
(1,203)	1:11:A:SER:H	1:12:A:ILE:HB	10	0.46
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	6	0.46
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	9	0.46
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	6	0.46
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	13	0.46
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	2	0.46
(1,150)	1:42:A:GLN:H	1:42:A:GLN:HB2	8	0.46
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	7	0.46
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	7	0.46
(1,80)	1:16:A:LYS:HA	1:19:A:GLN:H	7	0.46
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	5	0.45
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	5	0.45
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	5	0.45
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	5	0.45
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	5	0.45
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	14	0.45
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	14	0.45
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	14	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	3	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	3	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	3	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	4	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	4	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	4	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	5	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	5	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	5	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	6	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	6	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	6	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	11	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	11	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	11	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	13	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	13	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	13	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	15	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	15	0.45
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	15	0.45
(1,314)	1:39:A:ASN:HB3	1:39:A:ASN:HD22	9	0.45
(1,314)	1:39:A:ASN:HB2	1:39:A:ASN:HD22	9	0.45
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	4	0.45
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	4	0.45
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG2	15	0.45
(1,243)	1:30:A:LYS:H	1:30:A:LYS:HG3	15	0.45
(1,233)	1:12:A:ILE:H	1:12:A:ILE:HG13	14	0.45
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	3	0.45
(1,203)	1:11:A:SER:H	1:12:A:ILE:HB	12	0.45
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	7	0.45
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	9	0.45
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	15	0.45
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	9	0.45
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	9	0.45
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	15	0.45
(1,148)	1:20:A:GLN:HB2	1:21:A:ASP:H	2	0.45
(1,148)	1:20:A:GLN:HB3	1:21:A:ASP:H	2	0.45
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	4	0.45
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	4	0.45
(1,124)	1:28:A:ALA:HA	1:31:A:GLY:H	12	0.45
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	15	0.45
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	10	0.45
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	10	0.45
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG21	15	0.44
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG22	15	0.44
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG23	15	0.44
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG21	15	0.44
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG22	15	0.44
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG23	15	0.44
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	10	0.44
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	10	0.44
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	4	0.44
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	4	0.44
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	4	0.44
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	4	0.44
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	4	0.44
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	4	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	2	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	2	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	2	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	10	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	10	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	10	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	12	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	12	0.44
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	12	0.44
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	9	0.44
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	9	0.44
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	9	0.44
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	10	0.44
(1,290)	1:22:A:PHE:HA	1:25:A:TRP:HD1	13	0.44
(1,277)	1:36:A:TRP:HE3	1:37:A:LYS:HA	14	0.44
(1,213)	1:8:A:SER:H	1:10:A:TYR:H	5	0.44
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	12	0.44
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	4	0.44
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	4	0.44
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	14	0.44
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	6	0.44
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	5	0.44
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	11	0.44
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	12	0.44
(1,150)	1:42:A:GLN:H	1:42:A:GLN:HB2	1	0.44
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	1	0.44
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	1	0.44
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	3	0.44
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	3	0.44
(1,84)	1:34:A:ASN:HA	1:37:A:LYS:H	10	0.44
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	9	0.43
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	9	0.43
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	9	0.43
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	14	0.43
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	14	0.43
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	14	0.43
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG21	10	0.43
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG22	10	0.43
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG23	10	0.43
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG21	10	0.43
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG22	10	0.43
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG23	10	0.43
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	8	0.43
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	8	0.43
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	8	0.43
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	8	0.43
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	8	0.43
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	8	0.43
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	7	0.43
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	7	0.43
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	7	0.43
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	12	0.43
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	12	0.43
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	12	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	2	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	2	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	2	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	3	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	3	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	5	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	5	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	5	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	6	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	6	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	6	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	7	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	7	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	7	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	9	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	9	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	9	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	15	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	15	0.43
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	15	0.43
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	14	0.43
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	14	0.43
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	14	0.43
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	11	0.43
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	9	0.43
(1,314)	1:39:A:ASN:HB3	1:39:A:ASN:HD22	6	0.43
(1,314)	1:39:A:ASN:HB2	1:39:A:ASN:HD22	6	0.43
(1,314)	1:39:A:ASN:HB3	1:39:A:ASN:HD22	15	0.43
(1,314)	1:39:A:ASN:HB2	1:39:A:ASN:HD22	15	0.43
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	1	0.43
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	4	0.43
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	4	0.43
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	4	0.43
(1,219)	1:30:A:LYS:HA	1:32:A:LYS:H	1	0.43
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	12	0.43
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	13	0.43
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	3	0.43
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	4	0.43
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	15	0.43
(1,84)	1:34:A:ASN:HA	1:37:A:LYS:H	7	0.43
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	7	0.42
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	7	0.42
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	7	0.42
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	6	0.42
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	6	0.42
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	6	0.42
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	6	0.42
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	6	0.42
(1,435)	1:41:A:THR:H	1:41:A:THR:HG21	13	0.42
(1,435)	1:41:A:THR:H	1:41:A:THR:HG22	13	0.42
(1,435)	1:41:A:THR:H	1:41:A:THR:HG23	13	0.42
(1,428)	1:28:A:ALA:HB1	1:29:A:GLN:H	11	0.42
(1,428)	1:28:A:ALA:HB2	1:29:A:GLN:H	11	0.42
(1,428)	1:28:A:ALA:HB3	1:29:A:GLN:H	11	0.42
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	1	0.42
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	1	0.42
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	1	0.42
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG21	4	0.42
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG22	4	0.42
(1,422)	1:17:A:ILE:H	1:17:A:ILE:HG23	4	0.42
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	15	0.42
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	15	0.42
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	15	0.42
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	1	0.42
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	1	0.42
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	1	0.42
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	7	0.42
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	7	0.42
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	2	0.42
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	5	0.42
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	7	0.42
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	5	0.42
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	6	0.42
(1,218)	1:29:A:GLN:HA	1:31:A:GLY:H	12	0.42
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	5	0.42
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	6	0.42
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	7	0.42
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	11	0.42
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	1	0.42
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	13	0.42
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	5	0.42
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	6	0.42
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	1	0.42
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	5	0.42
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	5	0.42
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	11	0.42
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	13	0.42
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	13	0.42
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	14	0.42
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	14	0.42
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	15	0.42
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	15	0.42
(1,119)	1:11:A:SER:HA	1:14:A:MET:H	12	0.42
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	11	0.42
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	13	0.42
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	12	0.42
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	5	0.41
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	5	0.41
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	5	0.41
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	2	0.41
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	2	0.41
(1,435)	1:41:A:THR:H	1:41:A:THR:HG21	10	0.41
(1,435)	1:41:A:THR:H	1:41:A:THR:HG22	10	0.41
(1,435)	1:41:A:THR:H	1:41:A:THR:HG23	10	0.41
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	8	0.41
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	8	0.41
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	8	0.41
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	6	0.41
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	6	0.41
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	6	0.41
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	15	0.41
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	15	0.41
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	15	0.41
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	9	0.41
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	14	0.41
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	15	0.41
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	15	0.41
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	9	0.41
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	9	0.41
(1,234)	1:14:A:MET:H	1:14:A:MET:HG2	4	0.41
(1,234)	1:14:A:MET:H	1:14:A:MET:HG3	4	0.41
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	8	0.41
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	9	0.41
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	9	0.41
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	13	0.41
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	7	0.41
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	14	0.41
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	5	0.41
(1,148)	1:20:A:GLN:HB2	1:21:A:ASP:H	7	0.41
(1,148)	1:20:A:GLN:HB3	1:21:A:ASP:H	7	0.41
(1,140)	1:41:A:THR:H	1:41:A:THR:HB	1	0.41
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	9	0.41
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	9	0.41
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	12	0.41
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	1	0.4
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	1	0.4
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	1	0.4
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	15	0.4
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	15	0.4
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	7	0.4
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	7	0.4
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	7	0.4
(1,435)	1:41:A:THR:H	1:41:A:THR:HG21	6	0.4
(1,435)	1:41:A:THR:H	1:41:A:THR:HG22	6	0.4
(1,435)	1:41:A:THR:H	1:41:A:THR:HG23	6	0.4
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	2	0.4
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	2	0.4
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	2	0.4
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	4	0.4
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	4	0.4
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	4	0.4
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	11	0.4
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	11	0.4
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	11	0.4
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	9	0.4
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	9	0.4
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	9	0.4
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	10	0.4
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	10	0.4
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	10	0.4
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	14	0.4
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	14	0.4
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	14	0.4
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	14	0.4
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	4	0.4
(1,254)	1:33:A:LYS:HG2	1:34:A:ASN:H	2	0.4
(1,254)	1:33:A:LYS:HG3	1:34:A:ASN:H	2	0.4
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	11	0.4
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	12	0.4
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	11	0.4
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	4	0.4
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	13	0.4
(1,198)	1:11:A:SER:H	1:12:A:ILE:H	13	0.4
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	4	0.4
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	11	0.4
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	9	0.4
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	3	0.4
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	13	0.4
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	11	0.4
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	4	0.4
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	2	0.4
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	2	0.4
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	2	0.4
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	5	0.4
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	1	0.4
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	2	0.39
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	2	0.39
(1,435)	1:41:A:THR:H	1:41:A:THR:HG21	4	0.39
(1,435)	1:41:A:THR:H	1:41:A:THR:HG22	4	0.39
(1,435)	1:41:A:THR:H	1:41:A:THR:HG23	4	0.39
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	10	0.39
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	10	0.39
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	10	0.39
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG21	1	0.39
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG22	1	0.39
(1,412)	1:7:A:ILE:H	1:7:A:ILE:HG23	1	0.39
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	5	0.39
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	5	0.39
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	5	0.39
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	14	0.39
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	14	0.39
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	14	0.39
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	10	0.39
(1,325)	1:14:A:MET:HB2	1:18:A:HIS:HD2	2	0.39
(1,325)	1:14:A:MET:HB3	1:18:A:HIS:HD2	2	0.39
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	1	0.39
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	1	0.39
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	10	0.39
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	10	0.39
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	12	0.39
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	14	0.39
(1,219)	1:30:A:LYS:HA	1:32:A:LYS:H	12	0.39
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	9	0.39
(1,203)	1:11:A:SER:H	1:12:A:ILE:HB	7	0.39
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	14	0.39
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	10	0.39
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	10	0.39
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	15	0.39
(1,82)	1:33:A:LYS:HA	1:35:A:ASP:H	4	0.39
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	10	0.39
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	15	0.39
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	15	0.39
(2,8)	1:1:A:TYR:HD1	1:4:A:GLY:HA2	13	0.38
(2,8)	1:1:A:TYR:HD2	1:4:A:GLY:HA2	13	0.38
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	4	0.38
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	4	0.38
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	4	0.38
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	14	0.38
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	14	0.38
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	14	0.38
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	6	0.38
(1,256)	1:32:A:LYS:HG2	1:33:A:LYS:H	15	0.38
(1,256)	1:32:A:LYS:HG3	1:33:A:LYS:H	15	0.38
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	12	0.38
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	12	0.38
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	14	0.38
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	5	0.38
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	9	0.38
(1,198)	1:11:A:SER:H	1:12:A:ILE:H	11	0.38
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	12	0.38
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	9	0.38
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	4	0.38
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	2	0.38
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	6	0.38
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	4	0.38
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	8	0.38
(2,20)	1:6:A:PHE:HD1	1:10:A:TYR:HD1	8	0.37
(2,20)	1:6:A:PHE:HD1	1:10:A:TYR:HD2	8	0.37
(2,20)	1:6:A:PHE:HD2	1:10:A:TYR:HD1	8	0.37
(2,20)	1:6:A:PHE:HD2	1:10:A:TYR:HD2	8	0.37
(1,428)	1:28:A:ALA:HB1	1:29:A:GLN:H	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:28:A:ALA:HB2	1:29:A:GLN:H	3	0.37
(1,428)	1:28:A:ALA:HB3	1:29:A:GLN:H	3	0.37
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	10	0.37
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	10	0.37
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	10	0.37
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	12	0.37
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG2	8	0.37
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG3	8	0.37
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	10	0.37
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	10	0.37
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	4	0.37
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	4	0.37
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	10	0.37
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	10	0.37
(1,239)	1:16:A:LYS:HG2	1:17:A:ILE:H	6	0.37
(1,239)	1:16:A:LYS:HG3	1:17:A:ILE:H	6	0.37
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	13	0.37
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	13	0.37
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	9	0.37
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	9	0.37
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	4	0.37
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	15	0.37
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	8	0.37
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	12	0.37
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	11	0.37
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	11	0.37
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	13	0.37
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	15	0.37
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	10	0.37
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	7	0.37
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	7	0.37
(1,53)	1:32:A:LYS:HB2	1:33:A:LYS:H	4	0.37
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	3	0.37
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	6	0.37
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	13	0.37
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	15	0.37
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	7	0.36
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	7	0.36
(1,435)	1:41:A:THR:H	1:41:A:THR:HG21	14	0.36
(1,435)	1:41:A:THR:H	1:41:A:THR:HG22	14	0.36
(1,435)	1:41:A:THR:H	1:41:A:THR:HG23	14	0.36
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	14	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	14	0.36
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	14	0.36
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	6	0.36
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	6	0.36
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	6	0.36
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	15	0.36
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	15	0.36
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	15	0.36
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	8	0.36
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	8	0.36
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	8	0.36
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	4	0.36
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG2	1	0.36
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG3	1	0.36
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG2	9	0.36
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG3	9	0.36
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	11	0.36
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	11	0.36
(1,213)	1:8:A:SER:H	1:10:A:TYR:H	1	0.36
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	5	0.36
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	14	0.36
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	9	0.36
(1,66)	1:35:A:ASP:HA	1:36:A:TRP:H	13	0.36
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	2	0.36
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	7	0.36
(1,1)	1:2:A:ALA:HA	1:3:A:GLU:H	7	0.36
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	3	0.35
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	3	0.35
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	3	0.35
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	3	0.35
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	3	0.35
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	3	0.35
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	7	0.35
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	7	0.35
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	7	0.35
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	11	0.35
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	11	0.35
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	11	0.35
(1,421)	1:14:A:MET:HE1	1:15:A:ASP:H	6	0.35
(1,421)	1:14:A:MET:HE2	1:15:A:ASP:H	6	0.35
(1,421)	1:14:A:MET:HE3	1:15:A:ASP:H	6	0.35
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	5	0.35
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	1	0.35
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	1	0.35
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	3	0.35
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	10	0.35
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	15	0.35
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	7	0.35
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG2	11	0.35
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG3	11	0.35
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG2	14	0.35
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG3	14	0.35
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG2	15	0.35
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG3	15	0.35
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	3	0.35
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	3	0.35
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	2	0.35
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	13	0.35
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	4	0.35
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	6	0.35
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	5	0.35
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	10	0.35
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	4	0.35
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	7	0.35
(1,134)	1:22:A:PHE:HB2	1:23:A:VAL:H	6	0.35
(1,134)	1:22:A:PHE:HB3	1:23:A:VAL:H	6	0.35
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	14	0.35
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	5	0.35
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	5	0.35
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	12	0.35
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	12	0.35
(1,1)	1:2:A:ALA:HA	1:3:A:GLU:H	2	0.35
(1,1)	1:2:A:ALA:HA	1:3:A:GLU:H	12	0.35
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD11	15	0.34
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD12	15	0.34
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD13	15	0.34
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	6	0.34
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	6	0.34
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	6	0.34
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	2	0.34
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	6	0.34
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	7	0.34
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	9	0.34
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	10	0.34
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	13	0.34
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	14	0.34
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	15	0.34
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	1	0.34
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	7	0.34
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	11	0.34
(1,318)	1:25:A:TRP:HD1	1:26:A:LEU:HG	10	0.34
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG2	12	0.34
(1,269)	1:20:A:GLN:H	1:20:A:GLN:HG3	12	0.34
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	3	0.34
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	3	0.34
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	8	0.34
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	8	0.34
(1,239)	1:16:A:LYS:HG2	1:17:A:ILE:H	1	0.34
(1,239)	1:16:A:LYS:HG3	1:17:A:ILE:H	1	0.34
(1,239)	1:16:A:LYS:HG2	1:17:A:ILE:H	2	0.34
(1,239)	1:16:A:LYS:HG3	1:17:A:ILE:H	2	0.34
(1,239)	1:16:A:LYS:HG2	1:17:A:ILE:H	14	0.34
(1,239)	1:16:A:LYS:HG3	1:17:A:ILE:H	14	0.34
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	15	0.34
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	15	0.34
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	10	0.34
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	15	0.34
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	15	0.34
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	13	0.34
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	1	0.34
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	11	0.34
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	12	0.34
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	15	0.34
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	10	0.34
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	8	0.34
(1,108)	1:3:A:GLU:HA	1:6:A:PHE:H	5	0.34
(1,84)	1:34:A:ASN:HA	1:37:A:LYS:H	2	0.34
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	6	0.34
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	6	0.34
(1,1)	1:2:A:ALA:HA	1:3:A:GLU:H	3	0.34
(1,1)	1:2:A:ALA:HA	1:3:A:GLU:H	11	0.34
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD21	14	0.33
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD22	14	0.33
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD23	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	14	0.33
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD22	14	0.33
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD23	14	0.33
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	14	0.33
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD22	14	0.33
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD23	14	0.33
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD11	14	0.33
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD12	14	0.33
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD13	14	0.33
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD11	14	0.33
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD12	14	0.33
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD13	14	0.33
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD11	14	0.33
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD12	14	0.33
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD13	14	0.33
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	3	0.33
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	3	0.33
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	3	0.33
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG12	13	0.33
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG13	13	0.33
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG12	13	0.33
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG13	13	0.33
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE22	4	0.33
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE21	4	0.33
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	3	0.33
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	11	0.33
(1,381)	1:25:A:TRP:HZ2	1:25:A:TRP:HE1	12	0.33
(1,254)	1:33:A:LYS:HG2	1:34:A:ASN:H	9	0.33
(1,254)	1:33:A:LYS:HG3	1:34:A:ASN:H	9	0.33
(1,251)	1:40:A:ILE:H	1:40:A:ILE:HG12	3	0.33
(1,251)	1:40:A:ILE:H	1:40:A:ILE:HG13	3	0.33
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	9	0.33
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	9	0.33
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	1	0.33
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	1	0.33
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	8	0.33
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	8	0.33
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	15	0.33
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	15	0.33
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	7	0.33
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	7	0.33
(1,202)	1:24:A:ASN:H	1:25:A:TRP:H	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	1	0.33
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	11	0.33
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	8	0.33
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	10	0.33
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	9	0.33
(1,115)	1:13:A:ALA:HA	1:14:A:MET:H	3	0.33
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	9	0.33
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	13	0.33
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	8	0.33
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	13	0.33
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	13	0.33
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	4	0.33
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	4	0.33
(1,1)	1:2:A:ALA:HA	1:3:A:GLU:H	13	0.33
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	2	0.32
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	2	0.32
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	2	0.32
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD21	11	0.32
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD22	11	0.32
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD23	11	0.32
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD11	11	0.32
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD12	11	0.32
(1,442)	1:25:A:TRP:HD1	1:26:A:LEU:HD13	11	0.32
(1,428)	1:28:A:ALA:HB1	1:29:A:GLN:H	15	0.32
(1,428)	1:28:A:ALA:HB2	1:29:A:GLN:H	15	0.32
(1,428)	1:28:A:ALA:HB3	1:29:A:GLN:H	15	0.32
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	1	0.32
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	1	0.32
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	1	0.32
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	7	0.32
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	7	0.32
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	7	0.32
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB2	9	0.32
(1,389)	1:19:A:GLN:HG2	1:20:A:GLN:HB3	9	0.32
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB2	9	0.32
(1,389)	1:19:A:GLN:HG3	1:20:A:GLN:HB3	9	0.32
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	9	0.32
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	9	0.32
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	8	0.32
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	3	0.32
(1,317)	1:6:A:PHE:HD1	1:7:A:ILE:HG13	1	0.32
(1,317)	1:6:A:PHE:HD2	1:7:A:ILE:HG13	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	2	0.32
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	8	0.32
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	2	0.32
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	2	0.32
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	8	0.32
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	8	0.32
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	13	0.32
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	13	0.32
(1,234)	1:14:A:MET:H	1:14:A:MET:HG2	11	0.32
(1,234)	1:14:A:MET:H	1:14:A:MET:HG3	11	0.32
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	11	0.32
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	3	0.32
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	2	0.32
(1,189)	1:32:A:LYS:H	1:33:A:LYS:H	13	0.32
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	12	0.32
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	13	0.32
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	5	0.32
(1,176)	1:35:A:ASP:H	1:36:A:TRP:H	2	0.32
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	14	0.32
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	11	0.32
(1,80)	1:16:A:LYS:HA	1:19:A:GLN:H	2	0.32
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	10	0.32
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	10	0.32
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	11	0.32
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	11	0.32
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	7	0.32
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	7	0.32
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	4	0.31
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	4	0.31
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB2	12	0.31
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB3	12	0.31
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB2	12	0.31
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB3	12	0.31
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB1	4	0.31
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB2	4	0.31
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB3	4	0.31
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	8	0.31
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	8	0.31
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	8	0.31
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	3	0.31
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	3	0.31
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	4	0.31
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	4	0.31
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	4	0.31
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	11	0.31
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	11	0.31
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	11	0.31
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG12	1	0.31
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG13	1	0.31
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG12	1	0.31
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG13	1	0.31
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	1	0.31
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	11	0.31
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	12	0.31
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	1	0.31
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	7	0.31
(1,251)	1:40:A:ILE:H	1:40:A:ILE:HG12	1	0.31
(1,251)	1:40:A:ILE:H	1:40:A:ILE:HG13	1	0.31
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	11	0.31
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	11	0.31
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	5	0.31
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	14	0.31
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	6	0.31
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	12	0.31
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	5	0.31
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	8	0.31
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	10	0.31
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	14	0.31
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	1	0.31
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	1	0.31
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	6	0.31
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	12	0.31
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	11	0.31
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	11	0.31
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	14	0.31
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	14	0.31
(1,480)	1:7:A:ILE:HG21	1:9:A:ASP:H	8	0.3
(1,480)	1:7:A:ILE:HG22	1:9:A:ASP:H	8	0.3
(1,480)	1:7:A:ILE:HG23	1:9:A:ASP:H	8	0.3
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	9	0.3
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	9	0.3
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	9	0.3
(1,437)	1:17:A:ILE:HG21	1:18:A:HIS:H	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:17:A:ILE:HG22	1:18:A:HIS:H	10	0.3
(1,437)	1:17:A:ILE:HG23	1:18:A:HIS:H	10	0.3
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	6	0.3
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	12	0.3
(1,341)	1:25:A:TRP:HE3	1:26:A:LEU:H	3	0.3
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	9	0.3
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	1	0.3
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	1	0.3
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	4	0.3
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	4	0.3
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG2	5	0.3
(1,236)	1:16:A:LYS:H	1:16:A:LYS:HG3	5	0.3
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	9	0.3
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	11	0.3
(1,216)	1:37:A:LYS:H	1:39:A:ASN:H	3	0.3
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	7	0.3
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	3	0.3
(1,179)	1:25:A:TRP:H	1:26:A:LEU:H	13	0.3
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	8	0.3
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	3	0.3
(1,173)	1:39:A:ASN:H	1:40:A:ILE:H	10	0.3
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	6	0.3
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	9	0.3
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	10	0.3
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	14	0.3
(1,115)	1:13:A:ALA:HA	1:14:A:MET:H	6	0.3
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	3	0.3
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	4	0.3
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	5	0.3
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	9	0.3
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	13	0.3
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	14	0.3
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	15	0.3
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	10	0.3
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	6	0.3
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	6	0.3
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	14	0.3
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	14	0.3
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD11	9	0.29
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD12	9	0.29
(2,28)	1:6:A:PHE:HE1	1:7:A:ILE:HD13	9	0.29
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD11	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD12	9	0.29
(2,28)	1:6:A:PHE:HE2	1:7:A:ILE:HD13	9	0.29
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	4	0.29
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	4	0.29
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	7	0.29
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	7	0.29
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	7	0.29
(1,254)	1:33:A:LYS:HG2	1:34:A:ASN:H	12	0.29
(1,254)	1:33:A:LYS:HG3	1:34:A:ASN:H	12	0.29
(1,246)	1:33:A:LYS:HD2	1:34:A:ASN:H	6	0.29
(1,246)	1:33:A:LYS:HD3	1:34:A:ASN:H	6	0.29
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	9	0.29
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	8	0.29
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	6	0.29
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	6	0.29
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	8	0.29
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	14	0.29
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	13	0.29
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	14	0.29
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	15	0.29
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	4	0.29
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	8	0.29
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	11	0.29
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	12	0.29
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	12	0.29
(1,146)	1:19:A:GLN:HB2	1:20:A:GLN:H	7	0.29
(1,146)	1:19:A:GLN:HB3	1:20:A:GLN:H	7	0.29
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	4	0.29
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	7	0.29
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	15	0.29
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	2	0.29
(1,28)	1:20:A:GLN:HA	1:21:A:ASP:H	7	0.29
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD11	9	0.28
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD12	9	0.28
(2,36)	1:10:A:TYR:HD1	1:12:A:ILE:HD13	9	0.28
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD11	9	0.28
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD12	9	0.28
(2,36)	1:10:A:TYR:HD2	1:12:A:ILE:HD13	9	0.28
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	1	0.28
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	1	0.28
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	11	0.28
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	11	0.28
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB1	4	0.28
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB2	4	0.28
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB3	4	0.28
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB1	4	0.28
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB2	4	0.28
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB3	4	0.28
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB1	4	0.28
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB2	4	0.28
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB3	4	0.28
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	5	0.28
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	5	0.28
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	5	0.28
(1,411)	1:5:A:THR:HG21	1:6:A:PHE:H	14	0.28
(1,411)	1:5:A:THR:HG22	1:6:A:PHE:H	14	0.28
(1,411)	1:5:A:THR:HG23	1:6:A:PHE:H	14	0.28
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE22	6	0.28
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE21	6	0.28
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	11	0.28
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	12	0.28
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	12	0.28
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	13	0.28
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	13	0.28
(1,230)	1:15:A:ASP:HA	1:18:A:HIS:H	7	0.28
(1,218)	1:29:A:GLN:HA	1:31:A:GLY:H	10	0.28
(1,216)	1:37:A:LYS:H	1:39:A:ASN:H	6	0.28
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	5	0.28
(1,198)	1:11:A:SER:H	1:12:A:ILE:H	4	0.28
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	13	0.28
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	2	0.28
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	12	0.28
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	2	0.28
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	5	0.28
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	2	0.28
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	8	0.28
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	10	0.28
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	8	0.28
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	8	0.28
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	8	0.28
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	9	0.28
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	6	0.28
(1,115)	1:13:A:ALA:HA	1:14:A:MET:H	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:13:A:ALA:HA	1:14:A:MET:H	5	0.28
(1,115)	1:13:A:ALA:HA	1:14:A:MET:H	15	0.28
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	5	0.28
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	12	0.28
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	12	0.28
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	12	0.28
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	15	0.28
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	15	0.28
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB1	2	0.27
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB2	2	0.27
(2,34)	1:25:A:TRP:HE3	1:28:A:ALA:HB3	2	0.27
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD21	10	0.27
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD22	10	0.27
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD23	10	0.27
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	10	0.27
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD22	10	0.27
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD23	10	0.27
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	10	0.27
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD22	10	0.27
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD23	10	0.27
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD11	10	0.27
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD12	10	0.27
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD13	10	0.27
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD11	10	0.27
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD12	10	0.27
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD13	10	0.27
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD11	10	0.27
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD12	10	0.27
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD13	10	0.27
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	5	0.27
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	5	0.27
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	5	0.27
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	2	0.27
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	15	0.27
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	3	0.27
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	3	0.27
(1,311)	1:10:A:TYR:HD1	1:11:A:SER:HB2	9	0.27
(1,311)	1:10:A:TYR:HD2	1:11:A:SER:HB2	9	0.27
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG2	6	0.27
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG3	6	0.27
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	5	0.27
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	6	0.27
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	6	0.27
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	9	0.27
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	9	0.27
(1,230)	1:15:A:ASP:HA	1:18:A:HIS:H	3	0.27
(1,224)	1:38:A:HIS:HA	1:42:A:GLN:H	8	0.27
(1,203)	1:11:A:SER:H	1:12:A:ILE:HB	13	0.27
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	1	0.27
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	7	0.27
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	5	0.27
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	12	0.27
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	4	0.27
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	7	0.27
(1,51)	1:30:A:LYS:HB2	1:31:A:GLY:H	15	0.27
(1,51)	1:30:A:LYS:HB3	1:31:A:GLY:H	15	0.27
(1,47)	1:30:A:LYS:HA	1:31:A:GLY:H	9	0.27
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	13	0.27
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	3	0.27
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	3	0.27
(1,437)	1:17:A:ILE:HG21	1:18:A:HIS:H	8	0.26
(1,437)	1:17:A:ILE:HG22	1:18:A:HIS:H	8	0.26
(1,437)	1:17:A:ILE:HG23	1:18:A:HIS:H	8	0.26
(1,437)	1:17:A:ILE:HG21	1:18:A:HIS:H	14	0.26
(1,437)	1:17:A:ILE:HG22	1:18:A:HIS:H	14	0.26
(1,437)	1:17:A:ILE:HG23	1:18:A:HIS:H	14	0.26
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	9	0.26
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	9	0.26
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	9	0.26
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	10	0.26
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD3	10	0.26
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE22	13	0.26
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE21	13	0.26
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	12	0.26
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	1	0.26
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	1	0.26
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	11	0.26
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	11	0.26
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	14	0.26
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	14	0.26
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	5	0.26
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	5	0.26
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	1	0.26
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	4	0.26
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	1	0.26
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	2	0.26
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	13	0.26
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	2	0.26
(1,172)	1:4:A:GLY:H	1:6:A:PHE:H	9	0.26
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	3	0.26
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	13	0.26
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	6	0.26
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	7	0.26
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	15	0.26
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	15	0.26
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	15	0.26
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	15	0.26
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	3	0.26
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	7	0.26
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	9	0.26
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	1	0.26
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	10	0.26
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	11	0.26
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	12	0.26
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	13	0.26
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	14	0.26
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	13	0.26
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	13	0.26
(2,26)	1:6:A:PHE:HD1	1:7:A:ILE:HG21	1	0.25
(2,26)	1:6:A:PHE:HD1	1:7:A:ILE:HG22	1	0.25
(2,26)	1:6:A:PHE:HD1	1:7:A:ILE:HG23	1	0.25
(2,26)	1:6:A:PHE:HD2	1:7:A:ILE:HG21	1	0.25
(2,26)	1:6:A:PHE:HD2	1:7:A:ILE:HG22	1	0.25
(2,26)	1:6:A:PHE:HD2	1:7:A:ILE:HG23	1	0.25
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB2	7	0.25
(2,9)	1:10:A:TYR:HD1	1:14:A:MET:HB3	7	0.25
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB2	7	0.25
(2,9)	1:10:A:TYR:HD2	1:14:A:MET:HB3	7	0.25
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	6	0.25
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	6	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	11	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	11	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	11	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	11	0.25
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	11	0.25
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB1	7	0.25
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB2	7	0.25
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB3	7	0.25
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB1	7	0.25
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB2	7	0.25
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB3	7	0.25
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB1	7	0.25
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB2	7	0.25
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB3	7	0.25
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD11	10	0.25
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD12	10	0.25
(1,443)	1:25:A:TRP:HE3	1:26:A:LEU:HD13	10	0.25
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	10	0.25
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	10	0.25
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	10	0.25
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	3	0.25
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	3	0.25
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG2	2	0.25
(1,240)	1:19:A:GLN:H	1:19:A:GLN:HG3	2	0.25
(1,234)	1:14:A:MET:H	1:14:A:MET:HG2	2	0.25
(1,234)	1:14:A:MET:H	1:14:A:MET:HG3	2	0.25
(1,230)	1:15:A:ASP:HA	1:18:A:HIS:H	12	0.25
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	14	0.25
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	6	0.25
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	7	0.25
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	7	0.25
(1,209)	1:8:A:SER:HB3	1:10:A:TYR:H	10	0.25
(1,209)	1:8:A:SER:HB2	1:10:A:TYR:H	10	0.25
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	9	0.25
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	5	0.25
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	10	0.25
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	15	0.25
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	14	0.25
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	10	0.25
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	1	0.25
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	5	0.25
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	13	0.25
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	6	0.25
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	8	0.25
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	14	0.25
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	2	0.25
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	13	0.25
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	2	0.25
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	3	0.25
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	5	0.25
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	11	0.25
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	13	0.25
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	9	0.25
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	9	0.25
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	2	0.25
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	4	0.25
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	7	0.25
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	15	0.25
(2,11)	1:10:A:TYR:HD1	1:14:A:MET:HG2	7	0.24
(2,11)	1:10:A:TYR:HD1	1:14:A:MET:HG3	7	0.24
(2,11)	1:10:A:TYR:HD2	1:14:A:MET:HG2	7	0.24
(2,11)	1:10:A:TYR:HD2	1:14:A:MET:HG3	7	0.24
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	1	0.24
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	1	0.24
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	1	0.24
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	1	0.24
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	1	0.24
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	1	0.24
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD11	2	0.24
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD12	2	0.24
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD13	2	0.24
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	13	0.24
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	13	0.24
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	13	0.24
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	12	0.24
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	12	0.24
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	12	0.24
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	7	0.24
(1,328)	1:34:A:ASN:HD22	1:38:A:HIS:HB2	13	0.24
(1,265)	1:26:A:LEU:HG	1:29:A:GLN:H	10	0.24
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD2	2	0.24
(1,244)	1:32:A:LYS:H	1:32:A:LYS:HD3	2	0.24
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	4	0.24
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	4	0.24
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	7	0.24
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	1:11:A:SER:H	1:12:A:ILE:HB	14	0.24
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	5	0.24
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	9	0.24
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	9	0.24
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	8	0.24
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	5	0.24
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	1	0.24
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	5	0.24
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	2	0.24
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	14	0.24
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	7	0.24
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	12	0.24
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	8	0.24
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	1	0.24
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	14	0.24
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	8	0.24
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	8	0.24
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	8	0.24
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	6	0.24
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	8	0.24
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	9	0.24
(1,7)	1:6:A:PHE:HB2	1:7:A:ILE:H	2	0.24
(1,7)	1:6:A:PHE:HB3	1:7:A:ILE:H	2	0.24
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	9	0.23
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	9	0.23
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	2	0.23
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	2	0.23
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	2	0.23
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	13	0.23
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	13	0.23
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	13	0.23
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE22	9	0.23
(1,385)	1:25:A:TRP:HE1	1:29:A:GLN:HE21	9	0.23
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	2	0.23
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	6	0.23
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG2	3	0.23
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG3	3	0.23
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	3	0.23
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	3	0.23
(1,228)	1:5:A:THR:H	1:5:A:THR:HA	1	0.23
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	1	0.23
(1,200)	1:14:A:MET:H	1:15:A:ASP:H	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	4	0.23
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	14	0.23
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	1	0.23
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	12	0.23
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	7	0.23
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	7	0.23
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	8	0.23
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	5	0.23
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	7	0.23
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	12	0.23
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	1	0.23
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	3	0.23
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	6	0.23
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	5	0.23
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	3	0.23
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	4	0.23
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	5	0.23
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	14	0.23
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	6	0.23
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	4	0.23
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	6	0.23
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	10	0.23
(1,17)	1:15:A:ASP:H	1:15:A:ASP:HB3	5	0.23
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	5	0.23
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB1	3	0.22
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB2	3	0.22
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB3	3	0.22
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	5	0.22
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	5	0.22
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	5	0.22
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	6	0.22
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	6	0.22
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	6	0.22
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	15	0.22
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	15	0.22
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	15	0.22
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE21	8	0.22
(1,378)	1:25:A:TRP:HD1	1:29:A:GLN:HE22	8	0.22
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	14	0.22
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	9	0.22
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	10	0.22
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	13	0.22
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG2	5	0.22
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG3	5	0.22
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	10	0.22
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	10	0.22
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	3	0.22
(1,180)	1:33:A:LYS:H	1:34:A:ASN:H	15	0.22
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	9	0.22
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	15	0.22
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	2	0.22
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	3	0.22
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	6	0.22
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	2	0.22
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	7	0.22
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	4	0.22
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	4	0.22
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	8	0.22
(1,19)	1:14:A:MET:HB2	1:15:A:ASP:H	7	0.22
(1,19)	1:14:A:MET:HB3	1:15:A:ASP:H	7	0.22
(1,17)	1:15:A:ASP:H	1:15:A:ASP:HB3	14	0.22
(1,10)	1:12:A:ILE:HA	1:13:A:ALA:H	3	0.22
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	13	0.21
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	13	0.21
(2,5)	1:10:A:TYR:HD1	1:12:A:ILE:HA	9	0.21
(2,5)	1:10:A:TYR:HD2	1:12:A:ILE:HA	9	0.21
(1,434)	1:13:A:ALA:HB1	1:14:A:MET:H	9	0.21
(1,434)	1:13:A:ALA:HB2	1:14:A:MET:H	9	0.21
(1,434)	1:13:A:ALA:HB3	1:14:A:MET:H	9	0.21
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	8	0.21
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	7	0.21
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	7	0.21
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	1	0.21
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	1	0.21
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	3	0.21
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	9	0.21
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	8	0.21
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	10	0.21
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	2	0.21
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	11	0.21
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	13	0.21
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	13	0.21
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	2	0.21
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	3	0.21
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	7	0.21
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	9	0.21
(1,111)	1:32:A:LYS:HA	1:34:A:ASN:H	15	0.21
(1,110)	1:5:A:THR:HB	1:6:A:PHE:H	9	0.21
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	8	0.21
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	3	0.21
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	15	0.21
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	14	0.21
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	2	0.21
(1,17)	1:15:A:ASP:H	1:15:A:ASP:HB3	7	0.21
(1,17)	1:15:A:ASP:H	1:15:A:ASP:HB3	8	0.21
(1,17)	1:15:A:ASP:H	1:15:A:ASP:HB3	9	0.21
(1,5)	1:8:A:SER:H	1:8:A:SER:HB2	9	0.21
(1,5)	1:8:A:SER:H	1:8:A:SER:HB3	9	0.21
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG21	14	0.2
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG22	14	0.2
(2,33)	1:1:A:TYR:HD1	1:5:A:THR:HG23	14	0.2
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG21	14	0.2
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG22	14	0.2
(2,33)	1:1:A:TYR:HD2	1:5:A:THR:HG23	14	0.2
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	15	0.2
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	15	0.2
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	15	0.2
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	15	0.2
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	15	0.2
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	15	0.2
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD11	7	0.2
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD12	7	0.2
(1,436)	1:40:A:ILE:H	1:40:A:ILE:HD13	7	0.2
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	1	0.2
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	1	0.2
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	1	0.2
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	2	0.2
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	2	0.2
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	2	0.2
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD11	8	0.2
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD12	8	0.2
(1,413)	1:7:A:ILE:H	1:7:A:ILE:HD13	8	0.2
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	10	0.2
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	13	0.2
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	6	0.2
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	6	0.2
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	7	0.2
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	7	0.2
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	13	0.2
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	13	0.2
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	15	0.2
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	15	0.2
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	12	0.2
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	12	0.2
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	7	0.2
(1,217)	1:1:A:TYR:HA	1:3:A:GLU:H	1	0.2
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	6	0.2
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	6	0.2
(1,186)	1:35:A:ASP:H	1:37:A:LYS:H	10	0.2
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	14	0.2
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	15	0.2
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	9	0.2
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	10	0.2
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	9	0.2
(1,136)	1:5:A:THR:HA	1:8:A:SER:H	1	0.2
(1,119)	1:11:A:SER:HA	1:14:A:MET:H	10	0.2
(1,108)	1:3:A:GLU:HA	1:6:A:PHE:H	4	0.2
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	13	0.2
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	1	0.2
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	6	0.2
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	9	0.2
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	11	0.2
(2,18)	1:6:A:PHE:HD1	1:10:A:TYR:HE1	8	0.19
(2,18)	1:6:A:PHE:HD1	1:10:A:TYR:HE2	8	0.19
(2,18)	1:6:A:PHE:HD2	1:10:A:TYR:HE1	8	0.19
(2,18)	1:6:A:PHE:HD2	1:10:A:TYR:HE2	8	0.19
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG2	3	0.19
(2,12)	1:10:A:TYR:HE1	1:14:A:MET:HG3	3	0.19
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG2	3	0.19
(2,12)	1:10:A:TYR:HE2	1:14:A:MET:HG3	3	0.19
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD21	8	0.19
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD22	8	0.19
(1,477)	1:22:A:PHE:H	1:26:A:LEU:HD23	8	0.19
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	8	0.19
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	8	0.19
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	9	0.19
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	9	0.19
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	9	0.19
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	7	0.19
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	7	0.19
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	8	0.19
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	8	0.19
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	5	0.19
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	9	0.19
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	11	0.19
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	13	0.19
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	14	0.19
(1,346)	1:36:A:TRP:H	1:36:A:TRP:HD1	12	0.19
(1,334)	1:14:A:MET:HA	1:18:A:HIS:HD2	15	0.19
(1,272)	1:11:A:SER:H	1:12:A:ILE:HG12	7	0.19
(1,260)	1:30:A:LYS:HD2	1:34:A:ASN:H	3	0.19
(1,260)	1:30:A:LYS:HD3	1:34:A:ASN:H	3	0.19
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG2	4	0.19
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG3	4	0.19
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG2	14	0.19
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG3	14	0.19
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD2	12	0.19
(1,245)	1:33:A:LYS:H	1:33:A:LYS:HD3	12	0.19
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	4	0.19
(1,198)	1:11:A:SER:H	1:12:A:ILE:H	1	0.19
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	7	0.19
(1,191)	1:16:A:LYS:H	1:17:A:ILE:H	6	0.19
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	6	0.19
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	10	0.19
(1,166)	1:10:A:TYR:HB2	1:11:A:SER:H	11	0.19
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	2	0.19
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	12	0.19
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	8	0.19
(1,84)	1:34:A:ASN:HA	1:37:A:LYS:H	12	0.19
(1,80)	1:16:A:LYS:HA	1:19:A:GLN:H	3	0.19
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	7	0.19
(1,36)	1:21:A:ASP:HB2	1:22:A:PHE:H	6	0.19
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	12	0.18
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	12	0.18
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	12	0.18
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	12	0.18
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	12	0.18
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB1	14	0.18
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB2	14	0.18
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB3	14	0.18
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB1	14	0.18
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB2	14	0.18
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB3	14	0.18
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB1	14	0.18
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB2	14	0.18
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB3	14	0.18
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG12	10	0.18
(1,397)	1:16:A:LYS:HG2	1:17:A:ILE:HG13	10	0.18
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG12	10	0.18
(1,397)	1:16:A:LYS:HG3	1:17:A:ILE:HG13	10	0.18
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	5	0.18
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	5	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	1	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	3	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	4	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	6	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	7	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	8	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	10	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	12	0.18
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	15	0.18
(1,346)	1:36:A:TRP:H	1:36:A:TRP:HD1	1	0.18
(1,325)	1:14:A:MET:HB2	1:18:A:HIS:HD2	11	0.18
(1,325)	1:14:A:MET:HB3	1:18:A:HIS:HD2	11	0.18
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	3	0.18
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	3	0.18
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	5	0.18
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	5	0.18
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	8	0.18
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	8	0.18
(1,219)	1:30:A:LYS:HA	1:32:A:LYS:H	3	0.18
(1,212)	1:6:A:PHE:HA	1:10:A:TYR:H	9	0.18
(1,206)	1:7:A:ILE:HB	1:9:A:ASP:H	1	0.18
(1,203)	1:11:A:SER:H	1:12:A:ILE:HB	11	0.18
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	4	0.18
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	12	0.18
(1,169)	1:5:A:THR:H	1:6:A:PHE:H	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	11	0.18
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	12	0.18
(1,98)	1:1:A:TYR:HB3	1:2:A:ALA:H	2	0.18
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	10	0.18
(1,84)	1:34:A:ASN:HA	1:37:A:LYS:H	8	0.18
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	12	0.18
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	10	0.18
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	14	0.18
(1,17)	1:15:A:ASP:H	1:15:A:ASP:HB3	10	0.18
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE1	3	0.17
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE2	3	0.17
(2,21)	1:10:A:TYR:HD1	1:14:A:MET:HE3	3	0.17
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE1	3	0.17
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE2	3	0.17
(2,21)	1:10:A:TYR:HD2	1:14:A:MET:HE3	3	0.17
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB2	15	0.17
(2,4)	1:1:A:TYR:HE1	1:6:A:PHE:HB3	15	0.17
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB2	15	0.17
(2,4)	1:1:A:TYR:HE2	1:6:A:PHE:HB3	15	0.17
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB1	2	0.17
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB2	2	0.17
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB3	2	0.17
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB1	2	0.17
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB2	2	0.17
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB3	2	0.17
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB1	2	0.17
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB2	2	0.17
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB3	2	0.17
(1,437)	1:17:A:ILE:HG21	1:18:A:HIS:H	11	0.17
(1,437)	1:17:A:ILE:HG22	1:18:A:HIS:H	11	0.17
(1,437)	1:17:A:ILE:HG23	1:18:A:HIS:H	11	0.17
(1,431)	1:27:A:LEU:HD21	1:28:A:ALA:H	12	0.17
(1,431)	1:27:A:LEU:HD22	1:28:A:ALA:H	12	0.17
(1,431)	1:27:A:LEU:HD23	1:28:A:ALA:H	12	0.17
(1,335)	1:17:A:ILE:HA	1:18:A:HIS:HD2	12	0.17
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	2	0.17
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	2	0.17
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	9	0.17
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	9	0.17
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	2	0.17
(1,175)	1:6:A:PHE:H	1:7:A:ILE:H	9	0.17
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	6	0.17
(1,152)	1:24:A:ASN:H	1:24:A:ASN:HB2	11	0.17
(1,140)	1:41:A:THR:H	1:41:A:THR:HB	4	0.17
(1,110)	1:5:A:THR:HB	1:6:A:PHE:H	3	0.17
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	11	0.17
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	3	0.17
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	6	0.17
(1,66)	1:35:A:ASP:HA	1:36:A:TRP:H	4	0.17
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	2	0.17
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	11	0.17
(1,61)	1:35:A:ASP:H	1:35:A:ASP:HB3	9	0.17
(1,61)	1:35:A:ASP:H	1:35:A:ASP:HB2	9	0.17
(1,41)	1:25:A:TRP:H	1:25:A:TRP:HB3	8	0.17
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG21	13	0.16
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG22	13	0.16
(1,453)	1:14:A:MET:HB2	1:17:A:ILE:HG23	13	0.16
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG21	13	0.16
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG22	13	0.16
(1,453)	1:14:A:MET:HB3	1:17:A:ILE:HG23	13	0.16
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD11	15	0.16
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD12	15	0.16
(1,416)	1:12:A:ILE:H	1:12:A:ILE:HD13	15	0.16
(1,380)	1:36:A:TRP:HZ2	1:36:A:TRP:HE1	2	0.16
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	1	0.16
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	1	0.16
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	6	0.16
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	6	0.16
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	14	0.16
(1,259)	1:30:A:LYS:HD2	1:31:A:GLY:H	1	0.16
(1,259)	1:30:A:LYS:HD3	1:31:A:GLY:H	1	0.16
(1,253)	1:33:A:LYS:H	1:33:A:LYS:HG2	10	0.16
(1,253)	1:33:A:LYS:H	1:33:A:LYS:HG3	10	0.16
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD2	9	0.16
(1,237)	1:16:A:LYS:H	1:16:A:LYS:HD3	9	0.16
(1,215)	1:36:A:TRP:H	1:38:A:HIS:H	7	0.16
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	1	0.16
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	2	0.16
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	8	0.16
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	15	0.16
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	9	0.16
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	2	0.16
(1,166)	1:10:A:TYR:HB2	1:11:A:SER:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:18:A:HIS:H	1:18:A:HIS:HB2	13	0.16
(1,137)	1:38:A:HIS:HA	1:40:A:ILE:H	12	0.16
(1,110)	1:5:A:THR:HB	1:6:A:PHE:H	12	0.16
(1,108)	1:3:A:GLU:HA	1:6:A:PHE:H	14	0.16
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	9	0.16
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	12	0.16
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	2	0.16
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	7	0.16
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	13	0.16
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	1	0.16
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	15	0.16
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	2	0.16
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	12	0.16
(1,36)	1:21:A:ASP:HB2	1:22:A:PHE:H	15	0.16
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	14	0.15
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	14	0.15
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	14	0.15
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	14	0.15
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	14	0.15
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	14	0.15
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB1	1	0.15
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB2	1	0.15
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB3	1	0.15
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB1	1	0.15
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB2	1	0.15
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB3	1	0.15
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB1	1	0.15
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB2	1	0.15
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB3	1	0.15
(1,409)	1:2:A:ALA:HB1	1:3:A:GLU:H	4	0.15
(1,409)	1:2:A:ALA:HB2	1:3:A:GLU:H	4	0.15
(1,409)	1:2:A:ALA:HB3	1:3:A:GLU:H	4	0.15
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	8	0.15
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD3	8	0.15
(1,346)	1:36:A:TRP:H	1:36:A:TRP:HD1	3	0.15
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	11	0.15
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	11	0.15
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	4	0.15
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	4	0.15
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	9	0.15
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	9	0.15
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG2	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG3	13	0.15
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.15
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	0.15
(1,214)	1:23:A:VAL:H	1:25:A:TRP:H	3	0.15
(1,198)	1:11:A:SER:H	1:12:A:ILE:H	6	0.15
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	6	0.15
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	8	0.15
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	4	0.15
(1,183)	1:9:A:ASP:H	1:10:A:TYR:H	6	0.15
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	14	0.15
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	14	0.15
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	1	0.15
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	2	0.15
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	3	0.15
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	5	0.15
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	9	0.15
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	13	0.15
(1,119)	1:11:A:SER:HA	1:14:A:MET:H	15	0.15
(1,115)	1:13:A:ALA:HA	1:14:A:MET:H	14	0.15
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	15	0.15
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	12	0.15
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	5	0.15
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	7	0.15
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	11	0.15
(1,89)	1:32:A:LYS:H	1:32:A:LYS:HB3	6	0.15
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	15	0.15
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	11	0.15
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	9	0.15
(1,45)	1:29:A:GLN:H	1:29:A:GLN:HB2	12	0.15
(1,45)	1:29:A:GLN:H	1:29:A:GLN:HB3	12	0.15
(1,41)	1:25:A:TRP:H	1:25:A:TRP:HB3	13	0.15
(1,41)	1:25:A:TRP:H	1:25:A:TRP:HB3	14	0.15
(1,5)	1:8:A:SER:H	1:8:A:SER:HB2	1	0.15
(1,5)	1:8:A:SER:H	1:8:A:SER:HB3	1	0.15
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	13	0.14
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD3	13	0.14
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	1	0.14
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	1	0.14
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	14	0.14
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	14	0.14
(1,338)	1:36:A:TRP:HE3	1:37:A:LYS:H	13	0.14
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	4	0.14
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	10	0.14
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	10	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	3	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	3	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	10	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	10	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	11	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	11	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	12	0.14
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	12	0.14
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG2	9	0.14
(1,250)	1:37:A:LYS:H	1:37:A:LYS:HG3	9	0.14
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.14
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG3	7	0.14
(1,228)	1:5:A:THR:H	1:5:A:THR:HA	8	0.14
(1,228)	1:5:A:THR:H	1:5:A:THR:HA	14	0.14
(1,223)	1:32:A:LYS:HA	1:36:A:TRP:H	2	0.14
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	9	0.14
(1,196)	1:28:A:ALA:H	1:29:A:GLN:H	14	0.14
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	7	0.14
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	10	0.14
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	3	0.14
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	5	0.14
(1,174)	1:38:A:HIS:H	1:39:A:ASN:H	4	0.14
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	14	0.14
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	13	0.14
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	4	0.14
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	7	0.14
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	10	0.14
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	11	0.14
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	14	0.14
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	15	0.14
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	11	0.14
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	3	0.14
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	10	0.14
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	14	0.14
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	2	0.14
(1,92)	1:9:A:ASP:HB2	1:10:A:TYR:H	3	0.14
(1,92)	1:9:A:ASP:HB3	1:10:A:TYR:H	3	0.14
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	4	0.14
(1,75)	1:39:A:ASN:HA	1:40:A:ILE:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	15	0.14
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	6	0.14
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	12	0.14
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	14	0.14
(1,55)	1:33:A:LYS:HA	1:34:A:ASN:H	12	0.14
(1,41)	1:25:A:TRP:H	1:25:A:TRP:HB3	5	0.14
(1,36)	1:21:A:ASP:HB2	1:22:A:PHE:H	13	0.14
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	6	0.14
(2,11)	1:10:A:TYR:HD1	1:14:A:MET:HG2	12	0.13
(2,11)	1:10:A:TYR:HD1	1:14:A:MET:HG3	12	0.13
(2,11)	1:10:A:TYR:HD2	1:14:A:MET:HG2	12	0.13
(2,11)	1:10:A:TYR:HD2	1:14:A:MET:HG3	12	0.13
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	5	0.13
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	5	0.13
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	5	0.13
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	5	0.13
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	5	0.13
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	5	0.13
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB1	6	0.13
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB2	6	0.13
(1,448)	1:25:A:TRP:HD1	1:28:A:ALA:HB3	6	0.13
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	14	0.13
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	4	0.13
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	5	0.13
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	5	0.13
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	13	0.13
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	13	0.13
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	14	0.13
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	14	0.13
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.13
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.13
(1,228)	1:5:A:THR:H	1:5:A:THR:HA	6	0.13
(1,228)	1:5:A:THR:H	1:5:A:THR:HA	7	0.13
(1,220)	1:33:A:LYS:HA	1:36:A:TRP:H	2	0.13
(1,203)	1:11:A:SER:H	1:12:A:ILE:HB	15	0.13
(1,199)	1:12:A:ILE:H	1:13:A:ALA:H	8	0.13
(1,187)	1:37:A:LYS:H	1:38:A:HIS:H	7	0.13
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	7	0.13
(1,165)	1:9:A:ASP:HB2	1:11:A:SER:H	14	0.13
(1,165)	1:9:A:ASP:HB3	1:11:A:SER:H	14	0.13
(1,150)	1:42:A:GLN:H	1:42:A:GLN:HB2	11	0.13
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	5	0.13
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	9	0.13
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	14	0.13
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	2	0.13
(1,132)	1:27:A:LEU:H	1:27:A:LEU:HA	8	0.13
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	9	0.13
(1,92)	1:9:A:ASP:HB2	1:10:A:TYR:H	9	0.13
(1,92)	1:9:A:ASP:HB3	1:10:A:TYR:H	9	0.13
(1,79)	1:14:A:MET:HA	1:17:A:ILE:H	11	0.13
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	15	0.13
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	1	0.13
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	4	0.13
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	5	0.13
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	7	0.13
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	10	0.13
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	8	0.13
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	5	0.13
(1,58)	1:33:A:LYS:H	1:33:A:LYS:HB2	11	0.13
(1,41)	1:25:A:TRP:H	1:25:A:TRP:HB3	15	0.13
(1,36)	1:21:A:ASP:HB2	1:22:A:PHE:H	11	0.13
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	7	0.13
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	15	0.13
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD21	2	0.12
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD22	2	0.12
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD23	2	0.12
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD11	2	0.12
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD12	2	0.12
(1,486)	1:25:A:TRP:HH2	1:26:A:LEU:HD13	2	0.12
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG21	9	0.12
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG22	9	0.12
(1,482)	1:2:A:ALA:H	1:5:A:THR:HG23	9	0.12
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB1	8	0.12
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB2	8	0.12
(1,470)	1:27:A:LEU:HD21	1:28:A:ALA:HB3	8	0.12
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB1	8	0.12
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB2	8	0.12
(1,470)	1:27:A:LEU:HD22	1:28:A:ALA:HB3	8	0.12
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB1	8	0.12
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB2	8	0.12
(1,470)	1:27:A:LEU:HD23	1:28:A:ALA:HB3	8	0.12
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	2	0.12
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE21	15	0.12
(1,386)	1:29:A:GLN:HA	1:29:A:GLN:HE22	15	0.12
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	3	0.12
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	5	0.12
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	8	0.12
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	9	0.12
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	12	0.12
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	13	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	1	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	2	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	3	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	5	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	6	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	9	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	11	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	13	0.12
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	14	0.12
(1,348)	1:36:A:TRP:HD1	1:37:A:LYS:H	9	0.12
(1,346)	1:36:A:TRP:H	1:36:A:TRP:HD1	10	0.12
(1,332)	1:38:A:HIS:HA	1:38:A:HIS:HD2	15	0.12
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	1	0.12
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	1	0.12
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	2	0.12
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	2	0.12
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	7	0.12
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	7	0.12
(1,253)	1:33:A:LYS:H	1:33:A:LYS:HG2	11	0.12
(1,253)	1:33:A:LYS:H	1:33:A:LYS:HG3	11	0.12
(1,218)	1:29:A:GLN:HA	1:31:A:GLY:H	8	0.12
(1,193)	1:13:A:ALA:H	1:14:A:MET:H	1	0.12
(1,190)	1:17:A:ILE:H	1:18:A:HIS:H	3	0.12
(1,188)	1:30:A:LYS:H	1:31:A:GLY:H	2	0.12
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	11	0.12
(1,164)	1:10:A:TYR:HB3	1:11:A:SER:H	3	0.12
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	10	0.12
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	12	0.12
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	3	0.12
(1,111)	1:32:A:LYS:HA	1:34:A:ASN:H	11	0.12
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	9	0.12
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	12	0.12
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	14	0.12
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	1	0.12
(1,90)	1:32:A:LYS:HB3	1:33:A:LYS:H	4	0.12
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	9	0.12
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	2	0.12
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	13	0.12
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	14	0.12
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	5	0.12
(1,45)	1:29:A:GLN:H	1:29:A:GLN:HB2	6	0.12
(1,45)	1:29:A:GLN:H	1:29:A:GLN:HB3	6	0.12
(2,13)	1:22:A:PHE:HE1	1:26:A:LEU:HG	3	0.11
(2,13)	1:22:A:PHE:HE2	1:26:A:LEU:HG	3	0.11
(2,7)	1:1:A:TYR:HD1	1:2:A:ALA:HA	11	0.11
(2,7)	1:1:A:TYR:HD2	1:2:A:ALA:HA	11	0.11
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD21	14	0.11
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD22	14	0.11
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD23	14	0.11
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD21	14	0.11
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD22	14	0.11
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD23	14	0.11
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD21	14	0.11
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD22	14	0.11
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD23	14	0.11
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD11	14	0.11
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD12	14	0.11
(1,473)	1:23:A:VAL:HG21	1:26:A:LEU:HD13	14	0.11
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD11	14	0.11
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD12	14	0.11
(1,473)	1:23:A:VAL:HG22	1:26:A:LEU:HD13	14	0.11
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD11	14	0.11
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD12	14	0.11
(1,473)	1:23:A:VAL:HG23	1:26:A:LEU:HD13	14	0.11
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD21	2	0.11
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD22	2	0.11
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD23	2	0.11
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	2	0.11
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD22	2	0.11
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD23	2	0.11
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	2	0.11
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD22	2	0.11
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD23	2	0.11
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD11	2	0.11
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD12	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:23:A:VAL:HG11	1:26:A:LEU:HD13	2	0.11
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD11	2	0.11
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD12	2	0.11
(1,471)	1:23:A:VAL:HG12	1:26:A:LEU:HD13	2	0.11
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD11	2	0.11
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD12	2	0.11
(1,471)	1:23:A:VAL:HG13	1:26:A:LEU:HD13	2	0.11
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	2	0.11
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD3	2	0.11
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	9	0.11
(1,402)	1:33:A:LYS:HB3	1:33:A:LYS:HD3	9	0.11
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	1	0.11
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	2	0.11
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	6	0.11
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	7	0.11
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	10	0.11
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	11	0.11
(1,383)	1:36:A:TRP:HD1	1:36:A:TRP:HE1	15	0.11
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	7	0.11
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	10	0.11
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	4	0.11
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	13	0.11
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	4	0.11
(1,356)	1:36:A:TRP:HZ3	1:36:A:TRP:HE3	4	0.11
(1,356)	1:36:A:TRP:HZ3	1:36:A:TRP:HE3	5	0.11
(1,356)	1:36:A:TRP:HZ3	1:36:A:TRP:HE3	13	0.11
(1,338)	1:36:A:TRP:HE3	1:37:A:LYS:H	4	0.11
(1,305)	1:24:A:ASN:HB2	1:24:A:ASN:HD21	14	0.11
(1,305)	1:24:A:ASN:HB3	1:24:A:ASN:HD21	14	0.11
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE1	8	0.11
(1,293)	1:22:A:PHE:HA	1:22:A:PHE:HE2	8	0.11
(1,278)	1:18:A:HIS:HA	1:18:A:HIS:HD2	9	0.11
(1,249)	1:37:A:LYS:HD2	1:38:A:HIS:H	6	0.11
(1,249)	1:37:A:LYS:HD3	1:38:A:HIS:H	6	0.11
(1,235)	1:14:A:MET:HG2	1:15:A:ASP:H	2	0.11
(1,235)	1:14:A:MET:HG3	1:15:A:ASP:H	2	0.11
(1,230)	1:15:A:ASP:HA	1:18:A:HIS:H	9	0.11
(1,228)	1:5:A:THR:H	1:5:A:THR:HA	10	0.11
(1,219)	1:30:A:LYS:HA	1:32:A:LYS:H	14	0.11
(1,197)	1:8:A:SER:H	1:9:A:ASP:H	4	0.11
(1,181)	1:34:A:ASN:H	1:35:A:ASP:H	12	0.11
(1,178)	1:34:A:ASN:H	1:36:A:TRP:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	4	0.11
(1,170)	1:19:A:GLN:H	1:20:A:GLN:H	10	0.11
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	2	0.11
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	7	0.11
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	10	0.11
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	11	0.11
(1,139)	1:42:A:GLN:H	1:42:A:GLN:HB3	10	0.11
(1,135)	1:5:A:THR:HB	1:8:A:SER:H	4	0.11
(1,116)	1:13:A:ALA:HA	1:16:A:LYS:H	11	0.11
(1,110)	1:5:A:THR:HB	1:6:A:PHE:H	4	0.11
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	1	0.11
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	3	0.11
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	7	0.11
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	4	0.11
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	5	0.11
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	6	0.11
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	13	0.11
(1,95)	1:1:A:TYR:HA	1:2:A:ALA:H	15	0.11
(1,72)	1:38:A:HIS:H	1:38:A:HIS:HA	1	0.11
(1,72)	1:38:A:HIS:H	1:38:A:HIS:HA	3	0.11
(1,69)	1:37:A:LYS:HA	1:38:A:HIS:H	5	0.11
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	3	0.11
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	8	0.11
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	9	0.11
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	12	0.11
(1,64)	1:36:A:TRP:H	1:36:A:TRP:HA	3	0.11
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	1	0.11
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	5	0.11
(1,12)	1:12:A:ILE:H	1:12:A:ILE:HB	7	0.11
(1,12)	1:12:A:ILE:H	1:12:A:ILE:HB	10	0.11
(1,12)	1:12:A:ILE:H	1:12:A:ILE:HB	12	0.11
(2,7)	1:1:A:TYR:HD1	1:2:A:ALA:HA	2	0.1
(2,7)	1:1:A:TYR:HD2	1:2:A:ALA:HA	2	0.1
(2,7)	1:1:A:TYR:HD1	1:2:A:ALA:HA	3	0.1
(2,7)	1:1:A:TYR:HD2	1:2:A:ALA:HA	3	0.1
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	8	0.1
(1,382)	1:25:A:TRP:HD1	1:25:A:TRP:HE1	12	0.1
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	2	0.1
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	3	0.1
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	8	0.1
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	11	0.1
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:25:A:TRP:HZ3	1:25:A:TRP:HE3	15	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	1	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	3	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	5	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	6	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	7	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	8	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	9	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	11	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	12	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	13	0.1
(1,360)	1:25:A:TRP:HH2	1:25:A:TRP:HZ2	14	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	1	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	2	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	3	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	4	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	5	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	6	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	7	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	8	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	9	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	10	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	11	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	12	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	13	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	14	0.1
(1,358)	1:36:A:TRP:HH2	1:36:A:TRP:HZ2	15	0.1
(1,356)	1:36:A:TRP:HZ3	1:36:A:TRP:HE3	9	0.1
(1,346)	1:36:A:TRP:H	1:36:A:TRP:HD1	2	0.1
(1,291)	1:22:A:PHE:HA	1:25:A:TRP:HE3	5	0.1
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG2	12	0.1
(1,231)	1:3:A:GLU:H	1:3:A:GLU:HG3	12	0.1
(1,184)	1:22:A:PHE:H	1:23:A:VAL:H	15	0.1
(1,147)	1:23:A:VAL:HB	1:24:A:ASN:H	12	0.1
(1,143)	1:8:A:SER:HA	1:9:A:ASP:H	6	0.1
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	10	0.1
(1,102)	1:21:A:ASP:H	1:21:A:ASP:HA	13	0.1
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	8	0.1
(1,94)	1:24:A:ASN:HB2	1:25:A:TRP:H	10	0.1
(1,77)	1:40:A:ILE:H	1:40:A:ILE:HB	8	0.1
(1,67)	1:36:A:TRP:HA	1:37:A:LYS:H	6	0.1
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:17:A:ILE:H	1:17:A:ILE:HB	9	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found