



Full wwPDB NMR Structure Validation Report ⓘ

Aug 30, 2026 – 01:14 am BST

PDB ID : 9RPN / pdb_00009rpn
BMRB ID : 35004
Title : PIN1 WW Domain Binding Mode with LYR-tide
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Deposited on : 2025-06-25

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
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 : v1.2.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

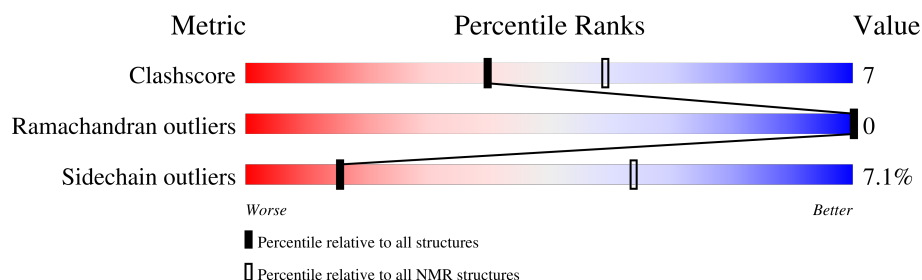
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 64%.

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	37	
2	B	12	

2 Ensemble composition and analysis

This entry contains 25 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:7-A:37, B:84-B:84, B:86-B:87 (34)	0.23	9

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 761 atoms, of which 371 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1.

Mol	Chain	Residues	Atoms						Trace
1	A	37	Total	C	H	N	O	S	0
			599	191	291	59	57	1	

- Molecule 2 is a protein called LYR-tide LYRpSPPLP.

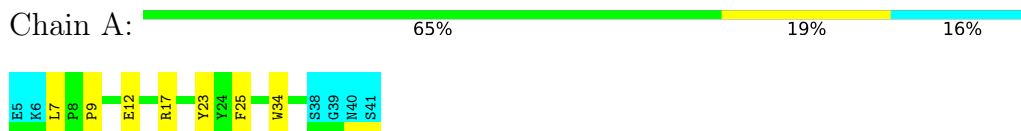
Mol	Chain	Residues	Atoms						Trace
2	B	12	Total	C	H	N	O	P	1
			162	51	80	14	16	1	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP

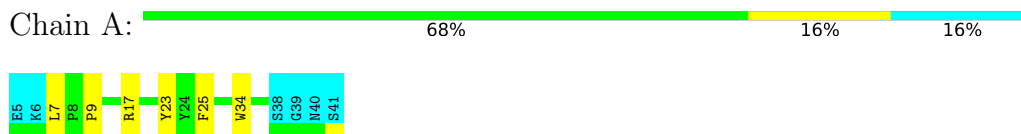


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP



4.2.2 Score per residue for model 2

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

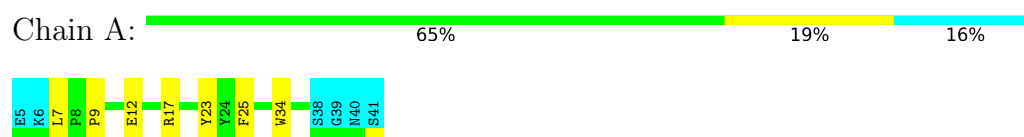


- Molecule 2: LYR-tide LYRpSPPLP



4.2.3 Score per residue for model 3

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP



4.2.4 Score per residue for model 4

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP



4.2.5 Score per residue for model 5

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP



4.2.6 Score per residue for model 6

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

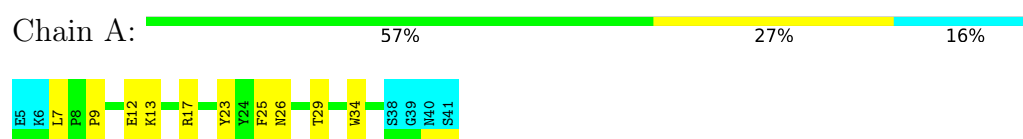


- Molecule 2: LYR-tide LYRpSPPLP



4.2.7 Score per residue for model 7

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP



4.2.8 Score per residue for model 8

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP



4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP



4.2.10 Score per residue for model 10

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



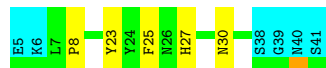
- Molecule 2: LYR-tide LYRpSPPLP



4.2.11 Score per residue for model 11

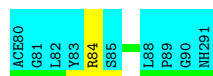
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  70% 14% 16%



- Molecule 2: LYR-tide LYRpSPPLP

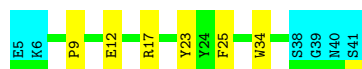
Chain B:  17% 8% 75%



4.2.12 Score per residue for model 12

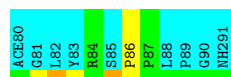
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  68% 16% 16%



- Molecule 2: LYR-tide LYRpSPPLP

Chain B:  17% 8% 75%



4.2.13 Score per residue for model 13

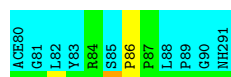
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  76% 8% 16%



- Molecule 2: LYR-tide LYRpSPPLP

Chain B:  17% 8% 75%



4.2.14 Score per residue for model 14

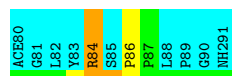
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: LYR-tide LYRpSPPLP

Chain B: 



4.2.15 Score per residue for model 15

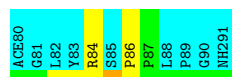
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: LYR-tide LYRpSPPLP

Chain B: 



4.2.16 Score per residue for model 16

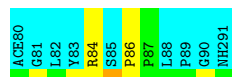
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: LYR-tide LYRpSPPLP

Chain B: 



4.2.17 Score per residue for model 17

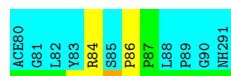
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  68% 16% 16%



- Molecule 2: LYR-tide LYRpSPPLP

Chain B:  8% 17% 75%



4.2.18 Score per residue for model 18

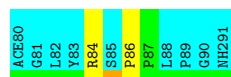
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  62% 19% 16%



- Molecule 2: LYR-tide LYRpSPPLP

Chain B:  8% 17% 75%



4.2.19 Score per residue for model 19

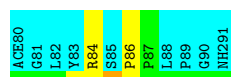
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  62% 22% 16%



- Molecule 2: LYR-tide LYRpSPPLP

Chain B:  8% 17% 75%



4.2.20 Score per residue for model 20

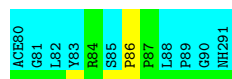
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: LYR-tide LYRpSPPLP

Chain B: 



4.2.21 Score per residue for model 21

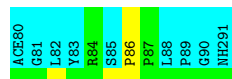
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: LYR-tide LYRpSPPLP

Chain B: 



4.2.22 Score per residue for model 22

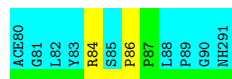
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: LYR-tide LYRpSPPLP

Chain B: 



4.2.23 Score per residue for model 23

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

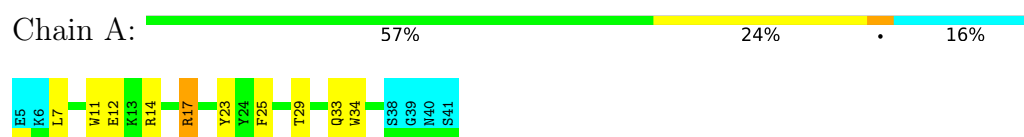


- Molecule 2: LYR-tide LYRpSPPLP



4.2.24 Score per residue for model 24

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

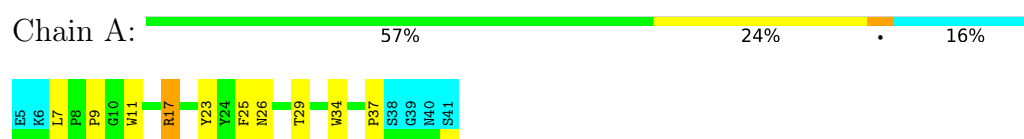


- Molecule 2: LYR-tide LYRpSPPLP



4.2.25 Score per residue for model 25

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: LYR-tide LYRpSPPLP



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure calculation	

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	429
Number of shifts mapped to atoms	381
Number of unparsed shifts	0
Number of shifts with mapping errors	48
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2, SEP

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [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	265	251	250	4±1
2	B	25	27	27	2±1
All	All	7250	6950	6925	100

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:CE2	1:A:25:PHE:HB2	0.70	2.21	22	14
1:A:23:TYR:CE1	1:A:25:PHE:HB2	0.65	2.27	5	11
1:A:23:TYR:CD2	2:B:86:PRO:HG3	0.59	2.32	22	6
1:A:8:PRO:HG2	1:A:11:TRP:CD1	0.57	2.34	9	4
1:A:34:TRP:NE1	2:B:86:PRO:HB2	0.55	2.16	4	22
1:A:25:PHE:CZ	1:A:30:ASN:HA	0.53	2.39	6	1
1:A:23:TYR:CD1	2:B:86:PRO:HG3	0.51	2.41	16	4
1:A:7:LEU:HD22	1:A:37:PRO:HD2	0.51	1.83	5	1
1:A:25:PHE:CE1	1:A:30:ASN:HA	0.50	2.41	11	1
1:A:34:TRP:CD1	2:B:86:PRO:HB2	0.50	2.41	4	3
1:A:32:SER:HB2	2:B:86:PRO:HG3	0.50	1.83	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:GLU:HG2	1:A:14:ARG:HG3	0.49	1.83	6	1
1:A:15:MET:HA	1:A:22:VAL:HA	0.49	1.84	16	1
1:A:11:TRP:HH2	1:A:33:GLN:OE1	0.48	1.92	24	2
1:A:12:GLU:OE2	1:A:25:PHE:HB3	0.48	2.09	6	1
1:A:26:ASN:OD1	1:A:29:THR:HG22	0.46	2.10	25	5
1:A:23:TYR:CD2	2:B:86:PRO:HD3	0.46	2.46	13	2
1:A:17:ARG:HD3	1:A:18:SER:N	0.45	2.26	8	2
1:A:26:ASN:OD1	1:A:28:ILE:HB	0.45	2.12	6	3
1:A:11:TRP:CD2	1:A:37:PRO:HG3	0.44	2.48	25	1
1:A:25:PHE:HD2	1:A:32:SER:OG	0.43	1.96	18	1
1:A:34:TRP:CE2	2:B:86:PRO:HB2	0.43	2.49	12	7
1:A:25:PHE:HD1	1:A:32:SER:OG	0.42	1.97	13	1
1:A:25:PHE:CE2	1:A:27:HIS:HA	0.42	2.50	11	1
1:A:16:SER:OG	1:A:19:SER:HB2	0.41	2.15	4	1
1:A:12:GLU:CG	1:A:14:ARG:HE	0.41	2.28	24	1
1:A:11:TRP:CE2	1:A:37:PRO:HB3	0.41	2.51	10	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	31/37 (84%)	29±0 (94±1%)	2±0 (6±1%)	0±0 (0±0%)	100	100
2	B	3/12 (25%)	3±0 (97±9%)	0±0 (3±9%)	0±0 (0±0%)	100	100
All	All	850/1225 (69%)	801 (94%)	49 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	28/33 (85%)	26±1 (93±4%)	2±1 (7±4%)	16	65
2	B	3/7 (43%)	3±0 (91±15%)	0±0 (9±15%)	11	56
All	All	775/1000 (78%)	720 (93%)	55 (7%)	15	64

All 8 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	7	LEU	15
1	A	17	ARG	14
1	A	12	GLU	11
2	B	84	ARG	7
1	A	29	THR	3
1	A	13	LYS	2
1	A	22	VAL	2
1	A	18	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	SEP	B	85	2	8,9,10	0.99±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	SEP	B	85	2	8,12,14	1.32±0.16	1±0 (12±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	B	85	2	-	0±0,5,8,10	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	85	SEP	OG-CB-CA	3.76	111.81	108.14	2	24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 58% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *default*

7.1.1 Bookkeeping

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

Total number of shifts	429
Number of shifts mapped to atoms	381
Number of unparsed shifts	0
Number of shifts with mapping errors	48
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 48 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	82	SER	H	7.80863987	.	1
1	B	82	SER	HA	3.348779634	.	1
1	B	82	SER	HB2	3.824167378	.	1
1	B	82	SER	HB3	3.857763047	.	1
1	B	82	SER	CB	64.90945182	0.03087790684	1
1	B	82	SER	N	125.765748	.	1
1	B	83	PRO	HA	3.648118573	0.007875391329	1
1	B	83	PRO	HB3	1.560833224	0.007606917336	1
1	B	83	PRO	HD2	3.478969344	0.01234724101	1
1	B	83	PRO	HD3	3.568468447	.	1
1	B	83	PRO	HG2	1.635240243	.	1
1	B	83	PRO	HG3	1.467984678	0.001520337198	1
1	B	83	PRO	CD	50.60450363	.	1
1	B	84	TYR	H	7.931468612	0.004024854893	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	84	TYR	HA	4.530741622	0.006477266682	1
1	B	84	TYR	HB2	2.901651715	0.001816490676	1
1	B	84	TYR	HB3	2.988383632	0.01511404067	1
1	B	84	TYR	HD1	7.019454915	0.002119262091	3
1	B	84	TYR	HD2	7.019454915	0.002119262091	3
1	B	84	TYR	HE1	6.740040027	0.001465965923	3
1	B	84	TYR	HE2	6.740040027	0.001465965923	3
1	B	84	TYR	CB	41.42150778	0.01304144335	1
1	B	87	PHE	H	8.131328494	0.003013355163	1
1	B	87	PHE	HA	4.777031208	0.002618783529	1
1	B	87	PHE	HB2	2.918226455	0.00859310348	1
1	B	87	PHE	HB3	3.100348185	0.008394355669	1
1	B	87	PHE	HD1	7.286603423	0.002778028386	3
1	B	87	PHE	HD2	7.286603423	0.002778028386	3
1	B	87	PHE	HE1	7.212394254	0.006075368195	3
1	B	87	PHE	HE2	7.212394254	0.006075368195	3
1	B	87	PHE	HZ	7.175088328	0.06827219181	1
1	B	87	PHE	CB	38.66571753	0.02791036905	1
1	B	88	PRO	HA	4.391591573	0.001873583633	1
1	B	88	PRO	HB3	2.212568307	0.003432494937	1
1	B	88	PRO	HD2	3.746432229	0.003872490502	1
1	B	88	PRO	HD3	3.39009697	0.00462945597	1
1	B	88	PRO	HG2	1.914829403	0.007486918559	1
1	B	88	PRO	CA	63.43030903	.	1
1	B	88	PRO	CB	35.71328563	.	1
1	B	88	PRO	CD	50.66128681	.	1
1	B	89	GLU	H	8.513170737	0.002963819428	1
1	B	89	GLU	HA	4.196999853	0.004057305478	1
1	B	89	GLU	HB2	1.901609602	0.002318466547	1
1	B	89	GLU	HB3	1.995385817	0.002717852704	1
1	B	89	GLU	HG3	2.229248387	0.005880574657	1
1	B	89	GLU	CA	57.02689962	.	1
1	B	89	GLU	CB	30.14137456	0.007495628342	1
1	B	89	GLU	CG	36.37058688	.	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	32	0.56 ± 0.19	Should be checked

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\beta$	40	-0.20 ± 0.30	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	26	0.22 ± 0.74	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 64%, i.e. 317 atoms were assigned a chemical shift out of a possible 494. 2 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	104/162 (64%)	59/65 (91%)	23/68 (34%)	22/29 (76%)
Sidechain	184/272 (68%)	125/174 (72%)	59/79 (75%)	0/19 (0%)
Aromatic	29/60 (48%)	27/29 (93%)	0/27 (0%)	2/4 (50%)
Overall	317/494 (64%)	211/268 (79%)	82/174 (47%)	24/52 (46%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 58%, i.e. 371 atoms were assigned a chemical shift out of a possible 635. 2 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	130/223 (58%)	75/91 (82%)	30/92 (33%)	25/40 (62%)
Sidechain	212/343 (62%)	145/220 (66%)	67/102 (66%)	0/21 (0%)
Aromatic	29/69 (42%)	27/33 (82%)	0/32 (0%)	2/4 (50%)
Overall	371/635 (58%)	247/344 (72%)	97/226 (43%)	27/65 (42%)

7.1.4 Statistically unusual chemical shifts [i](#)

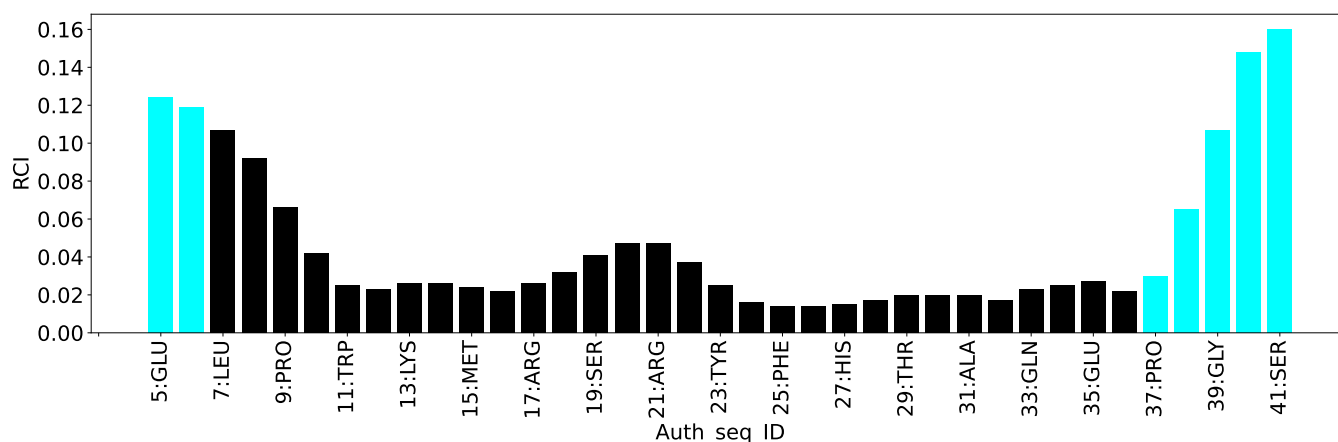
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	11	TRP	CE2	41.94	105.29 – 170.61	-14.7
1	A	26	ASN	HB3	-0.76	1.12 – 4.38	-10.8
1	A	14	ARG	HB2	-0.17	0.52 – 3.08	-7.7
1	A	37	PRO	HG2	-0.22	0.41 – 3.45	-7.1
1	A	26	ASN	HD21	4.12	4.94 – 9.72	-6.7

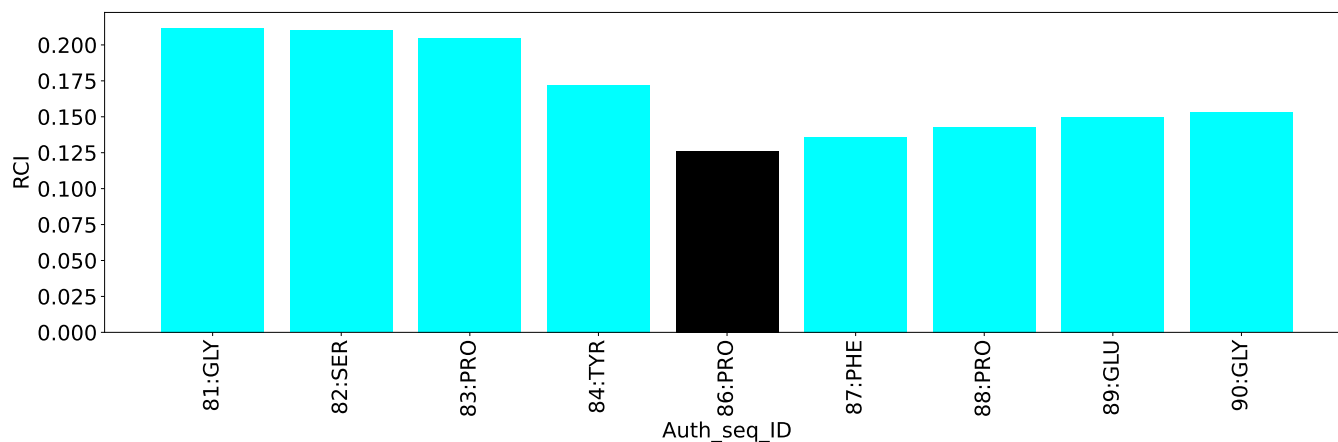
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



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	886
Intra-residue ($ i-j =0$)	156
Sequential ($ i-j =1$)	232
Medium range ($ i-j >1$ and $ i-j <5$)	102
Long range ($ i-j \geq 5$)	298
Inter-chain	98
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	48
Number of unmapped restraints	130
Number of restraints per residue	19.1
Number of long range restraints per residue ¹	6.1

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)	17.4	0.2
0.2-0.5 (Medium)	24.8	0.5
>0.5 (Large)	66.1	11.87

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	11.6	9.96
10.0-20.0 (Medium)	7.1	19.89
>20.0 (Large)	1.9	132.06

9 Distance violation analysis ⓘ

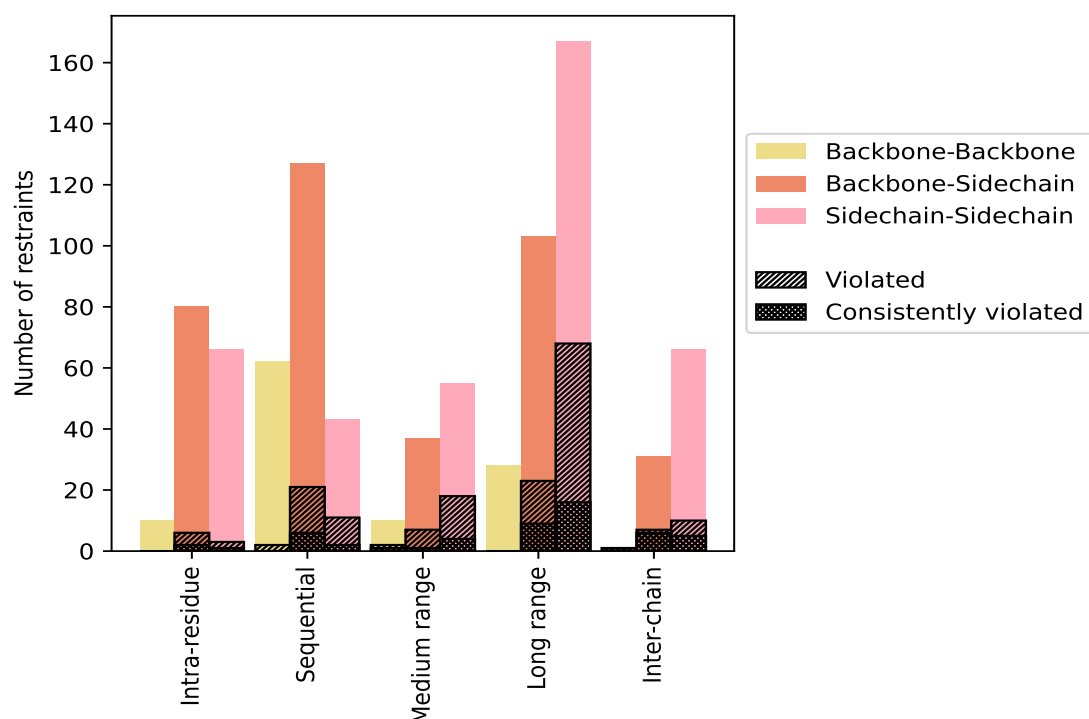
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	156	17.6	9	5.8	1.0	3	1.9	0.3
Backbone-Backbone	10	1.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	80	9.0	6	7.5	0.7	2	2.5	0.2
Sidechain-Sidechain	66	7.4	3	4.5	0.3	1	1.5	0.1
Sequential (i-j =1)	232	26.2	34	14.7	3.8	8	3.4	0.9
Backbone-Backbone	62	7.0	2	3.2	0.2	0	0.0	0.0
Backbone-Sidechain	127	14.3	21	16.5	2.4	6	4.7	0.7
Sidechain-Sidechain	43	4.9	11	25.6	1.2	2	4.7	0.2
Medium range (i-j >1 & i-j <5)	102	11.5	27	26.5	3.0	6	5.9	0.7
Backbone-Backbone	10	1.1	2	20.0	0.2	1	10.0	0.1
Backbone-Sidechain	37	4.2	7	18.9	0.8	1	2.7	0.1
Sidechain-Sidechain	55	6.2	18	32.7	2.0	4	7.3	0.5
Long range (i-j ≥5)	298	33.6	91	30.5	10.3	25	8.4	2.8
Backbone-Backbone	28	3.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	103	11.6	23	22.3	2.6	9	8.7	1.0
Sidechain-Sidechain	167	18.8	68	40.7	7.7	16	9.6	1.8
Inter-chain	98	11.1	18	18.4	2.0	12	12.2	1.4
Backbone-Backbone	1	0.1	1	100.0	0.1	1	100.0	0.1
Backbone-Sidechain	31	3.5	7	22.6	0.8	6	19.4	0.7
Sidechain-Sidechain	66	7.4	10	15.2	1.1	5	7.6	0.6
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	886	100.0	179	20.2	20.2	54	6.1	6.1
Backbone-Backbone	111	12.5	5	4.5	0.6	2	1.8	0.2
Backbone-Sidechain	378	42.7	64	16.9	7.2	24	6.3	2.7
Sidechain-Sidechain	397	44.8	110	27.7	12.4	28	7.1	3.2

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	5	20	17	55	16	113	1.13	9.74	1.58	0.65
2	7	20	15	54	17	113	1.15	9.45	1.63	0.67
3	6	22	15	54	15	112	1.13	11.38	1.64	0.64
4	7	19	14	48	14	102	1.21	11.31	1.88	0.64
5	4	20	14	51	14	103	1.17	9.77	1.66	0.69
6	5	22	14	59	17	117	1.12	10.57	1.55	0.65
7	6	19	15	54	15	109	1.21	9.96	1.56	0.75
8	6	21	15	51	14	107	1.2	11.68	1.91	0.63
9	6	22	15	52	13	108	1.08	9.0	1.58	0.67
10	6	19	16	53	14	108	1.17	11.71	1.66	0.69

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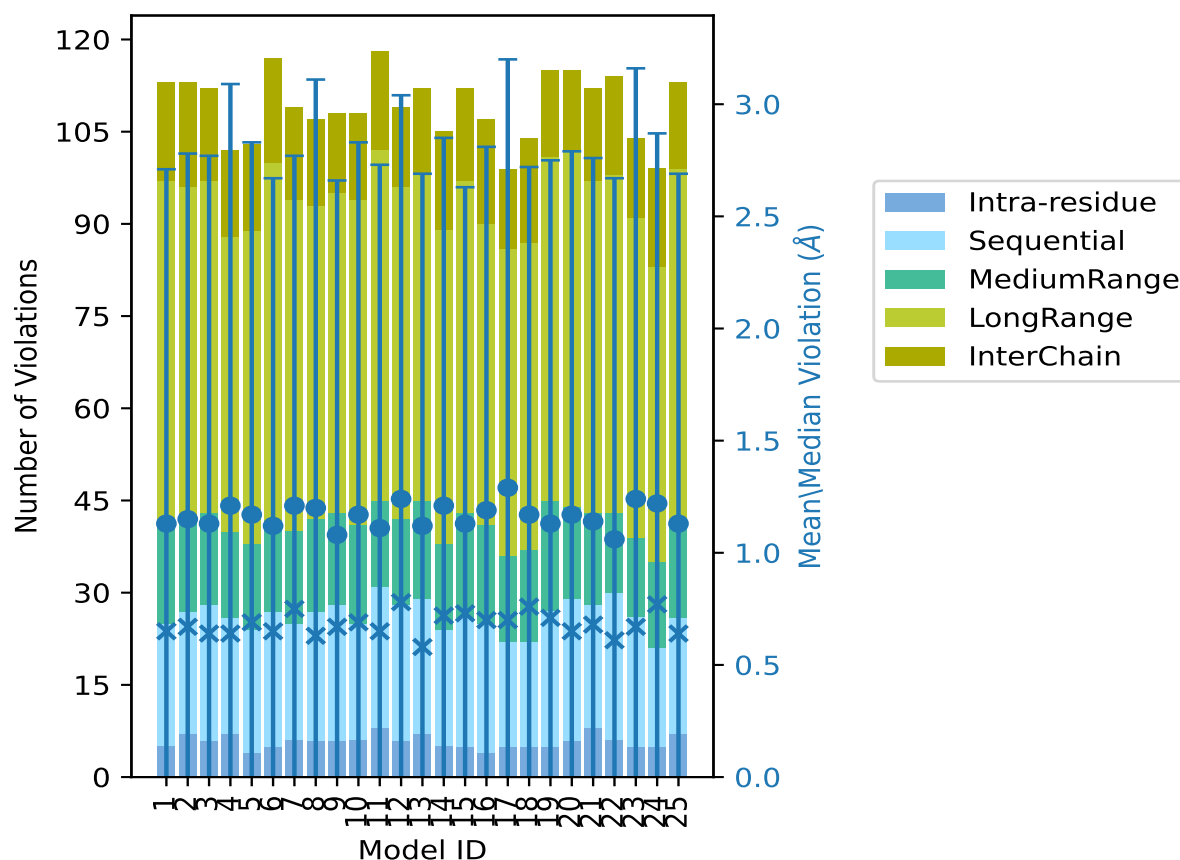
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	8	23	14	57	16	118	1.11	10.77	1.62	0.65
12	6	22	14	54	13	109	1.24	10.68	1.8	0.78
13	7	22	16	53	14	112	1.12	10.82	1.57	0.58
14	5	19	14	51	16	105	1.21	9.69	1.64	0.72
15	5	21	17	54	15	112	1.13	9.91	1.5	0.73
16	4	21	16	49	17	107	1.19	10.59	1.62	0.7
17	5	17	14	50	13	99	1.29	10.77	1.91	0.7
18	5	17	15	50	17	104	1.17	9.5	1.55	0.76
19	5	22	18	56	14	115	1.13	10.57	1.62	0.71
20	6	23	15	58	13	115	1.17	10.15	1.62	0.65
21	8	20	15	54	15	112	1.14	11.15	1.62	0.68
22	6	24	13	55	16	114	1.06	10.99	1.61	0.61
23	5	21	13	52	13	104	1.24	11.87	1.92	0.67
24	5	16	14	48	16	99	1.22	10.63	1.65	0.77
25	7	19	15	58	14	113	1.13	9.18	1.56	0.64

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 707(IR:147, SQ:198, MR:75, LR:207, IC:80) 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	%
0	1	4	9	0	14	1	4.0
1	4	2	5	0	12	2	8.0
0	2	1	5	1	9	3	12.0
0	0	1	5	0	6	4	16.0
0	1	1	2	0	4	5	20.0
1	1	0	3	0	5	6	24.0

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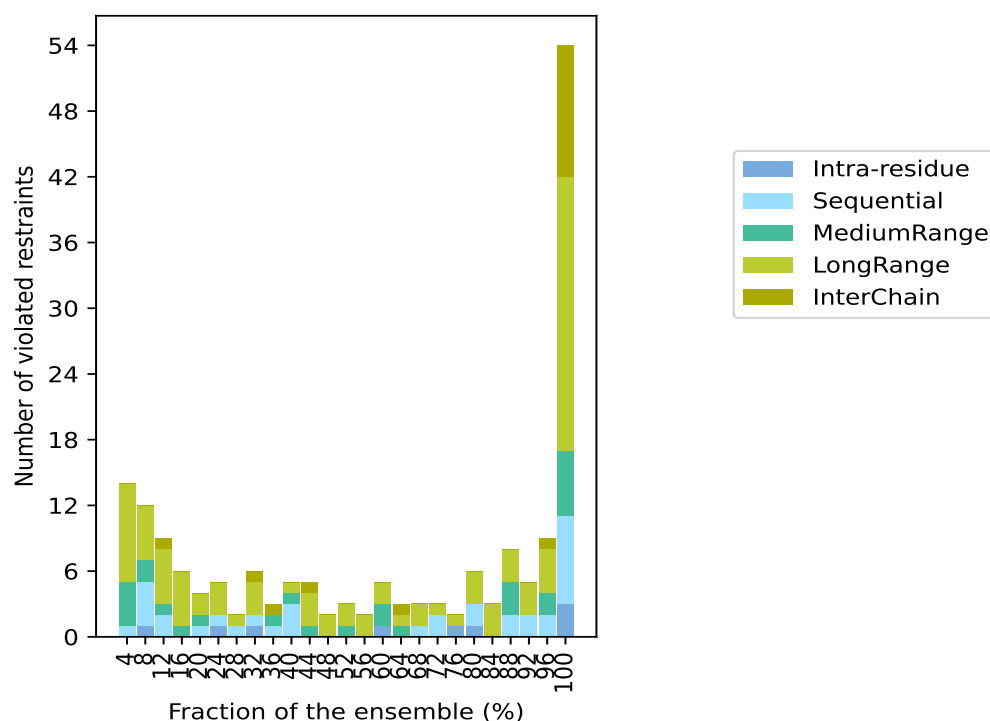
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	0	1	0	2	7	28.0
1	1	0	3	1	6	8	32.0
0	1	1	0	1	3	9	36.0
0	3	1	1	0	5	10	40.0
0	0	1	3	1	5	11	44.0
0	0	0	2	0	2	12	48.0
0	0	1	2	0	3	13	52.0
0	0	0	2	0	2	14	56.0
1	0	2	2	0	5	15	60.0
0	0	1	1	1	3	16	64.0
0	1	0	2	0	3	17	68.0
0	2	0	1	0	3	18	72.0
1	0	0	1	0	2	19	76.0
1	2	0	3	0	6	20	80.0
0	0	0	3	0	3	21	84.0
0	2	3	3	0	8	22	88.0
0	2	0	3	0	5	23	92.0
0	2	2	4	1	9	24	96.0
3	8	6	25	12	54	25	100.0

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

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

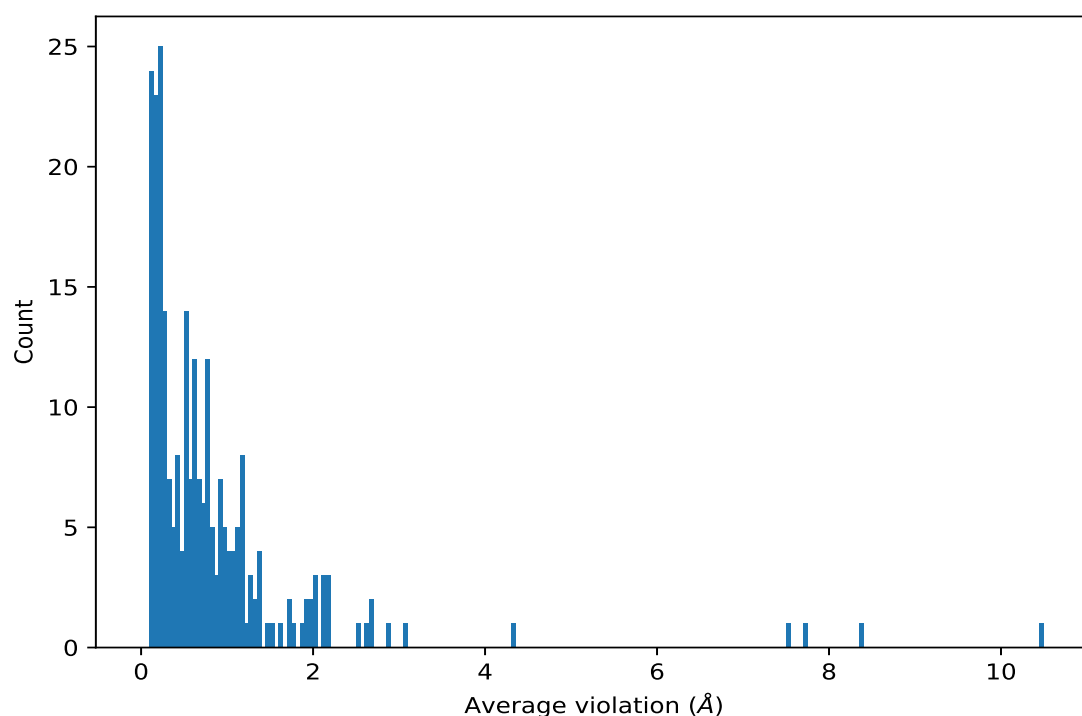
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	25	10.47	0.79	10.59
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	25	8.39	1.5	8.13
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	25	7.72	0.58	7.52
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	25	7.53	0.84	7.49
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	25	4.3	0.44	4.36
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	25	3.07	0.38	3.2
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	25	2.89	0.3	2.88
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	25	2.66	0.31	2.69
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	25	2.66	0.25	2.61
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	25	2.63	0.59	2.77
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	25	2.54	0.3	2.55
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	25	2.17	0.2	2.27
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	25	2.17	0.2	2.27
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	25	2.17	0.2	2.27
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	25	2.14	0.62	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	25	2.14	0.62	2.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	25	2.14	0.62	2.19
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	25	2.02	0.18	2.01
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	25	2.02	0.18	2.01
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	25	2.02	0.18	2.01
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	25	1.99	0.13	1.95
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	25	1.99	0.13	1.95
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	25	1.95	0.17	1.93
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	25	1.95	0.17	1.93
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	25	1.89	0.34	2.01
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	25	1.79	0.33	1.87
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	25	1.74	0.36	1.86
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	25	1.74	0.36	1.86
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	25	1.6	0.17	1.65
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	25	1.38	0.11	1.4
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	25	1.25	0.34	1.3
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	25	1.25	0.34	1.35
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	25	1.25	0.34	1.35
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	25	1.19	0.19	1.24
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	25	1.16	0.09	1.17
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	25	1.16	0.09	1.17
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	25	1.16	0.34	1.12
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	25	1.14	0.1	1.14
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	25	1.11	0.34	1.05
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	25	1.06	0.21	1.03
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	25	1.05	0.29	0.98
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	25	1.0	0.14	1.01
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	25	0.92	0.1	0.91
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	25	0.91	0.19	0.92
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	25	0.91	0.19	0.92
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	25	0.87	0.11	0.86
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	25	0.87	0.11	0.86
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	25	0.82	0.36	0.72
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	25	0.82	0.36	0.72
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	25	0.79	0.13	0.79
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	25	0.77	0.15	0.77
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	25	0.75	0.08	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	25	0.75	0.08	0.74
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	25	0.75	0.19	0.71
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	25	0.71	0.14	0.73
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	25	0.71	0.14	0.73
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	25	0.71	0.27	0.72
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	25	0.65	0.18	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	25	0.62	0.07	0.6
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	25	0.61	0.09	0.63
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	25	0.59	0.07	0.58
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	25	0.57	0.18	0.6
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	25	0.54	0.1	0.57
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	25	0.51	0.14	0.52
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	25	0.47	0.11	0.47
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	25	0.47	0.16	0.43
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	25	0.44	0.12	0.45
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	25	0.35	0.01	0.35
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	25	0.3	0.07	0.27
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	25	0.23	0.07	0.24
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	24	1.33	0.07	1.33
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	24	1.05	0.07	1.05
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	24	1.05	0.07	1.05
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	24	0.92	0.11	0.92
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	24	0.92	0.11	0.92
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	24	0.77	0.43	0.66
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	24	0.5	0.16	0.5
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	24	0.35	0.16	0.34
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	24	0.24	0.07	0.22
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	24	0.24	0.07	0.22
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	24	0.21	0.06	0.2
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	24	0.21	0.06	0.2
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	24	0.21	0.06	0.2
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	24	0.15	0.02	0.15
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	24	0.15	0.02	0.15
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	23	1.22	0.18	1.24
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	23	1.18	0.13	1.16
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	23	0.98	0.2	1.01
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	23	0.33	0.32	0.23
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	23	0.33	0.32	0.23
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	22	1.5	0.08	1.5
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	22	0.88	0.16	0.92
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	22	0.57	0.19	0.59
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	22	0.41	0.12	0.45
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	22	0.39	0.06	0.38
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	22	0.3	0.08	0.29
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	22	0.25	0.11	0.24
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	22	0.19	0.05	0.2
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	21	0.98	0.32	1.02
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	21	0.48	0.17	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	21	0.25	0.08	0.25
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	20	1.3	0.08	1.28
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	20	0.91	0.02	0.91
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	20	0.42	0.01	0.42
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	20	0.23	0.09	0.24
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	20	0.23	0.09	0.24
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	20	0.21	0.07	0.19
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	20	0.15	0.01	0.15
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	19	0.13	0.02	0.12
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	19	0.13	0.02	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	19	0.11	0.01	0.11
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	18	0.19	0.04	0.19
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	18	0.18	0.05	0.17
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	18	0.16	0.04	0.15
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	17	1.36	0.18	1.39
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	17	1.36	0.18	1.39
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	17	1.36	0.18	1.39
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	17	0.69	0.29	0.7
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	17	0.69	0.29	0.7
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	17	0.69	0.29	0.7
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	17	0.59	0.1	0.59
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	17	0.59	0.1	0.59
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	17	0.59	0.1	0.59
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	16	0.31	0.17	0.23
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	16	0.23	0.09	0.2
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	16	0.15	0.04	0.15
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	16	0.15	0.04	0.15
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	15	0.97	0.55	0.92
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	15	0.97	0.55	0.92
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	15	0.97	0.55	0.92
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	15	0.56	0.28	0.49
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	15	0.34	0.12	0.42
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	15	0.29	0.05	0.28
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	15	0.29	0.05	0.28
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	15	0.29	0.05	0.28
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	15	0.12	0.01	0.12
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	14	0.41	0.16	0.36
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	14	0.41	0.16	0.36
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	14	0.41	0.16	0.36
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	14	0.36	0.17	0.32
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	14	0.36	0.17	0.32
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	13	0.54	0.69	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	13	0.54	0.69	0.15
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	13	0.19	0.05	0.19
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	13	0.19	0.05	0.19
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	13	0.19	0.05	0.19
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	13	0.17	0.04	0.17
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	12	0.28	0.08	0.24
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	12	0.22	0.12	0.16
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	11	0.5	0.16	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	11	0.5	0.16	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	11	0.5	0.16	0.44
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	11	0.29	0.1	0.28
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	11	0.29	0.1	0.28
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	11	0.24	0.08	0.23
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	11	0.16	0.05	0.14
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	11	0.16	0.05	0.14
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	11	0.15	0.04	0.14
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	11	0.15	0.04	0.14
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	10	1.1	0.13	1.08
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	10	1.1	0.13	1.08
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	10	1.1	0.13	1.08
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	10	0.75	0.08	0.78
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	10	0.75	0.08	0.78
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	10	0.75	0.08	0.78
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	10	0.61	0.16	0.64
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	10	0.61	0.16	0.64
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	10	0.61	0.16	0.64
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	10	0.51	0.03	0.52
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	10	0.51	0.03	0.52
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	10	0.51	0.03	0.52
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	10	0.37	0.31	0.27
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	9	0.22	0.07	0.17
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	9	0.19	0.06	0.19
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	9	0.18	0.04	0.17
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	8	1.0	0.15	1.02
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	8	1.0	0.15	1.02
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	8	1.0	0.15	1.02
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	8	0.52	0.22	0.5
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	8	0.44	0.12	0.44
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	8	0.2	0.1	0.18
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	8	0.2	0.1	0.18
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	8	0.2	0.1	0.18
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	8	0.2	0.1	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	8	0.2	0.1	0.18
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	8	0.2	0.1	0.18
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	8	0.12	0.02	0.12
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG11	7	0.74	0.25	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG12	7	0.74	0.25	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG13	7	0.74	0.25	0.83
(1,744)	1:39:A:GLY:H	1:38:A:SER:H	7	0.24	0.07	0.22
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD21	6	1.16	0.16	1.13
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD22	6	1.16	0.16	1.13
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD23	6	1.16	0.16	1.13
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG21	6	0.76	0.15	0.8
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG22	6	0.76	0.15	0.8
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG23	6	0.76	0.15	0.8
(1,813)	1:22:A:VAL:HG11	1:23:A:TYR:HA	6	0.62	0.05	0.62
(1,813)	1:22:A:VAL:HG12	1:23:A:TYR:HA	6	0.62	0.05	0.62
(1,813)	1:22:A:VAL:HG13	1:23:A:TYR:HA	6	0.62	0.05	0.62
(1,701)	1:14:A:ARG:HA	1:14:A:ARG:HD3	6	0.22	0.22	0.12
(1,555)	1:34:A:TRP:HH2	1:23:A:TYR:HB3	6	0.16	0.05	0.15
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG21	5	0.83	0.27	0.77
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG22	5	0.83	0.27	0.77
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG23	5	0.83	0.27	0.77
(1,87)	1:23:A:TYR:HE1	1:16:A:SER:HB3	5	0.62	0.11	0.61
(1,87)	1:23:A:TYR:HE2	1:16:A:SER:HB3	5	0.62	0.11	0.61
(1,375)	1:28:A:ILE:H	1:29:A:THR:HB	5	0.37	0.05	0.38
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD21	5	0.16	0.04	0.17
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD22	5	0.16	0.04	0.17
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD23	5	0.16	0.04	0.17
(1,755)	1:27:A:HIS:HE1	1:12:A:GLU:HG2	4	0.46	0.6	0.12
(1,376)	1:39:A:GLY:H	1:8:A:PRO:HG3	4	0.41	0.16	0.39
(1,833)	1:11:A:TRP:HZ2	1:8:A:PRO:HB2	4	0.31	0.07	0.3
(1,362)	1:7:A:LEU:H	1:36:A:ARG:HG3	4	0.2	0.05	0.2
(1,483)	1:24:A:TYR:HD1	1:37:A:PRO:HB2	4	0.18	0.03	0.18
(1,483)	1:24:A:TYR:HD2	1:37:A:PRO:HB2	4	0.18	0.03	0.18
(1,313)	1:11:A:TRP:HE3	1:24:A:TYR:HB2	4	0.15	0.01	0.15
(1,227)	1:34:A:TRP:HE3	1:21:A:ARG:HB2	3	0.52	0.04	0.52
(1,135)	1:34:A:TRP:HE3	1:16:A:SER:HB3	3	0.29	0.09	0.24
(1,633)	1:18:A:SER:HB2	1:17:A:ARG:HB3	3	0.21	0.06	0.19
(1,758)	1:30:A:ASN:H	1:26:A:ASN:HD22	3	0.2	0.03	0.19
(1,575)	1:34:A:TRP:HZ2	2:86:B:PRO:HG3	3	0.16	0.02	0.17
(1,484)	1:24:A:TYR:HE1	1:36:A:ARG:HG2	3	0.16	0.02	0.16
(1,484)	1:24:A:TYR:HE2	1:36:A:ARG:HG2	3	0.16	0.02	0.16
(1,129)	1:7:A:LEU:HB2	1:8:A:PRO:HD3	3	0.15	0.03	0.17

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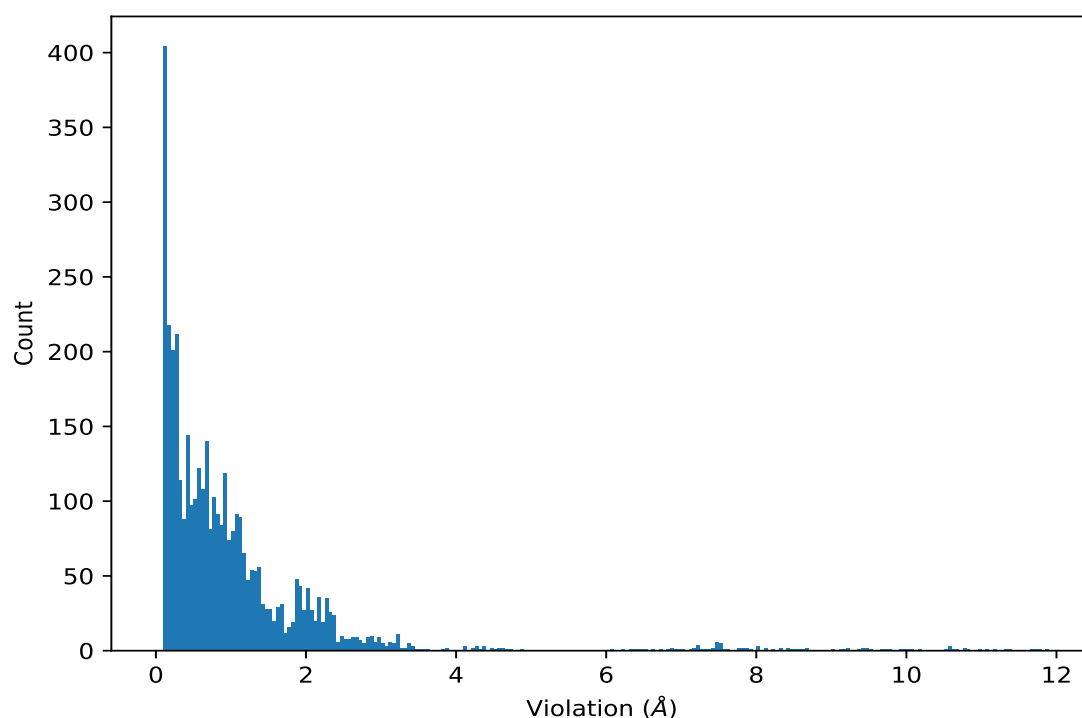
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,792)	1:11:A:TRP:HE3	1:33:A:GLN:HE21	3	0.14	0.02	0.15
(1,481)	1:25:A:PHE:HD1	1:14:A:ARG:HB2	3	0.11	0.01	0.11
(1,481)	1:25:A:PHE:HD2	1:14:A:ARG:HB2	3	0.11	0.01	0.11
(1,810)	1:11:A:TRP:HE3	1:33:A:GLN:HG2	2	1.48	0.01	1.48
(1,214)	1:14:A:ARG:H	1:13:A:LYS:HE2	2	0.9	0.02	0.9
(1,858)	1:22:A:VAL:HG11	1:13:A:LYS:HB2	2	0.68	0.06	0.68
(1,858)	1:22:A:VAL:HG12	1:13:A:LYS:HB2	2	0.68	0.06	0.68
(1,858)	1:22:A:VAL:HG13	1:13:A:LYS:HB2	2	0.68	0.06	0.68
(1,770)	1:25:A:PHE:HE1	1:14:A:ARG:HD2	2	0.64	0.2	0.64
(1,770)	1:25:A:PHE:HE2	1:14:A:ARG:HD2	2	0.64	0.2	0.64
(1,435)	1:33:A:GLN:HE21	1:37:A:PRO:HB2	2	0.54	0.1	0.54
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD21	2	0.3	0.01	0.3
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD22	2	0.3	0.01	0.3
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD23	2	0.3	0.01	0.3
(1,527)	1:11:A:TRP:HD1	1:8:A:PRO:HB2	2	0.21	0.0	0.21
(1,520)	1:11:A:TRP:HZ3	1:33:A:GLN:HA	2	0.18	0.03	0.18
(1,192)	1:9:A:PRO:HD3	1:8:A:PRO:HG3	2	0.16	0.01	0.16
(1,667)	1:37:A:PRO:HD3	1:36:A:ARG:HB2	2	0.11	0.0	0.11
(1,851)	1:7:A:LEU:HD11	1:37:A:PRO:HD3	2	0.11	0.01	0.11
(1,851)	1:7:A:LEU:HD12	1:37:A:PRO:HD3	2	0.11	0.01	0.11
(1,851)	1:7:A:LEU:HD13	1:37:A:PRO:HD3	2	0.11	0.01	0.11
(1,591)	1:22:A:VAL:HG11	1:22:A:VAL:HA	2	0.11	0.0	0.11
(1,591)	1:22:A:VAL:HG12	1:22:A:VAL:HA	2	0.11	0.0	0.11
(1,591)	1:22:A:VAL:HG13	1:22:A:VAL: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)
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	23	11.87
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	23	11.79
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	10	11.71
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	8	11.68
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	3	11.38
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	4	11.31
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	21	11.15
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	4	11.05
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	22	10.99
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	13	10.82
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	11	10.77
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	17	10.77
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	12	10.68
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	24	10.63
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	16	10.59
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	6	10.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	19	10.57
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	17	10.5
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	20	10.15
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	8	10.06
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	12	10.01
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	7	9.96
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	15	9.91
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	5	9.77
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	1	9.74
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	14	9.69
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	18	9.5
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	5	9.47
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	19	9.46
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	2	9.45
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	12	9.4
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	8	9.37
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	2	9.23
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	14	9.22
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	25	9.18
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	20	9.1
(1,322)	1:17:A:ARG:HD3	2:81:B:GLY:HA2	9	9.0
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	17	8.68
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	8	8.65
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	17	8.6
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	9	8.57
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	11	8.5
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	7	8.47
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	10	8.44
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	11	8.43
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	9	8.33
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	4	8.31
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	6	8.22
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	24	8.14
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	1	8.13
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	15	8.03
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	21	8.03
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	23	8.0
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	2	7.91
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	22	7.89
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	25	7.86
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	3	7.85
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	20	7.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	25	7.77
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	16	7.77
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	25	7.61
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	22	7.56
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	16	7.54
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	1	7.52
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	1	7.51
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	2	7.5
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	21	7.5
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	6	7.49
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	4	7.49
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	22	7.47
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	13	7.46
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	12	7.45
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	6	7.45
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	18	7.43
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	23	7.4
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	3	7.36
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	9	7.33
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	7	7.28
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	18	7.24
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	5	7.22
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	16	7.21
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	19	7.21
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	5	7.17
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	18	7.17
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	3	7.14
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	20	7.0
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	13	6.95
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	21	6.9
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	14	6.88
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	14	6.87
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	10	6.83
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	10	6.71
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	24	6.63
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	15	6.54
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	11	6.46
(1,756)	1:41:A:SER:H	1:6:A:LYS:HB2	19	6.42
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	13	6.39
(1,722)	2:90:B:GLY:HA2	1:21:A:ARG:HG3	24	6.31
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	15	6.24
(1,248)	2:90:B:GLY:HA2	1:18:A:SER:HA	7	6.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	2	4.89
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	18	4.71
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	1	4.66
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	11	4.64
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	16	4.64
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	19	4.58
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	25	4.56
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	5	4.5
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	7	4.48
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	10	4.48
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	20	4.38
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	15	4.37
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	24	4.36
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	12	4.33
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	9	4.28
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	17	4.25
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	21	4.25
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	14	4.23
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	3	4.2
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	23	4.14
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	13	4.13
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	22	4.12
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	4	3.87
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	8	3.85
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	24	3.81
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	14	3.61
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	13	3.58
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	23	3.5
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	12	3.45
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	5	3.44
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	4	3.42
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	13	3.41
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	17	3.4
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	5	3.39
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	3	3.38
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	14	3.36
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	20	3.36
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	24	3.33
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	10	3.31
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	3	3.3
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	19	3.3
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	13	3.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	13	3.22
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	13	3.22
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	17	3.21
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	17	3.21
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	17	3.21
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	24	3.21
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	12	3.2
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	12	3.2
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	12	3.2
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	21	3.2
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	8	3.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	8	3.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	8	3.18
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	14	3.17
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	17	3.17
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	22	3.14
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	16	3.13
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	8	3.13
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	24	3.13
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	23	3.12
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	2	3.1
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	1	3.08
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	18	3.07
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	25	3.07
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	11	3.04
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	12	3.02
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	19	3.02
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	14	3.02
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	17	3.0
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	9	2.99
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	4	2.98
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	7	2.98
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	1	2.97
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	2	2.97
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	16	2.97
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	1	2.96
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	8	2.96
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	18	2.95
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	25	2.94
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	16	2.93
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	8	2.92
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	21	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	25	2.92
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	15	2.91
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	6	2.9
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	20	2.9
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	7	2.89
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	11	2.88
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	11	2.88
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	11	2.87
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	2	2.86
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	20	2.86
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	6	2.85
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	3	2.85
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	12	2.84
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	21	2.84
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	15	2.83
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	10	2.82
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	20	2.82
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	13	2.82
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	23	2.82
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	12	2.82
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	13	2.81
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	22	2.79
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	16	2.78
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	19	2.78
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	15	2.77
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	16	2.77
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	7	2.73
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	10	2.72
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	9	2.72
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	20	2.72
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	2	2.72
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	11	2.7
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	6	2.7
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	12	2.69
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	6	2.68
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	8	2.68
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	7	2.67
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	18	2.67
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	19	2.67
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	15	2.66
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	5	2.66
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	22	2.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	4	2.64
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	22	2.63
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	7	2.63
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	4	2.62
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	1	2.62
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	2	2.61
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	12	2.61
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	8	2.61
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	14	2.6
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	18	2.58
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	21	2.58
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	3	2.57
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	5	2.57
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	2	2.57
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	3	2.56
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	19	2.56
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	23	2.56
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	15	2.55
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	13	2.55
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	20	2.54
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	21	2.54
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	1	2.53
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	25	2.53
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	17	2.52
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	1	2.5
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	7	2.49
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	17	2.49
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	10	2.48
(1,468)	2:85:B:SEP:H	1:14:A:ARG:HB3	6	2.48
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	7	2.47
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	25	2.47
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	19	2.47
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	10	2.46
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	14	2.45
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	21	2.45
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	13	2.44
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	25	2.43
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	10	2.43
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	9	2.43
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	17	2.42
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	6	2.41
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	16	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	16	2.4
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	16	2.4
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	17	2.4
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	17	2.4
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	17	2.4
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	1	2.38
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	1	2.38
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	1	2.38
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	3	2.38
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	15	2.37
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	15	2.37
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	15	2.37
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	7	2.36
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	7	2.36
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	7	2.36
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	22	2.35
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	18	2.35
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	18	2.35
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	18	2.35
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	24	2.35
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	24	2.35
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	24	2.35
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	4	2.35
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	20	2.34
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	20	2.34
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	20	2.34
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	3	2.34
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	3	2.34
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	3	2.34
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	4	2.34
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	2	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	2	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	2	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	10	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	10	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	10	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	21	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	21	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	21	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	23	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	23	2.32
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	23	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:34:A:TRP:HH2	1:17:A:ARG:HG2	9	2.31
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	7	2.31
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	7	2.31
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	11	2.31
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	11	2.31
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	23	2.31
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	23	2.31
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	23	2.3
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	14	2.3
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	4	2.29
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	4	2.29
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	4	2.29
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	7	2.29
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	7	2.29
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	7	2.29
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	4	2.28
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	4	2.28
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	4	2.28
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	18	2.28
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	18	2.28
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	18	2.28
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	18	2.27
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	8	2.27
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	8	2.27
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	8	2.27
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	6	2.26
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	6	2.26
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	6	2.26
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	16	2.26
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	16	2.26
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	16	2.26
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	15	2.26
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	14	2.25
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	14	2.25
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	5	2.25
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	5	2.25
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	5	2.25
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	19	2.25
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	19	2.25
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	19	2.25
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	1	2.25
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	1	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	21	2.22
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	21	2.22
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	21	2.22
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	14	2.22
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	14	2.22
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	14	2.22
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	17	2.21
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	17	2.21
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	17	2.21
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	23	2.21
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	23	2.21
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	23	2.21
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	25	2.21
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	25	2.21
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	25	2.21
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	20	2.21
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	20	2.21
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	22	2.2
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	20	2.2
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	23	2.19
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	23	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	2	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	2	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	2	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	4	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	4	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	4	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	25	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	25	2.19
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	25	2.19
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	6	2.19
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	6	2.19
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	15	2.18
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	15	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	3	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	3	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	3	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	15	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	15	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	15	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	16	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	16	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	16	2.18
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	24	2.18
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	11	2.17
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	11	2.17
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	11	2.17
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	7	2.17
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	25	2.17
(1,697)	2:85:B:SEP:HB3	1:17:A:ARG:HA	24	2.16
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	20	2.16
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	20	2.16
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	7	2.15
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	7	2.15
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	7	2.15
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	3	2.14
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	3	2.14
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	21	2.14
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	21	2.14
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	24	2.14
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	24	2.14
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	22	2.13
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	22	2.13
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	6	2.12
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	11	2.12
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	20	2.11
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	20	2.11
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	20	2.11
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	15	2.11
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	15	2.11
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	25	2.1
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	14	2.1
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	14	2.1
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	14	2.1
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	15	2.1
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	16	2.09
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	8	2.09
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	6	2.09
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	6	2.09
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	2	2.08
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	2	2.08
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	2	2.08
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	15	2.08
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	15	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	15	2.08
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	12	2.08
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	12	2.08
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	12	2.08
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	22	2.08
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	22	2.08
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	22	2.08
(1,643)	2:85:B:SEP:HB2	1:17:A:ARG:HG2	9	2.08
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	17	2.08
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	17	2.08
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	3	2.07
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	5	2.07
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	12	2.07
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	12	2.07
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	5	2.06
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	5	2.06
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	5	2.06
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	1	2.06
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	3	2.05
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	3	2.05
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	3	2.05
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	15	2.05
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	13	2.05
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	13	2.05
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	13	2.05
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	19	2.05
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	14	2.04
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	14	2.04
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	14	2.04
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	10	2.04
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	5	2.04
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	5	2.04
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	20	2.03
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	20	2.03
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	20	2.03
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	2	2.03
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	4	2.03
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	9	2.03
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	11	2.03
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	12	2.03
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	20	2.03
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	5	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	5	2.03
(1,641)	2:85:B:SEP:HB2	1:17:A:ARG:HB2	24	2.03
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	13	2.03
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	13	2.03
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	19	2.02
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	19	2.02
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	18	2.01
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	18	2.01
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	18	2.01
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	7	2.01
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	8	2.01
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	8	2.01
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	14	2.01
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	25	2.0
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	25	2.0
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	25	2.0
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	13	2.0
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	24	2.0
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	24	1.99
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	24	1.99
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	24	1.99
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	24	1.99
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	24	1.99
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	12	1.99
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	21	1.98
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	10	1.97
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	10	1.97
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	12	1.97
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	12	1.97
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	25	1.97
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	25	1.97
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	8	1.96
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	8	1.96
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	8	1.96
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	19	1.96
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	21	1.96
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	19	1.96
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	19	1.96
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	19	1.96
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	1	1.96
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	1	1.96
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	8	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	8	1.96
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	16	1.96
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	16	1.96
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	8	1.95
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	25	1.95
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	25	1.95
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	2	1.95
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	2	1.95
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	10	1.94
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	10	1.94
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	4	1.94
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	4	1.94
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	3	1.94
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	3	1.94
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	16	1.94
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	16	1.94
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	16	1.94
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	9	1.93
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	9	1.93
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	9	1.93
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	13	1.93
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	13	1.93
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	13	1.93
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	14	1.93
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	23	1.93
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	2	1.93
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	2	1.93
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	11	1.93
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	11	1.93
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	19	1.93
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	19	1.93
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	10	1.92
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	10	1.92
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	10	1.92
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	5	1.92
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	16	1.92
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	18	1.92
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	18	1.92
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	17	1.91
(1,621)	1:33:A:GLN:HG2	1:37:A:PRO:HD2	18	1.91
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	2	1.91
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	2	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	13	1.91
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	13	1.91
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	10	1.91
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	10	1.91
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	16	1.9
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	16	1.9
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	23	1.9
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	11	1.9
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	11	1.9
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	11	1.9
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	4	1.9
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	4	1.9
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	1	1.89
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	1	1.89
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	1	1.89
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	9	1.89
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	9	1.89
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	21	1.89
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	21	1.89
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	1	1.89
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	10	1.89
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	18	1.89
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	18	1.89
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	18	1.89
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	11	1.88
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	11	1.88
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	11	1.88
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	12	1.88
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	12	1.88
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	11	1.88
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	9	1.88
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	9	1.88
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	21	1.88
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	21	1.88
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	6	1.88
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	6	1.88
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	6	1.88
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	25	1.87
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	25	1.87
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	3	1.87
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	14	1.87
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	14	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	19	1.86
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	19	1.86
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	4	1.86
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	4	1.86
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	7	1.86
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	7	1.86
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	19	1.85
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	19	1.85
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	19	1.85
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	2	1.85
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	6	1.84
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	6	1.84
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	6	1.84
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	22	1.84
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	22	1.84
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	23	1.83
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	23	1.83
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	23	1.83
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	20	1.83
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	20	1.83
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	22	1.83
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	18	1.82
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	18	1.82
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	13	1.82
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	13	1.82
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	11	1.81
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	11	1.81
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD1	8	1.8
(1,145)	1:27:A:HIS:HE1	1:25:A:PHE:HD2	8	1.8
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	1	1.78
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	1	1.78
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	17	1.78
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	17	1.78
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	18	1.78
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	18	1.78
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	4	1.77
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	4	1.77
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	8	1.77
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	22	1.77
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	22	1.77
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	6	1.76
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	6	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	12	1.75
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	12	1.75
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	12	1.75
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	8	1.74
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	9	1.74
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	9	1.74
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	9	1.74
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	5	1.74
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	13	1.71
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	13	1.71
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	6	1.71
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD21	5	1.71
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD22	5	1.71
(1,736)	1:33:A:GLN:H	1:7:A:LEU:HD23	5	1.71
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	20	1.71
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	12	1.7
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	17	1.7
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	3	1.7
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	3	1.7
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	23	1.69
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	23	1.69
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	19	1.69
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	24	1.69
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	14	1.68
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	9	1.68
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	9	1.68
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	6	1.68
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	2	1.67
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	1	1.67
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	1	1.67
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	1	1.67
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	21	1.67
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	24	1.67
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	14	1.67
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	12	1.67
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	12	1.67
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	12	1.67
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	8	1.66
(1,762)	1:23:A:TYR:HE1	1:17:A:ARG:HG3	11	1.66
(1,762)	1:23:A:TYR:HE2	1:17:A:ARG:HG3	11	1.66
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	5	1.66
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	7	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	15	1.66
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	16	1.66
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	7	1.66
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	7	1.66
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	11	1.65
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	13	1.65
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	25	1.65
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	20	1.65
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	8	1.64
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	1	1.64
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	2	1.64
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	6	1.64
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	23	1.64
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	23	1.64
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	4	1.64
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	4	1.64
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB1	22	1.63
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB2	22	1.63
(1,857)	1:28:A:ILE:HG13	1:31:A:ALA:HB3	22	1.63
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	17	1.63
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	24	1.63
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	10	1.62
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	15	1.62
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	15	1.62
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	17	1.62
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	17	1.62
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	16	1.62
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	16	1.62
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	16	1.62
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	14	1.62
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	10	1.61
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	9	1.6
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	25	1.6
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	20	1.59
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	7	1.59
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	13	1.58
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	6	1.58
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	6	1.58
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	6	1.58
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	7	1.57
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	7	1.57
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	20	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	13	1.57
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	15	1.57
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	15	1.57
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	15	1.57
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	23	1.57
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	10	1.55
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	10	1.55
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	10	1.55
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	3	1.55
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	4	1.55
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	15	1.55
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	19	1.54
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	6	1.54
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	6	1.53
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	25	1.53
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	5	1.53
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	5	1.53
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	9	1.53
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	9	1.53
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	9	1.53
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	23	1.53
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	1	1.52
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	3	1.52
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	21	1.52
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	21	1.52
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	21	1.52
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	14	1.52
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	6	1.52
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	6	1.52
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	6	1.52
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	15	1.51
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	16	1.51
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	17	1.51
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	24	1.51
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	24	1.51
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	7	1.51
(1,755)	1:27:A:HIS:HE1	1:12:A:GLU:HG2	6	1.5
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	16	1.5
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	16	1.5
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	22	1.49
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	19	1.49
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	6	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	23	1.49
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	20	1.49
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	20	1.49
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	20	1.49
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	7	1.48
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	12	1.48
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	21	1.48
(1,810)	1:11:A:TRP:HE3	1:33:A:GLN:HG2	14	1.48
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	12	1.48
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	24	1.48
(1,810)	1:11:A:TRP:HE3	1:33:A:GLN:HG2	24	1.47
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	11	1.47
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	11	1.47
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	21	1.47
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	21	1.47
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD21	24	1.47
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD22	24	1.47
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD23	24	1.47
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	14	1.46
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	22	1.46
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	24	1.46
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	24	1.46
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	24	1.46
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	10	1.46
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	22	1.46
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	9	1.45
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	13	1.45
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	22	1.45
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	25	1.45
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	6	1.44
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	13	1.44
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	6	1.44
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	10	1.44
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	18	1.44
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	15	1.44
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	2	1.44
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	2	1.44
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	5	1.44
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	5	1.44
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	23	1.43
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	14	1.43
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	17	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	19	1.42
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	18	1.42
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	15	1.42
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	16	1.42
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	19	1.42
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	20	1.42
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	20	1.41
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	24	1.41
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	16	1.41
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	19	1.41
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	19	1.41
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	19	1.41
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	17	1.41
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	17	1.41
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	10	1.4
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	5	1.4
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	20	1.4
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	1	1.4
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	23	1.4
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	23	1.4
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	10	1.4
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	10	1.4
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	10	1.4
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	18	1.4
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	18	1.4
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	18	1.4
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	2	1.39
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	1	1.39
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	1	1.39
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	1	1.39
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	3	1.38
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	4	1.38
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	23	1.38
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	4	1.38
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	16	1.38
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	25	1.38
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	25	1.38
(1,820)	1:21:A:ARG:HB3	1:19:A:SER:HA	11	1.37
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	7	1.37
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	22	1.37
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	22	1.37
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	5	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	7	1.37
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	3	1.37
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	18	1.37
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	21	1.37
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	14	1.37
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	14	1.37
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	21	1.36
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	23	1.36
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	9	1.36
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	9	1.36
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	9	1.36
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	15	1.36
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	7	1.36
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	7	1.36
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	15	1.36
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	15	1.36
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	11	1.35
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	21	1.35
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	3	1.35
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	21	1.35
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	13	1.35
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	21	1.35
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	21	1.35
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	21	1.35
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	1	1.35
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	1	1.35
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	20	1.35
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	20	1.35
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	3	1.34
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	8	1.34
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	20	1.34
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	20	1.34
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	19	1.34
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	19	1.34
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	9	1.34
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	1	1.33
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	18	1.33
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	25	1.33
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	23	1.33
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	24	1.33
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	10	1.33
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	12	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	6	1.33
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	6	1.33
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	22	1.33
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	22	1.33
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	10	1.33
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	10	1.33
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	12	1.33
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	12	1.33
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	18	1.33
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	6	1.32
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	12	1.32
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	7	1.32
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	20	1.32
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	20	1.32
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	3	1.32
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	3	1.32
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	6	1.32
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	6	1.32
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	4	1.32
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	16	1.32
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	21	1.31
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	9	1.31
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	9	1.31
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	4	1.31
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	11	1.31
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	14	1.31
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	8	1.31
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	14	1.31
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	18	1.3
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	7	1.3
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	9	1.3
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	8	1.3
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	8	1.3
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	24	1.3
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	17	1.3
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	18	1.3
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	10	1.3
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	10	1.3
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	10	1.3
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	1	1.29
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	22	1.29
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	25	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	11	1.29
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	14	1.29
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	25	1.29
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	9	1.29
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	9	1.29
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	2	1.28
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	5	1.28
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	5	1.28
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	5	1.28
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	13	1.28
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	10	1.28
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	19	1.28
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	2	1.28
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	19	1.28
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	22	1.28
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	17	1.27
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	16	1.27
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	5	1.27
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	6	1.27
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	21	1.27
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	25	1.27
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	4	1.27
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	15	1.27
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	10	1.27
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	1	1.27
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	22	1.27
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	22	1.27
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	22	1.27
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	5	1.26
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	2	1.26
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	4	1.26
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	22	1.26
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	22	1.26
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	10	1.26
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	10	1.26
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	5	1.26
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	6	1.26
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	24	1.26
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	5	1.26
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	16	1.26
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	12	1.25
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	5	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	7	1.25
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	5	1.25
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	3	1.25
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	3	1.25
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	3	1.25
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	1	1.25
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	1	1.25
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	8	1.25
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	8	1.25
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	7	1.24
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	25	1.24
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	2	1.24
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	15	1.24
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	18	1.24
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	18	1.24
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	2	1.24
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	9	1.24
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	17	1.24
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	24	1.23
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	2	1.23
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	14	1.23
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	14	1.23
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	23	1.23
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	23	1.23
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	23	1.23
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	1	1.23
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	4	1.23
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	4	1.23
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	4	1.23
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	11	1.23
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	11	1.23
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	19	1.23
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	19	1.23
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	22	1.23
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	22	1.23
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	15	1.22
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	11	1.22
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	17	1.22
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	3	1.22
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	2	1.22
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	11	1.22
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	16	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	19	1.22
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	11	1.22
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	11	1.22
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	11	1.22
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	17	1.22
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG21	23	1.21
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG22	23	1.21
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG23	23	1.21
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	5	1.21
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	20	1.21
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	8	1.21
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	8	1.21
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	12	1.21
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	12	1.21
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	3	1.2
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	11	1.2
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	8	1.2
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	25	1.2
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	25	1.2
(1,751)	1:33:A:GLN:HE21	1:8:A:PRO:HG3	9	1.2
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	16	1.2
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	8	1.2
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	21	1.2
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	8	1.2
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	20	1.2
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	2	1.2
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	2	1.2
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	18	1.2
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	18	1.2
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	10	1.2
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	13	1.2
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD21	7	1.2
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD22	7	1.2
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD23	7	1.2
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	25	1.19
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	4	1.19
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	4	1.19
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	23	1.19
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	23	1.19
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	10	1.19
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	23	1.19
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	6	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	14	1.19
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	14	1.19
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	12	1.18
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	19	1.18
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	19	1.18
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	19	1.18
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	1	1.18
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	13	1.18
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	3	1.18
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	10	1.18
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	13	1.18
(1,370)	1:22:A:VAL:H	1:16:A:SER:HB2	12	1.18
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	23	1.18
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	23	1.18
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	6	1.18
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	6	1.18
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	6	1.18
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	25	1.18
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	18	1.17
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	16	1.17
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	9	1.17
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	11	1.17
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	15	1.17
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	21	1.17
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	21	1.17
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	18	1.16
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	1	1.16
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	22	1.16
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	22	1.16
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	2	1.16
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	2	1.16
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	2	1.16
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	23	1.16
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	18	1.16
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	12	1.16
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	12	1.16
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	12	1.16
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	11	1.15
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	1	1.15
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	4	1.15
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	4	1.15
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	25	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	25	1.15
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	1	1.15
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	17	1.15
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	16	1.15
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	16	1.15
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	8	1.14
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	19	1.14
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	24	1.14
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	7	1.14
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	11	1.14
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	20	1.14
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	25	1.14
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD21	17	1.14
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD22	17	1.14
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD23	17	1.14
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	22	1.13
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	24	1.13
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	12	1.13
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	13	1.13
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	13	1.13
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	25	1.13
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	10	1.13
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	10	1.13
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	14	1.13
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	14	1.13
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	14	1.13
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	9	1.13
(1,352)	1:16:A:SER:H	1:14:A:ARG:HB3	8	1.13
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	2	1.13
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	3	1.13
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	1	1.12
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	5	1.12
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	5	1.12
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	4	1.12
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	20	1.12
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	12	1.12
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	11	1.12
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	16	1.12
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	16	1.12
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	1	1.12
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	1	1.12
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	12	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	13	1.12
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	25	1.12
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	25	1.12
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	25	1.12
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	16	1.12
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD21	23	1.12
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD22	23	1.12
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD23	23	1.12
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	8	1.11
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	1	1.11
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	1	1.11
(1,760)	2:85:B:SEP:H	1:34:A:TRP:HZ2	19	1.11
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	13	1.11
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	13	1.11
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	13	1.11
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	15	1.11
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	6	1.11
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	12	1.11
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	12	1.11
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	18	1.11
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	18	1.11
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	23	1.11
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	23	1.11
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	17	1.11
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	21	1.11
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	5	1.11
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	5	1.11
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	15	1.11
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	15	1.11
(1,217)	1:16:A:SER:HB2	1:21:A:ARG:HG2	13	1.11
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	2	1.11
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	23	1.11
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD21	25	1.11
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD22	25	1.11
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD23	25	1.11
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	2	1.1
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	3	1.1
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	1	1.1
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	2	1.1
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	2	1.1
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	9	1.1
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	9	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	1	1.09
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	12	1.09
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	12	1.09
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	12	1.09
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	18	1.09
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	21	1.09
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	3	1.09
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	3	1.09
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	19	1.09
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	15	1.09
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	22	1.08
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	22	1.08
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	22	1.08
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	10	1.08
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	24	1.08
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	24	1.08
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	24	1.08
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	4	1.08
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	4	1.08
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	24	1.08
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	24	1.08
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	12	1.08
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	18	1.08
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	13	1.08
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	23	1.07
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	6	1.07
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	13	1.07
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	2	1.07
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	2	1.07
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	12	1.07
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	12	1.07
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	20	1.07
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	20	1.07
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	12	1.07
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	13	1.07
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	19	1.07
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	20	1.07
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	14	1.07
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	15	1.07
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	8	1.07
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	8	1.07
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	8	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	17	1.07
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	17	1.07
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	17	1.07
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	18	1.07
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	13	1.07
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	13	1.07
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	25	1.07
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	25	1.07
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	12	1.07
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	12	1.07
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	12	1.07
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	6	1.07
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	6	1.07
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	4	1.07
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	8	1.07
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	19	1.06
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	20	1.06
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	15	1.06
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	15	1.06
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	16	1.06
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	16	1.06
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	17	1.06
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	17	1.06
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	3	1.06
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	10	1.06
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	7	1.06
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	21	1.06
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	6	1.06
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	6	1.06
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	23	1.06
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	23	1.06
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	22	1.06
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	22	1.06
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	25	1.05
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	21	1.05
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	11	1.05
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	11	1.05
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	11	1.05
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	3	1.05
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	4	1.05
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	22	1.05
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	13	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	13	1.05
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	25	1.05
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	9	1.05
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	1	1.05
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	3	1.05
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	17	1.05
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	21	1.05
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	3	1.04
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	3	1.04
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	11	1.04
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	11	1.04
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	7	1.04
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	3	1.04
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	10	1.04
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	25	1.04
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	22	1.04
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	7	1.04
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	7	1.04
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	9	1.03
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	6	1.03
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	6	1.03
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	14	1.03
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	14	1.03
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	14	1.03
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	14	1.03
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	14	1.03
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	2	1.03
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	19	1.03
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	6	1.03
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	20	1.03
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	11	1.03
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	11	1.03
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	3	1.03
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	5	1.03
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	3	1.03
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	5	1.03
(1,298)	1:24:A:TYR:HE1	1:34:A:TRP:HA	17	1.03
(1,298)	1:24:A:TYR:HE2	1:34:A:TRP:HA	17	1.03
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	4	1.03
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	1	1.03
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	6	1.03
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	9	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	2	1.02
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	17	1.02
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	14	1.02
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	20	1.02
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	7	1.02
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	7	1.02
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	10	1.02
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	10	1.02
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	17	1.02
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	5	1.02
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	9	1.02
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	9	1.02
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	13	1.02
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	13	1.02
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	10	1.02
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	18	1.02
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	20	1.01
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	11	1.01
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	17	1.01
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	23	1.01
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	2	1.01
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	20	1.01
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	20	1.01
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	14	1.01
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	22	1.01
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG11	7	1.01
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG12	7	1.01
(1,305)	1:13:A:LYS:HA	1:22:A:VAL:HG13	7	1.01
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	12	1.01
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	12	1.01
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	23	1.01
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	8	1.0
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	19	1.0
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	19	1.0
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	21	1.0
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	21	1.0
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	12	1.0
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	3	1.0
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	16	1.0
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	16	1.0
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	24	1.0
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	11	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	11	1.0
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	16	1.0
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	25	1.0
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	7	0.99
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	21	0.99
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG21	1	0.99
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG22	1	0.99
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG23	1	0.99
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	14	0.99
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	18	0.99
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	18	0.99
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	4	0.99
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	5	0.99
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	22	0.99
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	1	0.99
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	1	0.99
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	18	0.99
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	23	0.99
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	20	0.99
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	20	0.99
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	4	0.98
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	19	0.98
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	8	0.98
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	8	0.98
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	9	0.98
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	9	0.98
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	19	0.98
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	14	0.98
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	17	0.98
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	25	0.98
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	18	0.98
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	5	0.98
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	5	0.98
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	13	0.98
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	20	0.98
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	20	0.98
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	20	0.98
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	1	0.98
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	16	0.98
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	21	0.98
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	21	0.97
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	15	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	17	0.97
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	20	0.97
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	15	0.97
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	16	0.97
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	19	0.97
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	19	0.97
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	6	0.97
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	9	0.97
(1,356)	1:16:A:SER:H	1:19:A:SER:HA	4	0.97
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	14	0.97
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	14	0.97
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	19	0.97
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	7	0.97
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	10	0.97
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	20	0.97
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	20	0.97
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	20	0.97
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	19	0.96
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	14	0.96
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	21	0.96
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	25	0.96
(1,501)	1:24:A:TYR:HE1	1:33:A:GLN:HG2	5	0.96
(1,501)	1:24:A:TYR:HE2	1:33:A:GLN:HG2	5	0.96
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	5	0.96
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	5	0.96
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	5	0.96
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	24	0.96
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	1	0.96
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	1	0.96
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	10	0.96
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	10	0.96
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	2	0.96
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	1	0.96
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	1	0.96
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	1	0.96
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	5	0.95
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	16	0.95
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	13	0.95
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	13	0.95
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	24	0.95
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	24	0.95
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	18	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	18	0.95
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	20	0.95
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	20	0.95
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	20	0.95
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	18	0.95
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	8	0.95
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	12	0.95
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	2	0.95
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	2	0.95
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	7	0.95
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	21	0.95
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	19	0.95
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	19	0.95
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	19	0.95
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	4	0.95
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	19	0.95
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	10	0.94
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	5	0.94
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	23	0.94
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	24	0.94
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	18	0.94
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	24	0.94
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	14	0.94
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	14	0.94
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	11	0.94
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	11	0.94
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	15	0.94
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	15	0.94
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	6	0.94
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	6	0.94
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	6	0.94
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	12	0.94
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	3	0.94
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	5	0.93
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	10	0.93
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	24	0.93
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	15	0.93
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	16	0.93
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	9	0.93
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG21	7	0.93
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG22	7	0.93
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG23	7	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	19	0.93
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	19	0.93
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	23	0.93
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	9	0.93
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD21	15	0.93
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD22	15	0.93
(1,23)	1:36:A:ARG:HD2	1:7:A:LEU:HD23	15	0.93
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	24	0.92
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	4	0.92
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	10	0.92
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	10	0.92
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	15	0.92
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	14	0.92
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	21	0.92
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	4	0.92
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	4	0.92
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	7	0.92
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	7	0.92
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG11	21	0.92
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG12	21	0.92
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG13	21	0.92
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	18	0.92
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	18	0.92
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	1	0.92
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	11	0.92
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	14	0.92
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	15	0.92
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	20	0.92
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	22	0.92
(1,214)	1:14:A:ARG:H	1:13:A:LYS:HE2	9	0.92
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	2	0.92
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	2	0.92
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	24	0.92
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	24	0.92
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	24	0.92
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	20	0.92
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	15	0.92
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	15	0.92
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	15	0.92
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	10	0.91
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	16	0.91
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	16	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	12	0.91
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	12	0.91
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	2	0.91
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	2	0.91
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	2	0.91
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	2	0.91
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	5	0.91
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	8	0.91
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	10	0.91
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	7	0.91
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	17	0.91
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	25	0.91
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	4	0.91
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	14	0.9
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	1	0.9
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	23	0.9
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	23	0.9
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	1	0.9
(1,764)	1:23:A:TYR:HD1	1:14:A:ARG:HB3	22	0.9
(1,764)	1:23:A:TYR:HD2	1:14:A:ARG:HB3	22	0.9
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	11	0.9
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	11	0.9
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD11	6	0.9
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD12	6	0.9
(1,676)	1:8:A:PRO:HD3	1:7:A:LEU:HD13	6	0.9
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	2	0.9
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	6	0.9
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	25	0.9
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	15	0.89
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	3	0.89
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	9	0.89
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	6	0.89
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	9	0.89
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	24	0.89
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	24	0.89
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	10	0.89
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	10	0.89
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	6	0.89
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	10	0.89
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	10	0.89
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	10	0.89
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	18	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	18	0.89
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	18	0.89
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	3	0.89
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	7	0.89
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	19	0.89
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	24	0.89
(1,214)	1:14:A:ARG:H	1:13:A:LYS:HE2	14	0.89
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	17	0.89
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	12	0.89
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	19	0.88
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	19	0.88
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	19	0.88
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	11	0.88
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	17	0.88
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	23	0.88
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	15	0.88
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	3	0.88
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	17	0.88
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	20	0.88
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	17	0.88
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	17	0.88
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	1	0.88
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	2	0.88
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	11	0.88
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	25	0.88
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	9	0.88
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	9	0.88
(1,219)	1:16:A:SER:HB2	1:15:A:MET:HA	21	0.88
(1,215)	1:14:A:ARG:H	1:13:A:LYS:HG2	16	0.88
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	15	0.88
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	12	0.87
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	8	0.87
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	8	0.87
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG21	3	0.87
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG22	3	0.87
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG23	3	0.87
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG21	21	0.87
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG22	21	0.87
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG23	21	0.87
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	9	0.87
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	9	0.87
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG11	3	0.87
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG12	3	0.87
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG13	3	0.87
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	1	0.87
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	1	0.87
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	1	0.87
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	23	0.87
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	16	0.87
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	16	0.87
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	17	0.86
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	6	0.86
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	6	0.86
(1,741)	1:14:A:ARG:H	1:15:A:MET:HG2	18	0.86
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	7	0.86
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	11	0.86
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	18	0.86
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	3	0.86
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	3	0.86
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	14	0.86
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	14	0.86
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	19	0.86
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	19	0.86
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	1	0.86
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	8	0.86
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	8	0.86
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	11	0.86
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	3	0.86
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	3	0.86
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	18	0.85
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	22	0.85
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	12	0.85
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	10	0.85
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	2	0.85
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	15	0.85
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	15	0.85
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	20	0.85
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	24	0.85
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	24	0.85
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	24	0.85
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	25	0.85
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	12	0.85
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	12	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	12	0.85
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	13	0.84
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	25	0.84
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	19	0.84
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	19	0.84
(1,770)	1:25:A:PHE:HE1	1:14:A:ARG:HD2	7	0.84
(1,770)	1:25:A:PHE:HE2	1:14:A:ARG:HD2	7	0.84
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	22	0.84
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	22	0.84
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	12	0.84
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	21	0.84
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	18	0.84
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	18	0.84
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	4	0.84
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	4	0.84
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	21	0.84
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	21	0.84
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	13	0.84
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	7	0.83
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	2	0.83
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	6	0.83
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	9	0.83
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	9	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG11	7	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG12	7	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG13	7	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG11	15	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG12	15	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG13	15	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG11	25	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG12	25	0.83
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG13	25	0.83
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	16	0.83
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	16	0.83
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	22	0.83
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	22	0.83
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	20	0.83
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	20	0.83
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	20	0.83
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	6	0.82
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	18	0.82
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	8	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	19	0.82
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	21	0.82
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	21	0.82
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	18	0.82
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	18	0.82
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	11	0.82
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	19	0.82
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	19	0.82
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	19	0.82
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	20	0.81
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	20	0.81
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	9	0.81
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	7	0.81
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	5	0.81
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	5	0.81
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	8	0.81
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	8	0.81
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	13	0.81
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	13	0.81
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	15	0.81
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	10	0.81
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	3	0.8
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	17	0.8
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	17	0.8
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	25	0.8
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	20	0.8
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	24	0.8
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	9	0.8
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	18	0.8
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	16	0.8
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	14	0.8
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	16	0.8
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	22	0.8
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	22	0.8
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	22	0.8
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	25	0.79
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	12	0.79
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	12	0.79
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	11	0.79
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	15	0.79
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	15	0.79
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	12	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:23:A:TYR:HE1	1:16:A:SER:HB3	18	0.79
(1,87)	1:23:A:TYR:HE2	1:16:A:SER:HB3	18	0.79
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	13	0.79
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	13	0.79
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	13	0.79
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	13	0.79
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	11	0.78
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	15	0.78
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	2	0.78
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	2	0.78
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	12	0.78
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	12	0.78
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	12	0.78
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	12	0.78
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	16	0.78
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	16	0.78
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	8	0.78
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	20	0.78
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	20	0.78
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	22	0.78
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG21	13	0.78
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG22	13	0.78
(1,383)	1:34:A:TRP:HE3	1:22:A:VAL:HG23	13	0.78
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	2	0.78
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	2	0.78
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	2	0.78
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	3	0.78
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	3	0.78
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	24	0.78
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	24	0.78
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	5	0.78
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	15	0.78
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	15	0.78
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	15	0.78
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	14	0.78
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	14	0.78
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	14	0.78
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	13	0.77
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG21	6	0.77
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG22	6	0.77
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG23	6	0.77
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG21	13	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG22	13	0.77
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG23	13	0.77
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	5	0.77
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	20	0.77
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	20	0.77
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	8	0.77
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	3	0.77
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	3	0.77
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG11	16	0.77
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG12	16	0.77
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG13	16	0.77
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	16	0.77
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	16	0.77
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	16	0.77
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	21	0.77
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	21	0.77
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	2	0.77
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	14	0.77
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	14	0.77
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	24	0.77
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	7	0.76
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	8	0.76
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	4	0.76
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	9	0.76
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	25	0.76
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	25	0.76
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	20	0.76
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	20	0.76
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	20	0.76
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	22	0.76
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	9	0.76
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	9	0.76
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	5	0.76
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	19	0.76
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	19	0.76
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	19	0.76
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	19	0.76
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	15	0.75
(1,830)	1:34:A:TRP:HD1	1:33:A:GLN:HG2	16	0.75
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	7	0.75
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	7	0.75
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	21	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	21	0.75
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	19	0.75
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	2	0.75
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	21	0.75
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	5	0.75
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	5	0.75
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	19	0.75
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	19	0.75
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	19	0.75
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	7	0.75
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	11	0.75
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	11	0.75
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	13	0.74
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	13	0.74
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	13	0.74
(1,858)	1:22:A:VAL:HG11	1:13:A:LYS:HB2	15	0.74
(1,858)	1:22:A:VAL:HG12	1:13:A:LYS:HB2	15	0.74
(1,858)	1:22:A:VAL:HG13	1:13:A:LYS:HB2	15	0.74
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	9	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	3	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	3	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	5	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	5	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	16	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	16	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	25	0.74
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	25	0.74
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	2	0.74
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	2	0.74
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	19	0.74
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	19	0.74
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	7	0.74
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	9	0.74
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	4	0.74
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	7	0.74
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	10	0.74
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	10	0.74
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	4	0.74
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	21	0.74
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	12	0.73
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	12	0.73
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	12	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:25:A:PHE:HB3	1:14:A:ARG:HB3	8	0.73
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	3	0.73
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	24	0.73
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	24	0.73
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	7	0.73
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	7	0.73
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	7	0.73
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	18	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	4	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	4	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	9	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	9	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	14	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	14	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	15	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	15	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	18	0.72
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	18	0.72
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	10	0.72
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	10	0.72
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	5	0.72
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	15	0.72
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	17	0.72
(1,442)	1:23:A:TYR:HE1	1:14:A:ARG:HB3	22	0.72
(1,442)	1:23:A:TYR:HE2	1:14:A:ARG:HB3	22	0.72
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG21	15	0.72
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG22	15	0.72
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG23	15	0.72
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	4	0.72
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	11	0.72
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	24	0.72
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	10	0.72
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	10	0.72
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	10	0.72
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	14	0.72
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	11	0.71
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	11	0.71
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	11	0.71
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	1	0.71
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	1	0.71
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	6	0.71
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	21	0.71
(1,701)	1:14:A:ARG:HA	1:14:A:ARG:HD3	7	0.71
(1,532)	1:11:A:TRP:HH2	1:26:A:ASN:HD22	16	0.71
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	11	0.71
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	11	0.71
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	21	0.71
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	21	0.71
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	8	0.71
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	19	0.71
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	9	0.7
(1,832)	1:11:A:TRP:HZ2	1:37:A:PRO:HD2	23	0.7
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	8	0.7
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	16	0.7
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	17	0.7
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	17	0.7
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	16	0.7
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	23	0.7
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	7	0.7
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	7	0.7
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	7	0.7
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	7	0.7
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	4	0.7
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	4	0.7
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	4	0.7
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	7	0.7
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	7	0.7
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	6	0.7
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	17	0.7
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	17	0.7
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	9	0.7
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	9	0.7
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	9	0.7
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	5	0.69
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	8	0.69
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	8	0.69
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	6	0.69
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	11	0.69
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	1	0.69
(1,674)	2:86:B:PRO:HD3	1:14:A:ARG:HD2	22	0.69
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	18	0.69
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	17	0.69
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	17	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	5	0.69
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	5	0.69
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	12	0.69
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	12	0.69
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	17	0.69
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	12	0.69
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	23	0.69
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	21	0.68
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	21	0.68
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	21	0.68
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	3	0.68
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	12	0.68
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	12	0.68
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	12	0.68
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	21	0.68
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	11	0.68
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	11	0.68
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	11	0.68
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD1	23	0.68
(1,258)	1:33:A:GLN:H	1:24:A:TYR:HD2	23	0.68
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	9	0.68
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	25	0.68
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	25	0.68
(1,87)	1:23:A:TYR:HE1	1:16:A:SER:HB3	16	0.68
(1,87)	1:23:A:TYR:HE2	1:16:A:SER:HB3	16	0.68
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	16	0.68
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	11	0.67
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	11	0.67
(1,813)	1:22:A:VAL:HG11	1:23:A:TYR:HA	21	0.67
(1,813)	1:22:A:VAL:HG12	1:23:A:TYR:HA	21	0.67
(1,813)	1:22:A:VAL:HG13	1:23:A:TYR:HA	21	0.67
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	22	0.67
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	7	0.67
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	7	0.67
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	2	0.67
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	5	0.67
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	23	0.67
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	17	0.67
(1,549)	1:11:A:TRP:HD1	1:28:A:ILE:HG13	4	0.67
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	1	0.67
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	22	0.67
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	17	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	6	0.67
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	23	0.67
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	12	0.67
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	16	0.67
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	16	0.67
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	16	0.67
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	6	0.67
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	6	0.67
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	7	0.67
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	2	0.67
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	24	0.66
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	24	0.66
(1,813)	1:22:A:VAL:HG11	1:23:A:TYR:HA	15	0.66
(1,813)	1:22:A:VAL:HG12	1:23:A:TYR:HA	15	0.66
(1,813)	1:22:A:VAL:HG13	1:23:A:TYR:HA	15	0.66
(1,813)	1:22:A:VAL:HG11	1:23:A:TYR:HA	16	0.66
(1,813)	1:22:A:VAL:HG12	1:23:A:TYR:HA	16	0.66
(1,813)	1:22:A:VAL:HG13	1:23:A:TYR:HA	16	0.66
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	18	0.66
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	9	0.66
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	9	0.66
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	5	0.66
(1,622)	1:33:A:GLN:HG2	1:24:A:TYR:HB3	22	0.66
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	5	0.66
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	10	0.66
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	13	0.66
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG21	25	0.66
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG22	25	0.66
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG23	25	0.66
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	2	0.66
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	18	0.66
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	1	0.66
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	1	0.66
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	1	0.66
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	1	0.66
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	1	0.66
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	12	0.66
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	13	0.66
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	5	0.66
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	5	0.66
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	5	0.66
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	11	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	11	0.66
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	11	0.66
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	14	0.65
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	14	0.65
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	14	0.65
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	12	0.65
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	17	0.65
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	1	0.65
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	1	0.65
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	6	0.65
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	22	0.65
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	13	0.65
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	17	0.65
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	17	0.65
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	12	0.65
(1,376)	1:39:A:GLY:H	1:8:A:PRO:HG3	8	0.65
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	4	0.65
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	8	0.65
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	10	0.65
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	22	0.65
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	2	0.65
(1,33)	1:24:A:TYR:H	1:33:A:GLN:HB2	22	0.65
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	20	0.65
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	22	0.64
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	22	0.64
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	22	0.64
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	6	0.64
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	10	0.64
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	16	0.64
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	3	0.64
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	17	0.64
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	6	0.64
(1,435)	1:33:A:GLN:HE21	1:37:A:PRO:HB2	14	0.64
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	19	0.64
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	1	0.64
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	3	0.64
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	20	0.64
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	25	0.64
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	4	0.64
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	4	0.64
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	4	0.64
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	12	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	12	0.64
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	12	0.64
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	3	0.64
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	18	0.64
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	19	0.64
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	19	0.64
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	23	0.64
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	6	0.64
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	11	0.64
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	21	0.63
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	15	0.63
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	15	0.63
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	6	0.63
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	7	0.63
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	13	0.63
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	19	0.63
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	25	0.63
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	23	0.63
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	23	0.63
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	7	0.63
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	15	0.63
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	17	0.63
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	8	0.63
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	20	0.63
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	20	0.63
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	9	0.63
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	9	0.63
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	9	0.63
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	9	0.63
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	21	0.63
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	15	0.62
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	25	0.62
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	12	0.62
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	9	0.62
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	12	0.62
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	19	0.62
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	16	0.62
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	16	0.62
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	16	0.62
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	16	0.62
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	14	0.62
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	16	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	12	0.62
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	1	0.62
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	4	0.62
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	10	0.62
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	20	0.62
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	12	0.62
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	17	0.62
(1,858)	1:22:A:VAL:HG11	1:13:A:LYS:HB2	21	0.61
(1,858)	1:22:A:VAL:HG12	1:13:A:LYS:HB2	21	0.61
(1,858)	1:22:A:VAL:HG13	1:13:A:LYS:HB2	21	0.61
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	24	0.61
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	22	0.61
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	25	0.61
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	25	0.61
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	8	0.61
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	17	0.61
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	18	0.61
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	22	0.61
(1,576)	1:34:A:TRP:HZ2	1:21:A:ARG:HG2	4	0.61
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	13	0.61
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	25	0.61
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	20	0.61
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	20	0.61
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	8	0.61
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	16	0.61
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	5	0.61
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	11	0.61
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	22	0.61
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	21	0.61
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	21	0.61
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	21	0.61
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	22	0.61
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	22	0.61
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	22	0.61
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	18	0.61
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	18	0.61
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	18	0.61
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	17	0.61
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	18	0.61
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	20	0.61
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	24	0.61
(1,87)	1:23:A:TYR:HE1	1:16:A:SER:HB3	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:23:A:TYR:HE2	1:16:A:SER:HB3	9	0.61
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	5	0.61
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD21	6	0.61
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD22	6	0.61
(1,8)	1:12:A:GLU:H	1:7:A:LEU:HD23	6	0.61
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	14	0.6
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	4	0.6
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	11	0.6
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	3	0.6
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	12	0.6
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	19	0.6
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	16	0.6
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	18	0.6
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	8	0.6
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	8	0.6
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	7	0.6
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	16	0.6
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	18	0.6
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	25	0.6
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	2	0.59
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	16	0.59
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	19	0.59
(1,813)	1:22:A:VAL:HG11	1:23:A:TYR:HA	3	0.59
(1,813)	1:22:A:VAL:HG12	1:23:A:TYR:HA	3	0.59
(1,813)	1:22:A:VAL:HG13	1:23:A:TYR:HA	3	0.59
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	9	0.59
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	10	0.59
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	18	0.59
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	2	0.59
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	12	0.59
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	4	0.59
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	9	0.59
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	10	0.59
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	18	0.59
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	21	0.59
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	25	0.59
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	16	0.59
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	15	0.59
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	15	0.59
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	2	0.59
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	22	0.59
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	22	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	22	0.59
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	25	0.59
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	3	0.59
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	14	0.59
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	13	0.58
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	24	0.58
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	24	0.58
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	14	0.58
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	9	0.58
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	11	0.58
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	14	0.58
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	8	0.58
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	13	0.58
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	6	0.58
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	6	0.58
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	2	0.58
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	2	0.58
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	2	0.58
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	15	0.58
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	10	0.58
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	11	0.58
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	11	0.58
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	11	0.58
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	1	0.58
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	8	0.58
(1,813)	1:22:A:VAL:HG11	1:23:A:TYR:HA	25	0.57
(1,813)	1:22:A:VAL:HG12	1:23:A:TYR:HA	25	0.57
(1,813)	1:22:A:VAL:HG13	1:23:A:TYR:HA	25	0.57
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	9	0.57
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	1	0.57
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	7	0.57
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	11	0.57
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	16	0.57
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	20	0.57
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	6	0.57
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	11	0.57
(1,463)	1:23:A:TYR:HE1	1:14:A:ARG:HD2	7	0.57
(1,463)	1:23:A:TYR:HE2	1:14:A:ARG:HD2	7	0.57
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	17	0.57
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	10	0.57
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	15	0.57
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	15	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	15	0.57
(1,227)	1:34:A:TRP:HE3	1:21:A:ARG:HB2	23	0.57
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	13	0.57
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	13	0.57
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	4	0.57
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	9	0.57
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	24	0.57
(1,813)	1:22:A:VAL:HG11	1:23:A:TYR:HA	7	0.56
(1,813)	1:22:A:VAL:HG12	1:23:A:TYR:HA	7	0.56
(1,813)	1:22:A:VAL:HG13	1:23:A:TYR:HA	7	0.56
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	5	0.56
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	1	0.56
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	2	0.56
(1,624)	1:25:A:PHE:HB2	1:14:A:ARG:HG2	6	0.56
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	2	0.56
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	14	0.56
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	15	0.56
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	17	0.56
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	24	0.56
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	6	0.56
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	21	0.56
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	16	0.56
(1,384)	1:34:A:TRP:HE3	1:21:A:ARG:HG2	8	0.56
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	19	0.56
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	15	0.56
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD1	22	0.55
(1,824)	1:34:A:TRP:HE1	1:23:A:TYR:HD2	22	0.55
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	20	0.55
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	25	0.55
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	21	0.55
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	10	0.55
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	21	0.55
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	21	0.55
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	6	0.55
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	6	0.55
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	6	0.55
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	11	0.55
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	11	0.55
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	11	0.55
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	2	0.55
(1,87)	1:23:A:TYR:HE1	1:16:A:SER:HB3	17	0.55
(1,87)	1:23:A:TYR:HE2	1:16:A:SER:HB3	17	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	14	0.55
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	9	0.54
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	9	0.54
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	9	0.54
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	3	0.54
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	3	0.54
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	3	0.54
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	20	0.54
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	17	0.54
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	17	0.54
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	17	0.54
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	6	0.54
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	5	0.54
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	3	0.54
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	20	0.53
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	12	0.53
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	12	0.53
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	12	0.53
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	14	0.53
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	14	0.53
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	14	0.53
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	19	0.53
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	19	0.53
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	19	0.53
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	3	0.53
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	25	0.53
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	7	0.53
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	14	0.53
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	14	0.53
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	21	0.53
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	6	0.53
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	19	0.53
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	21	0.53
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	21	0.53
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	21	0.53
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	21	0.53
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	18	0.53
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	4	0.52
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	13	0.52
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	13	0.52
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	13	0.52
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	22	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	22	0.52
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	22	0.52
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	21	0.52
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	4	0.52
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	4	0.52
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	8	0.52
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	8	0.52
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	7	0.52
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	10	0.52
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	18	0.52
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	23	0.52
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	15	0.52
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	16	0.52
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	24	0.52
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	23	0.52
(1,516)	1:11:A:TRP:HH2	1:37:A:PRO:HD2	23	0.52
(1,227)	1:34:A:TRP:HE3	1:21:A:ARG:HB2	5	0.52
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	11	0.52
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	23	0.52
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	23	0.52
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	8	0.52
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	4	0.52
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	4	0.52
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	4	0.52
(1,849)	1:14:A:ARG:HB3	1:15:A:MET:HG3	6	0.51
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	13	0.51
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	7	0.51
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	14	0.51
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	6	0.51
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	7	0.51
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	13	0.51
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	10	0.51
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	10	0.51
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	10	0.51
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	2	0.51
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	23	0.51
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	15	0.51
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	15	0.51
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	15	0.51
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	2	0.51
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	2	0.51
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	2	0.51
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	2	0.51
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	2	0.51
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	11	0.5
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	11	0.5
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	11	0.5
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	4	0.5
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	24	0.5
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	13	0.5
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	19	0.5
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	19	0.5
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	19	0.5
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	19	0.5
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	3	0.5
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	9	0.5
(1,175)	1:30:A:ASN:H	1:26:A:ASN:HB2	13	0.5
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	10	0.5
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	24	0.5
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	10	0.49
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	4	0.49
(1,761)	1:23:A:TYR:HE1	1:21:A:ARG:HB2	13	0.49
(1,761)	1:23:A:TYR:HE2	1:21:A:ARG:HB2	13	0.49
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	10	0.49
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	17	0.49
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	19	0.49
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	11	0.49
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	1	0.49
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	11	0.49
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	2	0.49
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	9	0.48
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	9	0.48
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	9	0.48
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	5	0.48
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	5	0.48
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	5	0.48
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	6	0.48
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	6	0.48
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	6	0.48
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	2	0.48
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	12	0.48
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	1	0.48
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	12	0.48
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	13	0.48
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG21	16	0.48
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG22	16	0.48
(1,414)	1:15:A:MET:H	1:22:A:VAL:HG23	16	0.48
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	19	0.48
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	23	0.48
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	13	0.48
(1,9)	1:34:A:TRP:HE1	2:86:B:PRO:HG3	22	0.48
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	20	0.47
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	20	0.47
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	20	0.47
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	1	0.47
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	12	0.47
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	5	0.47
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	16	0.47
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	16	0.47
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	16	0.47
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	13	0.47
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	22	0.47
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	15	0.47
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	18	0.47
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	18	0.47
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	1	0.47
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	23	0.47
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	9	0.47
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	21	0.47
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	21	0.47
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	21	0.47
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	6	0.47
(1,227)	1:34:A:TRP:HE3	1:21:A:ARG:HB2	4	0.47
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	18	0.47
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	6	0.47
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	14	0.47
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	6	0.46
(1,815)	1:7:A:LEU:HD11	1:8:A:PRO:HA	20	0.46
(1,815)	1:7:A:LEU:HD12	1:8:A:PRO:HA	20	0.46
(1,815)	1:7:A:LEU:HD13	1:8:A:PRO:HA	20	0.46
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	14	0.46
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	22	0.46
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	2	0.46
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	11	0.46
(1,652)	1:8:A:PRO:HD2	1:9:A:PRO:HA	20	0.46
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	11	0.46
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	21	0.46
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	24	0.46
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	17	0.46
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	9	0.46
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	25	0.46
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	25	0.46
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	25	0.46
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	25	0.46
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	21	0.46
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	3	0.46
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	19	0.46
(1,87)	1:23:A:TYR:HE1	1:16:A:SER:HB3	13	0.46
(1,87)	1:23:A:TYR:HE2	1:16:A:SER:HB3	13	0.46
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	24	0.46
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	16	0.46
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	23	0.45
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	7	0.45
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	17	0.45
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	12	0.45
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	12	0.45
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	22	0.45
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	2	0.45
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	2	0.45
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	2	0.45
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	10	0.45
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	14	0.45
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	17	0.45
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	9	0.45
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	7	0.44
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	13	0.44
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	2	0.44
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	12	0.44
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	13	0.44
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	5	0.44
(1,435)	1:33:A:GLN:HE21	1:37:A:PRO:HB2	24	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	1	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	1	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	1	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	4	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	4	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	18	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	18	0.44
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	18	0.44
(1,375)	1:28:A:ILE:H	1:29:A:THR:HB	13	0.44
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	3	0.44
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	3	0.44
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	3	0.44
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	1	0.44
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	5	0.44
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	3	0.44
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	21	0.44
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	22	0.44
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	23	0.43
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	24	0.43
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	23	0.43
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	23	0.43
(1,770)	1:25:A:PHE:HE1	1:14:A:ARG:HD2	6	0.43
(1,770)	1:25:A:PHE:HE2	1:14:A:ARG:HD2	6	0.43
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	9	0.43
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	6	0.43
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	20	0.43
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	24	0.43
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	20	0.43
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	25	0.43
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	14	0.43
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	19	0.43
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	20	0.43
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	24	0.43
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	3	0.43
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	3	0.43
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	3	0.43
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	11	0.43
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	14	0.43
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	20	0.43
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG11	7	0.43
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG12	7	0.43
(1,229)	1:23:A:TYR:H	1:22:A:VAL:HG13	7	0.43
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	8	0.43
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	21	0.43
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	18	0.43
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	1	0.43
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	6	0.43
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	1	0.42
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	24	0.42
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE1	22	0.42
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE2	22	0.42
(1,742)	1:14:A:ARG:H	1:15:A:MET:HE3	22	0.42
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	16	0.42
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	1	0.42
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	4	0.42
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	8	0.42
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	10	0.42
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	14	0.42
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	19	0.42
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	25	0.42
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	3	0.42
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	16	0.42
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	8	0.42
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	22	0.42
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	23	0.42
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	10	0.42
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	12	0.42
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	18	0.42
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	24	0.42
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	25	0.42
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	25	0.42
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	25	0.42
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	13	0.42
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	13	0.42
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	16	0.42
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	10	0.42
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	6	0.41
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	6	0.41
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	6	0.41
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	7	0.41
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	10	0.41
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	17	0.41
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	3	0.41
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	7	0.41
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	11	0.41
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	15	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	3	0.41
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	6	0.41
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	22	0.41
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	22	0.41
(1,499)	1:25:A:PHE:HE1	1:12:A:GLU:HG2	6	0.41
(1,499)	1:25:A:PHE:HE2	1:12:A:GLU:HG2	6	0.41
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	14	0.41
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	11	0.41
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	11	0.41
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	11	0.41
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	14	0.41
(1,376)	1:39:A:GLY:H	1:8:A:PRO:HG3	11	0.41
(1,375)	1:28:A:ILE:H	1:29:A:THR:HB	23	0.41
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	13	0.41
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	13	0.41
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	10	0.41
(1,135)	1:34:A:TRP:HE3	1:16:A:SER:HB3	13	0.41
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	18	0.41
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	13	0.41
(1,833)	1:11:A:TRP:HZ2	1:8:A:PRO:HB2	23	0.4
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	1	0.4
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	1	0.4
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	11	0.4
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	18	0.4
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	19	0.4
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	24	0.4
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	20	0.4
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	22	0.4
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	21	0.4
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	22	0.4
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	12	0.4
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	19	0.4
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	19	0.4
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	20	0.4
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	20	0.4
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	20	0.4
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	1	0.4
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	5	0.4
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	15	0.4
(1,379)	1:40:A:ASN:H	1:9:A:PRO:HD3	8	0.4
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	17	0.4
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	12	0.4
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	20	0.4
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	1	0.4
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	22	0.4
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	13	0.4
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	13	0.4
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	13	0.4
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	13	0.39
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG21	5	0.39
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG22	5	0.39
(1,828)	1:11:A:TRP:HZ2	1:29:A:THR:HG23	5	0.39
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	15	0.39
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	5	0.39
(1,704)	1:16:A:SER:HB3	1:17:A:ARG:HA	23	0.39
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	2	0.39
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	22	0.39
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	19	0.39
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	2	0.39
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	3	0.39
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	19	0.39
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	20	0.39
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	11	0.39
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	14	0.39
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD11	5	0.38
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD12	5	0.38
(1,863)	1:8:A:PRO:HD2	1:7:A:LEU:HD13	5	0.38
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	5	0.38
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	5	0.38
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	5	0.38
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	5	0.38
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	5	0.38
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	5	0.38
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	9	0.38
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	20	0.38
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	16	0.38
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	16	0.38
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	16	0.38
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	25	0.38
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	20	0.38
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	13	0.38
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	4	0.38
(1,375)	1:28:A:ILE:H	1:29:A:THR:HB	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	7	0.38
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	11	0.38
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	25	0.38
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	18	0.37
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	18	0.37
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	18	0.37
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	3	0.37
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	11	0.37
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	20	0.37
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	21	0.37
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	22	0.37
(1,495)	1:24:A:TYR:HE1	1:35:A:GLU:HB2	25	0.37
(1,495)	1:24:A:TYR:HE2	1:35:A:GLU:HB2	25	0.37
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	8	0.37
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	14	0.37
(1,376)	1:39:A:GLY:H	1:8:A:PRO:HG3	19	0.37
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	24	0.37
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	20	0.37
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	20	0.37
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	20	0.37
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	18	0.37
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	18	0.37
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	24	0.37
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	5	0.37
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	17	0.37
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	18	0.37
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	1	0.36
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	1	0.36
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	1	0.36
(1,801)	1:34:A:TRP:HH2	1:22:A:VAL:HA	15	0.36
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	17	0.36
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	10	0.36
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	10	0.36
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	10	0.36
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	25	0.36
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	13	0.36
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	16	0.36
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	2	0.36
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	10	0.36
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	13	0.36
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	17	0.36
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	11	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	12	0.36
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	5	0.36
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	23	0.36
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	16	0.36
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	18	0.36
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	18	0.36
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	18	0.36
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	15	0.36
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	6	0.36
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	9	0.36
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	15	0.36
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	20	0.35
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	20	0.35
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	5	0.35
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	1	0.35
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	8	0.35
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	16	0.35
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	18	0.35
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	19	0.35
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	25	0.35
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	4	0.35
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	4	0.35
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	20	0.35
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	11	0.35
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	18	0.35
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	3	0.35
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	10	0.35
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	2	0.35
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	20	0.35
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	5	0.34
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	5	0.34
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	5	0.34
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	8	0.34
(1,833)	1:11:A:TRP:HZ2	1:8:A:PRO:HB2	8	0.34
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	23	0.34
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	4	0.34
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	8	0.34
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	20	0.34
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	9	0.34
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	1	0.34
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	4	0.34
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	6	0.34
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	12	0.34
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	14	0.34
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	23	0.34
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	6	0.34
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	6	0.34
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	8	0.34
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	8	0.34
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	10	0.34
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	10	0.34
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	1	0.34
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	6	0.34
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	14	0.34
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	19	0.34
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	17	0.33
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	8	0.33
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	8	0.33
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	23	0.33
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	8	0.33
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	7	0.33
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	9	0.33
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	15	0.33
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	24	0.33
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	19	0.33
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	19	0.33
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	9	0.33
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	6	0.33
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	11	0.33
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	22	0.33
(1,375)	1:28:A:ILE:H	1:29:A:THR:HB	6	0.33
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	16	0.33
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	23	0.33
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	14	0.33
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	19	0.33
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	13	0.32
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	13	0.32
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	13	0.32
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	8	0.32
(1,744)	1:39:A:GLY:H	1:38:A:SER:H	19	0.32
(1,744)	1:39:A:GLY:H	1:38:A:SER:H	22	0.32
(1,518)	1:11:A:TRP:HZ3	1:11:A:TRP:HB2	3	0.32
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG11	22	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG12	22	0.32
(1,415)	1:15:A:MET:H	1:22:A:VAL:HG13	22	0.32
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	8	0.32
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	8	0.32
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	8	0.32
(1,291)	1:25:A:PHE:HE1	1:32:A:SER:HB2	11	0.32
(1,291)	1:25:A:PHE:HE2	1:32:A:SER:HB2	11	0.32
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	12	0.32
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	23	0.31
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	23	0.31
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	23	0.31
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	19	0.31
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	17	0.31
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	17	0.31
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	15	0.31
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	15	0.31
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	18	0.31
(1,744)	1:39:A:GLY:H	1:38:A:SER:H	11	0.31
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	11	0.31
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	11	0.31
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD21	8	0.31
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD22	8	0.31
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD23	8	0.31
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	4	0.31
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	16	0.31
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	4	0.31
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	2	0.31
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	2	0.31
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	20	0.31
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	20	0.31
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	13	0.31
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	13	0.31
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	10	0.31
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	6	0.31
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	2	0.31
(1,375)	1:28:A:ILE:H	1:29:A:THR:HB	5	0.31
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	25	0.31
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	13	0.31
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	16	0.31
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	23	0.31
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	7	0.31
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	15	0.3
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	3	0.3
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	25	0.3
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	2	0.3
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	2	0.3
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	2	0.3
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	17	0.3
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	17	0.3
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	17	0.3
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	1	0.3
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	1	0.3
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	6	0.3
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	6	0.3
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	13	0.3
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	13	0.3
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	6	0.3
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	6	0.3
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	7	0.3
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	7	0.3
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	7	0.3
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	5	0.3
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	1	0.3
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	1	0.3
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	24	0.3
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	22	0.3
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	2	0.3
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD1	4	0.3
(1,144)	2:85:B:SEP:H	1:23:A:TYR:HD2	4	0.3
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	2	0.3
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	5	0.3
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	21	0.3
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	7	0.3
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	4	0.3
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	6	0.29
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	6	0.29
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	6	0.29
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	6	0.29
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	6	0.29
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	6	0.29
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	15	0.29
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	16	0.29
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	3	0.29
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	3	0.29
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	25	0.29
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	25	0.29
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	25	0.29
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	24	0.29
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	19	0.29
(1,633)	1:18:A:SER:HB2	1:17:A:ARG:HB3	15	0.29
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	10	0.29
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	10	0.29
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	1	0.29
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	1	0.29
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	13	0.29
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	8	0.29
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	17	0.29
(1,362)	1:7:A:LEU:H	1:36:A:ARG:HG3	22	0.29
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	10	0.29
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	10	0.29
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	10	0.29
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	4	0.29
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	5	0.29
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	9	0.29
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	1	0.29
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	10	0.29
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	12	0.29
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	19	0.29
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	20	0.29
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	11	0.28
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	13	0.28
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	19	0.28
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	4	0.28
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	9	0.28
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	4	0.28
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	4	0.28
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	4	0.28
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	24	0.28
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	24	0.28
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	24	0.28
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	10	0.28
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	10	0.28
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	18	0.28
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	18	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD21	23	0.28
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD22	23	0.28
(1,675)	1:8:A:PRO:HD3	1:7:A:LEU:HD23	23	0.28
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	6	0.28
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	6	0.28
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	3	0.28
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	3	0.28
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	3	0.28
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	19	0.28
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	22	0.28
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	7	0.28
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	20	0.28
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	25	0.28
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	3	0.28
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	9	0.28
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	20	0.28
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	2	0.27
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	5	0.27
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	14	0.27
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	21	0.27
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	7	0.27
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	7	0.27
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	7	0.27
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	15	0.27
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	15	0.27
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	15	0.27
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	23	0.27
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	23	0.27
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	25	0.27
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	25	0.27
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	4	0.27
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	17	0.27
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	6	0.27
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	15	0.27
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	15	0.27
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	15	0.27
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	2	0.27
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	6	0.27
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	7	0.27
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	15	0.27
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	23	0.27
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	25	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:22:A:VAL:H	1:21:A:ARG:HG3	8	0.27
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	5	0.27
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	8	0.27
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	18	0.26
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	18	0.26
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	18	0.26
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	9	0.26
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	9	0.26
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	9	0.26
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	9	0.26
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	9	0.26
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	9	0.26
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	22	0.26
(1,833)	1:11:A:TRP:HZ2	1:8:A:PRO:HB2	5	0.26
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	5	0.26
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	13	0.26
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	13	0.26
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	13	0.26
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	8	0.26
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	8	0.26
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	8	0.26
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	21	0.26
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	8	0.26
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	8	0.26
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	18	0.26
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	18	0.26
(1,413)	1:32:A:SER:H	1:26:A:ASN:HB2	12	0.26
(1,365)	1:34:A:TRP:H	1:35:A:GLU:HB2	14	0.26
(1,342)	1:25:A:PHE:H	1:14:A:ARG:HG2	6	0.26
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	7	0.26
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	7	0.26
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	7	0.26
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	1	0.26
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	10	0.26
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	12	0.26
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	8	0.26
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	11	0.26
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	21	0.26
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	6	0.25
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	7	0.25
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	24	0.25
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	12	0.25
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	16	0.25
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	25	0.25
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	12	0.25
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	16	0.25
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	25	0.25
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	8	0.25
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	21	0.25
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	21	0.25
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	21	0.25
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	6	0.25
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	1	0.25
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	1	0.25
(1,555)	1:34:A:TRP:HH2	1:23:A:TYR:HB3	8	0.25
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	1	0.25
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	1	0.25
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	1	0.25
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	5	0.25
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	5	0.25
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	2	0.25
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	2	0.25
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	21	0.25
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	21	0.25
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	1	0.25
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	23	0.25
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	23	0.25
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	23	0.25
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	5	0.25
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	3	0.25
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	16	0.25
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	9	0.25
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	9	0.25
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	9	0.25
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	6	0.25
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	17	0.25
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	21	0.25
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	7	0.25
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	22	0.25
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	24	0.25
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	4	0.25
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	13	0.25
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	25	0.25
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	2	0.24
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	2	0.24
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	2	0.24
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	6	0.24
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	6	0.24
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	6	0.24
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	14	0.24
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	2	0.24
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	2	0.24
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	16	0.24
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	16	0.24
(1,758)	1:30:A:ASN:H	1:26:A:ASN:HD22	15	0.24
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	24	0.24
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	24	0.24
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	15	0.24
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	2	0.24
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	1	0.24
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	10	0.24
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	23	0.24
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	24	0.24
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	12	0.24
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	12	0.24
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	25	0.24
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	25	0.24
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	10	0.24
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	20	0.24
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	15	0.24
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	11	0.24
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB1	14	0.24
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB2	14	0.24
(1,309)	1:26:A:ASN:HD21	1:31:A:ALA:HB3	14	0.24
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	4	0.24
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	24	0.24
(1,135)	1:34:A:TRP:HE3	1:16:A:SER:HB3	9	0.24
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	15	0.24
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	5	0.23
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	24	0.23
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	5	0.23
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	24	0.23
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	2	0.23
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	1	0.23
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	1	0.23
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	1	0.23
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	18	0.23
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	18	0.23
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	22	0.23
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	22	0.23
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	5	0.23
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	12	0.23
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	14	0.23
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	21	0.23
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	21	0.23
(1,483)	1:24:A:TYR:HD1	1:37:A:PRO:HB2	4	0.23
(1,483)	1:24:A:TYR:HD2	1:37:A:PRO:HB2	4	0.23
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	6	0.23
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	19	0.23
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	18	0.23
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	1	0.23
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	10	0.23
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	13	0.23
(1,65)	1:34:A:TRP:H	1:33:A:GLN:HB2	22	0.23
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	18	0.23
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	22	0.23
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	4	0.22
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	4	0.22
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	4	0.22
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	20	0.22
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	20	0.22
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	20	0.22
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	24	0.22
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	24	0.22
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	24	0.22
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	22	0.22
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	22	0.22
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	22	0.22
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	22	0.22
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	22	0.22
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	22	0.22
(1,833)	1:11:A:TRP:HZ2	1:8:A:PRO:HB2	9	0.22
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	16	0.22
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	21	0.22
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	23	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	14	0.22
(1,744)	1:39:A:GLY:H	1:38:A:SER:H	13	0.22
(1,710)	1:34:A:TRP:HB3	2:86:B:PRO:HD2	8	0.22
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	11	0.22
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	25	0.22
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	10	0.22
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	10	0.22
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	10	0.22
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	7	0.22
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	22	0.22
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	24	0.22
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	9	0.22
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	9	0.22
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	15	0.22
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	15	0.22
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	10	0.22
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	10	0.22
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	18	0.22
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	18	0.22
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	13	0.22
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	25	0.22
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	25	0.22
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	5	0.22
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	11	0.22
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	13	0.22
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	5	0.22
(1,221)	2:85:B:SEP:HB3	1:17:A:ARG:HD3	25	0.22
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	25	0.22
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	11	0.22
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	3	0.22
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	3	0.22
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	1	0.22
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	16	0.22
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	20	0.22
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	4	0.22
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	21	0.22
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	15	0.21
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	15	0.21
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	15	0.21
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	9	0.21
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	2	0.21
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:34:A:TRP:HH2	1:23:A:TYR:HA	6	0.21
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	21	0.21
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	11	0.21
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	11	0.21
(1,744)	1:39:A:GLY:H	1:38:A:SER:H	9	0.21
(1,717)	1:33:A:GLN:HE22	1:37:A:PRO:HD3	23	0.21
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	6	0.21
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	10	0.21
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	21	0.21
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	21	0.21
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	21	0.21
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	24	0.21
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	24	0.21
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	24	0.21
(1,527)	1:11:A:TRP:HD1	1:8:A:PRO:HB2	20	0.21
(1,527)	1:11:A:TRP:HD1	1:8:A:PRO:HB2	22	0.21
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	1	0.21
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	8	0.21
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	10	0.21
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	16	0.21
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	16	0.21
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	24	0.21
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	24	0.21
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	11	0.21
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	11	0.21
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	22	0.21
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	22	0.21
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	13	0.21
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	13	0.21
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	22	0.21
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	24	0.21
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	1	0.21
(1,376)	1:39:A:GLY:H	1:8:A:PRO:HG3	12	0.21
(1,362)	1:7:A:LEU:H	1:36:A:ARG:HG3	3	0.21
(1,135)	1:34:A:TRP:HE3	1:16:A:SER:HB3	17	0.21
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	19	0.21
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	15	0.21
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	10	0.21
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	1	0.21
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	8	0.21
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	12	0.2
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	12	0.2
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	17	0.2
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	17	0.2
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	17	0.2
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	3	0.2
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	1	0.2
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	11	0.2
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	15	0.2
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	11	0.2
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	15	0.2
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD11	23	0.2
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD12	23	0.2
(1,779)	1:11:A:TRP:HZ3	1:7:A:LEU:HD13	23	0.2
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	10	0.2
(1,555)	1:34:A:TRP:HH2	1:23:A:TYR:HB3	16	0.2
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	11	0.2
(1,520)	1:11:A:TRP:HZ3	1:33:A:GLN:HA	14	0.2
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	1	0.2
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	12	0.2
(1,483)	1:24:A:TYR:HD1	1:37:A:PRO:HB2	25	0.2
(1,483)	1:24:A:TYR:HD2	1:37:A:PRO:HB2	25	0.2
(1,455)	1:20:A:GLY:H	1:15:A:MET:HB3	4	0.2
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	21	0.2
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD21	13	0.2
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD22	13	0.2
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD23	13	0.2
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	19	0.2
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	7	0.2
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	15	0.2
(1,254)	1:11:A:TRP:HE1	1:37:A:PRO:HD3	23	0.2
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	14	0.2
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	15	0.2
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	2	0.2
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	25	0.2
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	16	0.19
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	16	0.19
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	16	0.19
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	3	0.19
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	8	0.19
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	4	0.19
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	18	0.19
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	18	0.19
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	18	0.19
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	17	0.19
(1,758)	1:30:A:ASN:H	1:26:A:ASN:HD22	19	0.19
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	21	0.19
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	21	0.19
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	14	0.19
(1,633)	1:18:A:SER:HB2	1:17:A:ARG:HB3	3	0.19
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	2	0.19
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	18	0.19
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	18	0.19
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	18	0.19
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	25	0.19
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	25	0.19
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	25	0.19
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	9	0.19
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	16	0.19
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	16	0.19
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	23	0.19
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	23	0.19
(1,484)	1:24:A:TYR:HE1	1:36:A:ARG:HG2	4	0.19
(1,484)	1:24:A:TYR:HE2	1:36:A:ARG:HG2	4	0.19
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	17	0.19
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD21	20	0.19
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD22	20	0.19
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD23	20	0.19
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	9	0.19
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	18	0.19
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	9	0.19
(1,180)	1:7:A:LEU:H	1:6:A:LYS:HE3	17	0.19
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	22	0.19
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	4	0.19
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	11	0.19
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	15	0.19
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	7	0.19
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	11	0.19
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	15	0.19
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	3	0.19
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	9	0.18
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	9	0.18
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	9	0.18
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	11	0.18
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	11	0.18
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	10	0.18
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	21	0.18
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	10	0.18
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	21	0.18
(1,744)	1:39:A:GLY:H	1:38:A:SER:H	16	0.18
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	1	0.18
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	18	0.18
(1,575)	1:34:A:TRP:HZ2	2:86:B:PRO:HG3	4	0.18
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	19	0.18
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	20	0.18
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	2	0.18
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	2	0.18
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	2	0.18
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	3	0.18
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	23	0.18
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	23	0.18
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	7	0.18
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	7	0.18
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	14	0.18
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	14	0.18
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	22	0.18
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	22	0.18
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	2	0.18
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	2	0.18
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	24	0.18
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	24	0.18
(1,487)	1:25:A:PHE:HD1	1:14:A:ARG:HB3	23	0.18
(1,487)	1:25:A:PHE:HD2	1:14:A:ARG:HB3	23	0.18
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	9	0.18
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	16	0.18
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	4	0.18
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	4	0.18
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	3	0.18
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	12	0.18
(1,362)	1:7:A:LEU:H	1:36:A:ARG:HG3	10	0.18
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	25	0.18
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	25	0.18
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	25	0.18
(1,247)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	25	0.18
(1,247)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	25	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:34:A:TRP:HE3	1:21:A:ARG:HG3	8	0.18
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	12	0.18
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	21	0.18
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	13	0.18
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	4	0.18
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	4	0.18
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	23	0.18
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	23	0.18
(1,75)	1:37:A:PRO:HD3	1:36:A:ARG:HD2	22	0.18
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	2	0.18
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	10	0.18
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	22	0.17
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	22	0.17
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	22	0.17
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	20	0.17
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	14	0.17
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	22	0.17
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	22	0.17
(1,792)	1:11:A:TRP:HE3	1:33:A:GLN:HE21	1	0.17
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	3	0.17
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	3	0.17
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	5	0.17
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	12	0.17
(1,575)	1:34:A:TRP:HZ2	2:86:B:PRO:HG3	13	0.17
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	13	0.17
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	16	0.17
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	8	0.17
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	8	0.17
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	4	0.17
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	4	0.17
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	24	0.17
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	24	0.17
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	1	0.17
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	1	0.17
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	18	0.17
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	18	0.17
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	1	0.17
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	2	0.17
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD21	22	0.17
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD22	22	0.17
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD23	22	0.17
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	15	0.17
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	2	0.17
(1,313)	1:11:A:TRP:HE3	1:24:A:TYR:HB2	6	0.17
(1,192)	1:9:A:PRO:HD3	1:8:A:PRO:HG3	23	0.17
(1,137)	2:85:B:SEP:HB2	1:17:A:ARG:HD3	20	0.17
(1,129)	1:7:A:LEU:HB2	1:8:A:PRO:HD3	8	0.17
(1,129)	1:7:A:LEU:HB2	1:8:A:PRO:HD3	9	0.17
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	13	0.17
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	4	0.17
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	16	0.17
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	12	0.17
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	12	0.17
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	12	0.17
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	3	0.17
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	12	0.17
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	19	0.17
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	21	0.17
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	14	0.16
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	14	0.16
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	14	0.16
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	21	0.16
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	21	0.16
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	21	0.16
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	25	0.16
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	25	0.16
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	25	0.16
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	25	0.16
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	2	0.16
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	3	0.16
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	19	0.16
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	19	0.16
(1,796)	1:11:A:TRP:HZ2	1:26:A:ASN:HD21	9	0.16
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	9	0.16
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	9	0.16
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	19	0.16
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	19	0.16
(1,758)	1:30:A:ASN:H	1:26:A:ASN:HD22	16	0.16
(1,633)	1:18:A:SER:HB2	1:17:A:ARG:HB3	20	0.16
(1,611)	1:21:A:ARG:HA	1:21:A:ARG:HD2	5	0.16
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	20	0.16
(1,555)	1:34:A:TRP:HH2	1:23:A:TYR:HB3	21	0.16
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	4	0.16
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	4	0.16
(1,528)	1:11:A:TRP:HH2	1:26:A:ASN:HD21	4	0.16
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	8	0.16
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	18	0.16
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	20	0.16
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	3	0.16
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	6	0.16
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	6	0.16
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	4	0.16
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	4	0.16
(1,484)	1:24:A:TYR:HE1	1:36:A:ARG:HG2	19	0.16
(1,484)	1:24:A:TYR:HE2	1:36:A:ARG:HG2	19	0.16
(1,483)	1:24:A:TYR:HD1	1:37:A:PRO:HB2	15	0.16
(1,483)	1:24:A:TYR:HD2	1:37:A:PRO:HB2	15	0.16
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	2	0.16
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	1	0.16
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	15	0.16
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	22	0.16
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	5	0.16
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	5	0.16
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	17	0.16
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	6	0.16
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	11	0.16
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	14	0.16
(1,336)	1:33:A:GLN:H	2:86:B:PRO:HD3	18	0.16
(1,192)	1:9:A:PRO:HD3	1:8:A:PRO:HG3	9	0.16
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	9	0.16
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	16	0.16
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	10	0.16
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	19	0.16
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	20	0.16
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	25	0.16
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	13	0.16
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	13	0.16
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	17	0.16
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	17	0.16
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	20	0.16
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	20	0.16
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	21	0.16
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	21	0.16
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	3	0.15
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	3	0.15
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	3	0.15
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	8	0.15
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	8	0.15
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	8	0.15
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	19	0.15
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	19	0.15
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	19	0.15
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	1	0.15
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	20	0.15
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	25	0.15
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	3	0.15
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	3	0.15
(1,798)	1:34:A:TRP:HZ2	1:18:A:SER:HB3	2	0.15
(1,792)	1:11:A:TRP:HE3	1:33:A:GLN:HE21	11	0.15
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	20	0.15
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	20	0.15
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	8	0.15
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	8	0.15
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	8	0.15
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	17	0.15
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	17	0.15
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	17	0.15
(1,520)	1:11:A:TRP:HZ3	1:33:A:GLN:HA	11	0.15
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	21	0.15
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	2	0.15
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	2	0.15
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	5	0.15
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	5	0.15
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	21	0.15
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	21	0.15
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	3	0.15
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	3	0.15
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	5	0.15
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	5	0.15
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	10	0.15
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	10	0.15
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	15	0.15
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	15	0.15
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	16	0.15
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:24:A:TYR:HD1	1:37:A:PRO:HB2	23	0.15
(1,483)	1:24:A:TYR:HD2	1:37:A:PRO:HB2	23	0.15
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	3	0.15
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	7	0.15
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	21	0.15
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	8	0.15
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	25	0.15
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	10	0.15
(1,396)	1:27:A:HIS:H	1:25:A:PHE:HZ	23	0.15
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	9	0.15
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	19	0.15
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	21	0.15
(1,313)	1:11:A:TRP:HE3	1:24:A:TYR:HB2	11	0.15
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG11	7	0.15
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG12	7	0.15
(1,267)	1:14:A:ARG:H	1:22:A:VAL:HG13	7	0.15
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	3	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	1	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	2	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	3	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	4	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	6	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	7	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	8	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	9	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	11	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	12	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	15	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	21	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	22	0.15
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	23	0.15
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	1	0.15
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	3	0.15
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	3	0.15
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	9	0.15
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	9	0.15
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	14	0.15
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	14	0.15
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	15	0.15
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	15	0.15
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	22	0.15
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	22	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG11	22	0.15
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG12	22	0.15
(1,24)	1:13:A:LYS:HE2	1:22:A:VAL:HG13	22	0.15
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	3	0.15
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	19	0.15
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	24	0.15
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	2	0.15
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	12	0.14
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	12	0.14
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	12	0.14
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	12	0.14
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	12	0.14
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	12	0.14
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	18	0.14
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	8	0.14
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	8	0.14
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	3	0.14
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	7	0.14
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	21	0.14
(1,629)	1:17:A:ARG:HG2	1:16:A:SER:HA	15	0.14
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	6	0.14
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	25	0.14
(1,575)	1:34:A:TRP:HZ2	2:86:B:PRO:HG3	19	0.14
(1,555)	1:34:A:TRP:HH2	1:23:A:TYR:HB3	20	0.14
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	13	0.14
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	15	0.14
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	2	0.14
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	2	0.14
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	19	0.14
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	19	0.14
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	22	0.14
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	22	0.14
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	2	0.14
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	2	0.14
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	11	0.14
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	11	0.14
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	12	0.14
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	12	0.14
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	13	0.14
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	13	0.14
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	14	0.14
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:26:A:ASN:HD22	1:28:A:ILE:HG12	19	0.14
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	24	0.14
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	7	0.14
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	7	0.14
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	3	0.14
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	12	0.14
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG11	14	0.14
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG12	14	0.14
(1,382)	1:34:A:TRP:HE3	1:22:A:VAL:HG13	14	0.14
(1,362)	1:7:A:LEU:H	1:36:A:ARG:HG3	24	0.14
(1,343)	1:25:A:PHE:H	1:14:A:ARG:HB3	6	0.14
(1,313)	1:11:A:TRP:HE3	1:24:A:TYR:HB2	22	0.14
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	1	0.14
(1,100)	1:33:A:GLN:HE22	1:33:A:GLN:HG2	17	0.14
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	1	0.14
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	1	0.14
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	5	0.14
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	5	0.14
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	7	0.14
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	7	0.14
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	8	0.14
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	8	0.14
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	10	0.14
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	10	0.14
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	16	0.14
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	16	0.14
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	24	0.14
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	24	0.14
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	25	0.14
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	25	0.14
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	24	0.14
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	6	0.14
(1,12)	1:21:A:ARG:H	1:16:A:SER:HB2	22	0.14
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	23	0.14
(1,827)	1:11:A:TRP:H	1:7:A:LEU:HB3	19	0.13
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	21	0.13
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	21	0.13
(1,755)	1:27:A:HIS:HE1	1:12:A:GLU:HG2	23	0.13
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	5	0.13
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	8	0.13
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	10	0.13
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	24	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:33:A:GLN:HE22	1:24:A:TYR:HB3	22	0.13
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	21	0.13
(1,555)	1:34:A:TRP:HH2	1:23:A:TYR:HB3	25	0.13
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	15	0.13
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	15	0.13
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	15	0.13
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	1	0.13
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	1	0.13
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	10	0.13
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	10	0.13
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	14	0.13
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	14	0.13
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	13	0.13
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	13	0.13
(1,505)	1:24:A:TYR:HE1	1:34:A:TRP:HB3	17	0.13
(1,505)	1:24:A:TYR:HE2	1:34:A:TRP:HB3	17	0.13
(1,502)	1:24:A:TYR:HD1	1:33:A:GLN:HG2	22	0.13
(1,502)	1:24:A:TYR:HD2	1:33:A:GLN:HG2	22	0.13
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	1	0.13
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	1	0.13
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	8	0.13
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	8	0.13
(1,484)	1:24:A:TYR:HE1	1:36:A:ARG:HG2	23	0.13
(1,484)	1:24:A:TYR:HE2	1:36:A:ARG:HG2	23	0.13
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	8	0.13
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	6	0.13
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	25	0.13
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	1	0.13
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	1	0.13
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	12	0.13
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	12	0.13
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	17	0.13
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	17	0.13
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	3	0.13
(1,313)	1:11:A:TRP:HE3	1:24:A:TYR:HB2	20	0.13
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	18	0.13
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	6	0.13
(1,99)	1:11:A:TRP:HD1	1:8:A:PRO:HG3	25	0.13
(1,98)	1:34:A:TRP:HZ3	1:21:A:ARG:HB3	5	0.13
(1,94)	1:34:A:TRP:HZ3	1:21:A:ARG:HG2	8	0.13
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	19	0.13
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:34:A:TRP:H	1:33:A:GLN:HA	22	0.13
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	16	0.13
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	19	0.12
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	19	0.12
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	19	0.12
(1,851)	1:7:A:LEU:HD11	1:37:A:PRO:HD3	13	0.12
(1,851)	1:7:A:LEU:HD12	1:37:A:PRO:HD3	13	0.12
(1,851)	1:7:A:LEU:HD13	1:37:A:PRO:HD3	13	0.12
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	19	0.12
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	19	0.12
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	19	0.12
(1,841)	1:5:A:GLU:HA	1:6:A:LYS:HB3	4	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	1	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	14	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	16	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	17	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	19	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	22	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	24	0.12
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	25	0.12
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	9	0.12
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	12	0.12
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	12	0.12
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	9	0.12
(1,754)	1:11:A:TRP:HE3	1:13:A:LYS:HB3	13	0.12
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	4	0.12
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	22	0.12
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	25	0.12
(1,744)	1:39:A:GLY:H	1:38:A:SER:H	20	0.12
(1,701)	1:14:A:ARG:HA	1:14:A:ARG:HD3	3	0.12
(1,701)	1:14:A:ARG:HA	1:14:A:ARG:HD3	4	0.12
(1,701)	1:14:A:ARG:HA	1:14:A:ARG:HD3	18	0.12
(1,562)	1:34:A:TRP:HZ2	1:16:A:SER:HB3	23	0.12
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	5	0.12
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	22	0.12
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	2	0.12
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	6	0.12
(1,514)	1:34:A:TRP:HZ3	1:21:A:ARG:HB2	11	0.12
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	3	0.12
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	3	0.12
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	7	0.12
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	9	0.12
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	9	0.12
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	17	0.12
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	17	0.12
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	21	0.12
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	21	0.12
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	24	0.12
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	24	0.12
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	8	0.12
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	8	0.12
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	21	0.12
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	21	0.12
(1,481)	1:25:A:PHE:HD1	1:14:A:ARG:HB2	23	0.12
(1,481)	1:25:A:PHE:HD2	1:14:A:ARG:HB2	23	0.12
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	2	0.12
(1,453)	1:11:A:TRP:HE3	1:7:A:LEU:HB2	16	0.12
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD21	14	0.12
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD22	14	0.12
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD23	14	0.12
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	2	0.12
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	7	0.12
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	20	0.12
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	15	0.12
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	11	0.12
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	6	0.12
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	6	0.12
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	11	0.12
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	11	0.12
(1,90)	1:23:A:TYR:HE1	1:25:A:PHE:HB2	18	0.12
(1,90)	1:23:A:TYR:HE2	1:25:A:PHE:HB2	18	0.12
(1,2)	1:13:A:LYS:H	1:12:A:GLU:HG2	17	0.12
(1,865)	1:28:A:ILE:HG21	1:27:A:HIS:HB2	7	0.11
(1,865)	1:28:A:ILE:HG22	1:27:A:HIS:HB2	7	0.11
(1,865)	1:28:A:ILE:HG23	1:27:A:HIS:HB2	7	0.11
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	11	0.11
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	11	0.11
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	11	0.11
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	11	0.11
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	11	0.11
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	11	0.11
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	2	0.11
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	10	0.11
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	11	0.11
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	15	0.11
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	18	0.11
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	20	0.11
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	21	0.11
(1,826)	1:29:A:THR:H	1:31:A:ALA:HA	10	0.11
(1,823)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	14	0.11
(1,822)	1:25:A:PHE:HZ	1:14:A:ARG:HD2	14	0.11
(1,808)	1:11:A:TRP:HE3	1:37:A:PRO:HD2	22	0.11
(1,792)	1:11:A:TRP:HE3	1:33:A:GLN:HE21	24	0.11
(1,755)	1:27:A:HIS:HE1	1:12:A:GLU:HG2	5	0.11
(1,755)	1:27:A:HIS:HE1	1:12:A:GLU:HG2	13	0.11
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	2	0.11
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	9	0.11
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	11	0.11
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	12	0.11
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	14	0.11
(1,701)	1:14:A:ARG:HA	1:14:A:ARG:HD3	13	0.11
(1,701)	1:14:A:ARG:HA	1:14:A:ARG:HD3	21	0.11
(1,667)	1:37:A:PRO:HD3	1:36:A:ARG:HB2	4	0.11
(1,667)	1:37:A:PRO:HD3	1:36:A:ARG:HB2	10	0.11
(1,634)	1:17:A:ARG:HB3	1:18:A:SER:HA	19	0.11
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	8	0.11
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	13	0.11
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	23	0.11
(1,591)	1:22:A:VAL:HG11	1:22:A:VAL:HA	2	0.11
(1,591)	1:22:A:VAL:HG12	1:22:A:VAL:HA	2	0.11
(1,591)	1:22:A:VAL:HG13	1:22:A:VAL:HA	2	0.11
(1,555)	1:34:A:TRP:HH2	1:23:A:TYR:HB3	3	0.11
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD11	3	0.11
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD12	3	0.11
(1,547)	1:11:A:TRP:HD1	1:7:A:LEU:HD13	3	0.11
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	25	0.11
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	12	0.11
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	12	0.11
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	15	0.11
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	15	0.11
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	25	0.11
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	25	0.11
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	1	0.11
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	14	0.11
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	14	0.11
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	6	0.11
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	6	0.11
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	9	0.11
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	9	0.11
(1,496)	1:24:A:TYR:HD1	1:35:A:GLU:HB2	19	0.11
(1,496)	1:24:A:TYR:HD2	1:35:A:GLU:HB2	19	0.11
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	3	0.11
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	3	0.11
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	7	0.11
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	7	0.11
(1,481)	1:25:A:PHE:HD1	1:14:A:ARG:HB2	7	0.11
(1,481)	1:25:A:PHE:HD2	1:14:A:ARG:HB2	7	0.11
(1,471)	1:33:A:GLN:HE22	1:37:A:PRO:HG2	25	0.11
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	8	0.11
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	11	0.11
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD21	12	0.11
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD22	12	0.11
(1,451)	1:11:A:TRP:HE3	1:7:A:LEU:HD23	12	0.11
(1,440)	1:26:A:ASN:HD22	1:29:A:THR:HG21	7	0.11
(1,440)	1:26:A:ASN:HD22	1:29:A:THR:HG22	7	0.11
(1,440)	1:26:A:ASN:HD22	1:29:A:THR:HG23	7	0.11
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	15	0.11
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	15	0.11
(1,431)	1:23:A:TYR:HD1	1:14:A:ARG:HB2	20	0.11
(1,431)	1:23:A:TYR:HD2	1:14:A:ARG:HB2	20	0.11
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	14	0.11
(1,407)	1:35:A:GLU:H	1:33:A:GLN:HE22	22	0.11
(1,140)	1:34:A:TRP:H	1:34:A:TRP:HD1	8	0.11
(1,129)	1:7:A:LEU:HB2	1:8:A:PRO:HD3	23	0.11
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	13	0.11
(1,16)	1:15:A:MET:H	1:14:A:ARG:HB3	23	0.11
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	20	0.1
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	20	0.1
(1,861)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	20	0.1
(1,851)	1:7:A:LEU:HD11	1:37:A:PRO:HD3	9	0.1
(1,851)	1:7:A:LEU:HD12	1:37:A:PRO:HD3	9	0.1
(1,851)	1:7:A:LEU:HD13	1:37:A:PRO:HD3	9	0.1
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD21	20	0.1
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD22	20	0.1
(1,842)	1:37:A:PRO:HD2	1:7:A:LEU:HD23	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	4	0.1
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	9	0.1
(1,840)	1:14:A:ARG:HD2	1:14:A:ARG:HA	12	0.1
(1,831)	1:34:A:TRP:HD1	1:23:A:TYR:HB2	4	0.1
(1,768)	1:24:A:TYR:HE1	1:37:A:PRO:HD3	14	0.1
(1,768)	1:24:A:TYR:HE2	1:37:A:PRO:HD3	14	0.1
(1,748)	1:27:A:HIS:H	1:27:A:HIS:HD2	13	0.1
(1,719)	1:23:A:TYR:HD1	2:85:B:SEP:HB2	14	0.1
(1,719)	1:23:A:TYR:HD2	2:85:B:SEP:HB2	14	0.1
(1,603)	1:33:A:GLN:HE22	1:33:A:GLN:HB3	11	0.1
(1,591)	1:22:A:VAL:HG11	1:22:A:VAL:HA	11	0.1
(1,591)	1:22:A:VAL:HG12	1:22:A:VAL:HA	11	0.1
(1,591)	1:22:A:VAL:HG13	1:22:A:VAL:HA	11	0.1
(1,525)	1:11:A:TRP:HZ3	1:26:A:ASN:HB2	19	0.1
(1,507)	1:25:A:PHE:HD1	1:32:A:SER:HB3	20	0.1
(1,507)	1:25:A:PHE:HD2	1:32:A:SER:HB3	20	0.1
(1,506)	1:25:A:PHE:HE1	1:32:A:SER:HB3	25	0.1
(1,506)	1:25:A:PHE:HE2	1:32:A:SER:HB3	25	0.1
(1,490)	1:23:A:TYR:HD1	2:86:B:PRO:HG3	11	0.1
(1,490)	1:23:A:TYR:HD2	2:86:B:PRO:HG3	11	0.1
(1,481)	1:25:A:PHE:HD1	1:14:A:ARG:HB2	17	0.1
(1,481)	1:25:A:PHE:HD2	1:14:A:ARG:HB2	17	0.1
(1,456)	1:20:A:GLY:H	1:21:A:ARG:HB3	10	0.1
(1,417)	1:11:A:TRP:HE3	1:26:A:ASN:HB3	17	0.1
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	7	0.1
(1,392)	1:34:A:TRP:HE3	1:22:A:VAL:HA	25	0.1

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

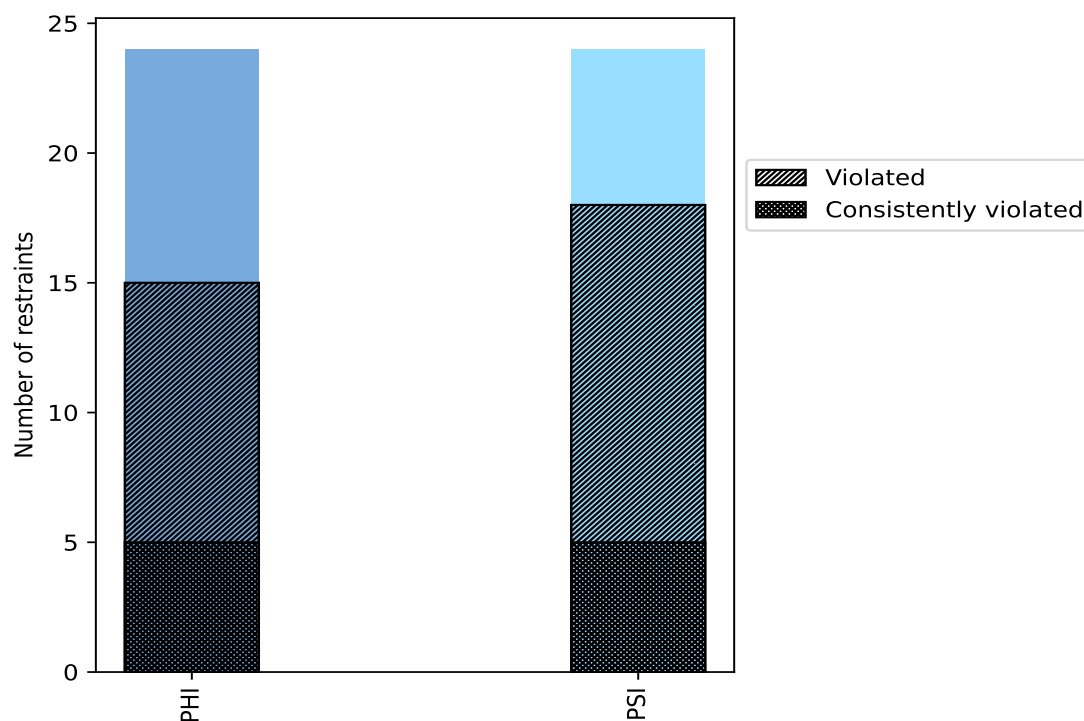
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	24	50.0	15	62.5	31.2	5	20.8	10.4
PSI	24	50.0	18	75.0	37.5	5	20.8	10.4
Total	48	100.0	33	68.8	68.8	10	20.8	20.8

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

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



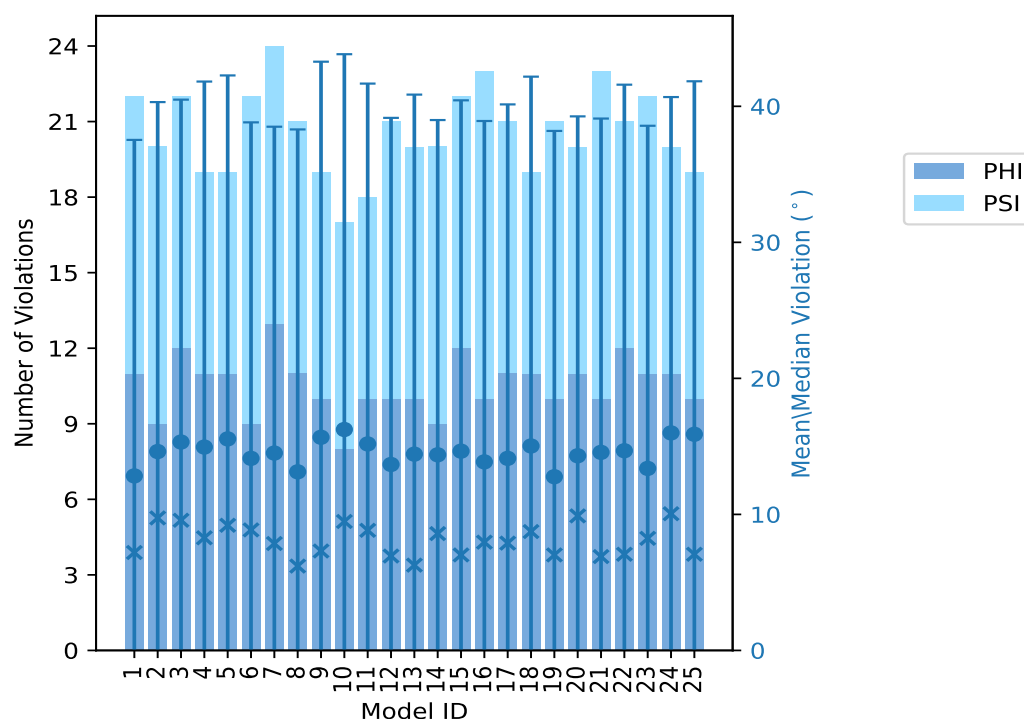
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	11	11	22	12.83	123.33	24.7	7.2
2	9	11	20	14.62	124.05	25.69	9.74
3	12	10	22	15.32	126.28	25.17	9.57
4	11	8	19	14.95	127.08	26.87	8.28
5	11	8	19	15.55	126.57	26.72	9.2
6	9	13	22	14.12	124.31	24.7	8.86
7	13	11	24	14.51	124.22	23.99	7.86
8	11	10	21	13.13	123.74	25.17	6.2
9	10	9	19	15.67	129.52	27.61	7.31
10	8	9	17	16.24	124.59	27.59	9.48
11	10	8	18	15.18	122.41	26.49	8.83
12	10	11	21	13.67	124.31	25.48	6.94
13	10	10	20	14.43	125.41	26.43	6.27
14	9	11	20	14.38	118.38	24.61	8.59
15	12	10	22	14.65	127.69	25.79	7.02
16	10	13	23	13.86	127.76	25.06	7.96
17	11	10	21	14.12	127.27	26.02	7.89
18	11	8	19	15.03	127.61	27.15	8.74
19	10	11	21	12.77	124.03	25.42	7.02
20	11	9	20	14.31	120.74	24.95	9.89
21	10	13	23	14.56	124.4	24.54	6.9
22	12	9	21	14.68	132.06	26.91	7.07
23	11	11	22	13.38	125.96	25.19	8.24
24	11	9	20	15.99	119.11	24.69	10.05
25	10	9	19	15.89	122.4	25.95	7.07

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	2	2	1	4.0
0	0	0	2	8.0
1	0	1	3	12.0
1	0	1	4	16.0
1	1	2	5	20.0
0	1	1	6	24.0
1	1	2	7	28.0
0	4	4	8	32.0
0	0	0	9	36.0
0	0	0	10	40.0
0	0	0	11	44.0

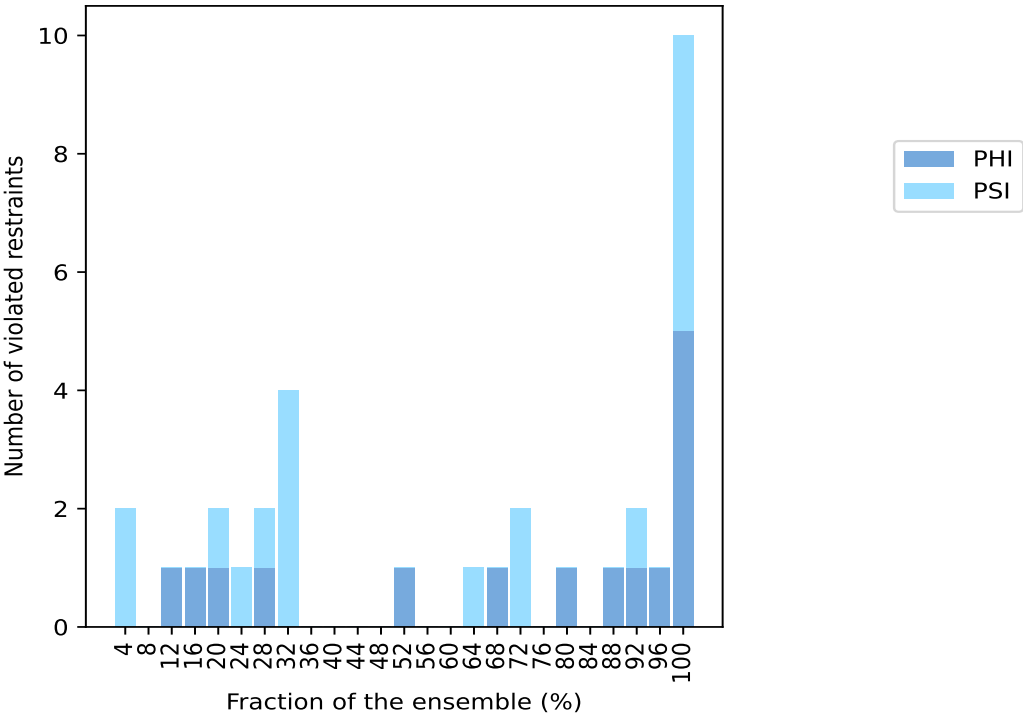
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	48.0
1	0	1	13	52.0
0	0	0	14	56.0
0	0	0	15	60.0
0	1	1	16	64.0
1	0	1	17	68.0
0	2	2	18	72.0
0	0	0	19	76.0
1	0	1	20	80.0
0	0	0	21	84.0
1	0	1	22	88.0
1	1	2	23	92.0
1	0	1	24	96.0
5	5	10	25	100.0

¹ Number of models with violations

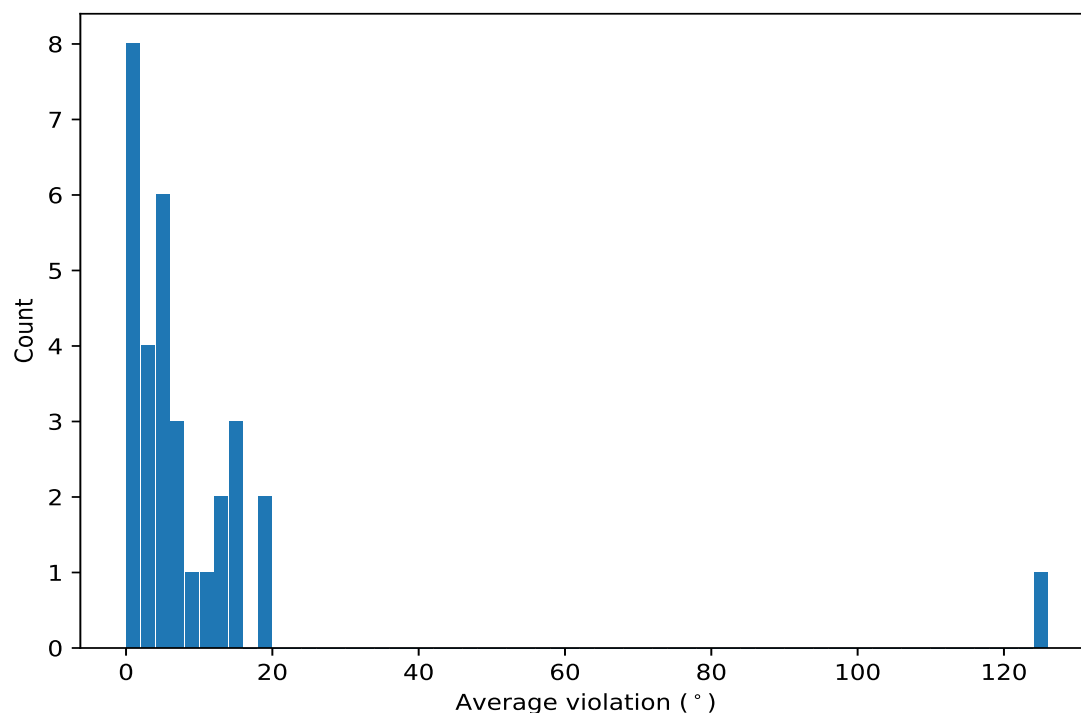
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	25	124.93	3.0	124.4
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	25	18.0	7.34	16.12
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	25	15.91	0.89	16.08
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	25	15.88	3.22	16.6
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	25	14.31	4.71	14.32
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	25	13.87	1.96	14.23
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	25	12.24	1.2	12.57
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	25	10.6	0.48	10.52
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	25	6.97	1.19	6.94
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	25	5.88	0.98	6.08
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	24	18.64	4.46	18.56
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	23	9.82	4.47	11.43
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	23	6.4	0.91	6.32

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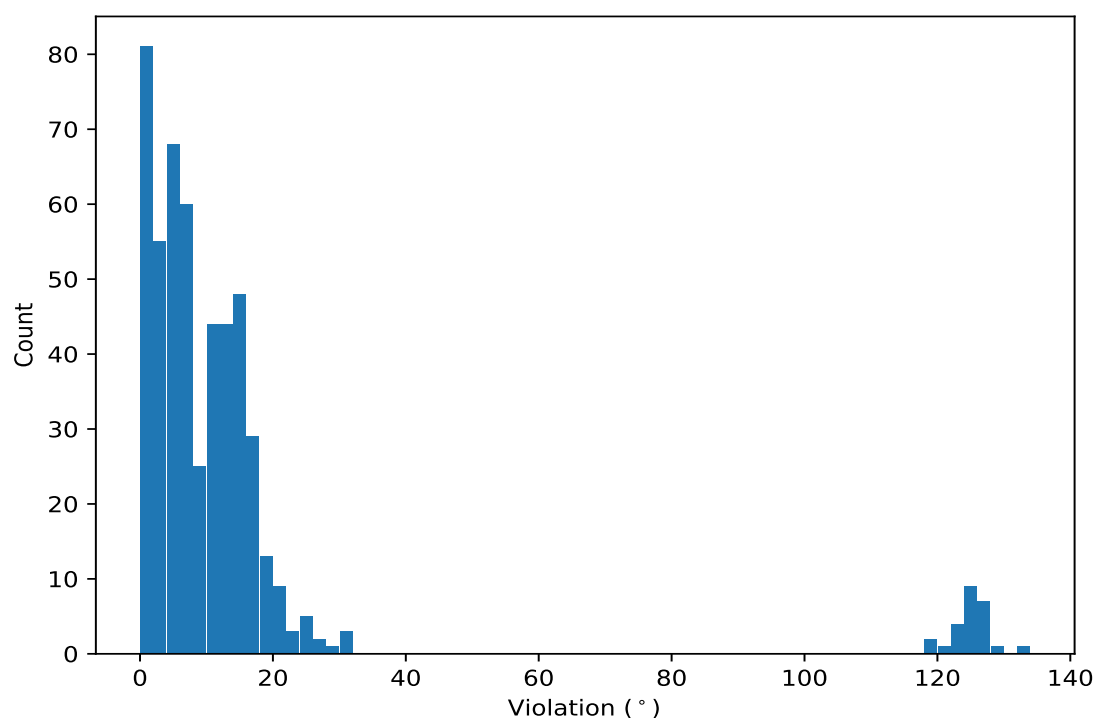
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	22	4.88	1.21	4.92
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	20	3.6	0.96	3.73
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	18	4.04	1.48	4.48
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	18	1.82	0.44	1.72
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	17	5.82	4.91	4.84
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	16	7.71	2.99	8.56
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	13	2.02	0.73	1.95
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	8	1.68	1.2	1.23
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	8	1.4	0.24	1.32
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	8	1.37	0.29	1.22
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	8	1.36	0.23	1.27
(1,24)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:SER:N	7	2.6	1.1	2.92
(1,5)	1:7:A:LEU:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	7	1.89	0.58	1.66
(1,30)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:TYR:N	6	4.89	0.46	4.87
(1,16)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:ARG:N	5	4.14	0.66	3.72
(1,1)	1:5:A:GLU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	5	1.21	0.21	1.15
(1,45)	1:36:A:ARG:C	1:37:A:PRO:N	1:37:A:PRO:CA	1:37:A:PRO:C	4	1.94	0.65	1.84
(1,25)	1:19:A:SER:C	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	3	2.91	0.53	2.79

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	22	132.06
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	9	129.52
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	16	127.76
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	15	127.69
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	18	127.61
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	17	127.27
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	4	127.08
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	5	126.57
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	3	126.28
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	23	125.96
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	13	125.41
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	10	124.59
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	21	124.4
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	6	124.31
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	12	124.31
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	7	124.22
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	2	124.05
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	19	124.03
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	8	123.74
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	1	123.33
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	11	122.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	25	122.4
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	20	120.74
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	24	119.11
(1,42)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:TRP:N	14	118.38
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	3	31.85
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	15	31.74
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	21	31.26
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	7	29.02
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	24	27.92
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	25	26.67
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	9	25.87
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	16	25.39
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	22	25.39
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	13	24.56
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	7	24.27
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	21	23.43
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	6	22.92
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	10	22.73
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	14	21.63
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	12	21.46
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	11	21.1
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	24	20.9
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	15	20.65
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	4	20.65
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	24	20.59
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	17	20.35
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	18	20.09
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	7	19.89
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	24	19.73
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	25	19.71
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	15	19.19
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1	19.14
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	2	18.96
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	14	18.51
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	13	18.45
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	5	18.4
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	13	18.39
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	3	18.38
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	21	18.09
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	9	18.02
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	14	17.98
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	23	17.7
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	20	17.64
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	13	17.63
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	16	17.43
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	17	17.34
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	6	17.03
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	23	16.99
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	2	16.95
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	20	16.88
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	12	16.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	2	16.84
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	5	16.83
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	13	16.72
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	19	16.7
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	22	16.66
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	25	16.63
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	25	16.6
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	19	16.5
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	1	16.48
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	18	16.45
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	15	16.38
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	6	16.31
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	5	16.21
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	10	16.21
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	18	16.16
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	5	16.12
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	12	16.08
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	9	16.04
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	23	15.99
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	7	15.97
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	5	15.95
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	7	15.92
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	21	15.89
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	14	15.88
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	3	15.87
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	8	15.86
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	18	15.83
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	16	15.57
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	3	15.55
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	17	15.51
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1	15.45
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	11	15.4
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	6	15.39
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	8	15.27
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	6	15.21
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	20	15.2
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	15	15.17
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	9	15.17
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	9	15.13
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	2	15.05
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	16	15.0
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	25	14.95
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	22	14.87
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	21	14.83
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	7	14.77
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	19	14.77
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	3	14.73
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	7	14.68
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	3	14.67
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	22	14.52
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	10	14.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	16	14.42
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	4	14.35
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	23	14.34
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	12	14.32
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	8	14.3
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	17	14.3
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	24	14.23
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	19	14.23
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	17	14.18
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	15	14.17
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	3	14.08
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	22	14.05
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	18	14.01
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	11	14.0
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	17	14.0
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	20	13.98
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	12	13.93
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	4	13.93
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	21	13.9
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	17	13.89
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	25	13.86
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	12	13.79
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	19	13.71
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	9	13.65
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	5	13.61
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	10	13.47
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	14	13.43
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	16	13.32
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	23	13.29
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	22	13.22
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	17	13.19
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	11	13.19
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	13	13.16
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	4	13.12
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	25	13.09
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	8	13.06
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	20	13.02
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1	13.02
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	24	13.01
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	16	12.96
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	14	12.94
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	23	12.92
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	23	12.88
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	11	12.84
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	10	12.82
(1,11)	1:10:A:GLY:C	1:11:A:TRP:N	1:11:A:TRP:CA	1:11:A:TRP:C	24	12.75
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	1	12.72
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	3	12.71
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	16	12.65
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	2	12.57
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	4	12.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	18	12.39
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	12	12.35
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	8	12.31
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	9	12.29
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	18	12.27
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	2	12.17
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	6	12.13
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	4	12.09
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	2	11.99
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	7	11.84
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	21	11.84
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	5	11.7
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	1	11.69
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	24	11.65
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	13	11.63
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	21	11.55
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	23	11.49
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	20	11.47
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	14	11.43
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	8	11.43
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	22	11.39
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	22	11.37
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	20	11.34
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	11	11.3
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	5	11.23
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	7	11.13
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	11	11.09
(1,17)	1:13:A:LYS:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	21	11.09
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	11	11.08
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	2	11.0
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	8	10.95
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	12	10.93
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	4	10.89
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	24	10.88
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	10	10.83
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	8	10.73
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	19	10.73
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	7	10.6
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	9	10.55
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	16	10.52
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	25	10.5
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	3	10.46
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	2	10.43
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	20	10.38
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	6	10.38
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	6	10.32
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	20	10.31
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	18	10.3
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	23	10.29
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	6	10.21
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	17	10.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	15	10.13
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	3	9.96
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	21	9.96
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	4	9.95
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1	9.93
(1,32)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:TYR:N	6	9.92
(1,13)	1:11:A:TRP:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	15	9.92
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	10	9.88
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	16	9.82
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	15	9.78
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	1	9.65
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	14	9.62
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	1	9.57
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	13	9.55
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	10	9.48
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	20	9.46
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	14	9.36
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	12	9.35
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	24	9.21
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	5	9.2
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	3	9.19
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	2	9.05
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	23	8.84
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	18	8.74
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	4	8.28
(1,31)	1:22:A:VAL:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	19	8.1
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	20	7.96
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	16	7.96
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	10	7.92
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	7	7.91
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	17	7.89
(1,38)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:THR:N	19	7.85
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	14	7.83
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	7	7.82
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	6	7.8
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	13	7.78
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	24	7.73
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	4	7.7
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	23	7.63
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	3	7.63
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	10	7.59
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	1	7.54
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	5	7.37
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	9	7.31
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	15	7.28
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	22	7.27
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	10	7.17
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	19	7.11
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	25	7.07
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	22	7.07
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	19	7.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	25	6.97
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	20	6.94
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	12	6.94
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	22	6.9
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	21	6.9
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	21	6.89
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1	6.86
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	20	6.85
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	19	6.84
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	4	6.84
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	25	6.83
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	15	6.75
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1	6.73
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	18	6.66
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	4	6.64
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	2	6.63
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	11	6.58
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	2	6.57
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	5	6.52
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	3	6.52
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	11	6.5
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	15	6.45
(1,18)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:MET:N	25	6.42
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	14	6.41
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	22	6.38
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	24	6.32
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	5	6.31
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	23	6.27
(1,29)	1:21:A:ARG:C	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	8	6.26
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	10	6.24
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	21	6.22
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	18	6.2
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	8	6.2
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	24	6.16
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	17	6.08
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	8	5.99
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	2	5.98
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	12	5.95
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	9	5.91
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	22	5.88
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	7	5.87
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	9	5.86
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	11	5.8
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	6	5.78
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	9	5.66
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	14	5.66
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	17	5.61
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	16	5.6
(1,30)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:TYR:N	3	5.57
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	6	5.36
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	18	5.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	16	5.32
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	20	5.28
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	24	5.26
(1,30)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:TYR:N	7	5.22
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	19	5.22
(1,16)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:ARG:N	6	5.21
(1,30)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:TYR:N	15	5.18
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	4	5.18
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	8	5.14
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	3	5.13
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	4	5.12
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	7	5.11
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	8	5.08
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	24	5.06
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	12	5.05
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	3	5.04
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	6	5.03
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	22	5.02
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	9	4.98
(1,27)	1:20:A:GLY:C	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	10	4.94
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	8	4.93
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	21	4.86
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	16	4.86
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	22	4.85
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	11	4.85
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	6	4.84
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	6	4.84
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	15	4.84
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	13	4.76
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	9	4.74
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	1	4.7
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	10	4.68
(1,16)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:ARG:N	7	4.62
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	15	4.59
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	25	4.59
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	11	4.58
(1,30)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:TYR:N	21	4.56
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	8	4.55
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	15	4.53
(1,30)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:TYR:N	16	4.5
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	12	4.5
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	25	4.47
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	4	4.39
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	21	4.39
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	13	4.3
(1,30)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:TYR:N	25	4.29
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	11	4.26
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	2	4.19
(1,24)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:SER:N	14	4.18
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	13	4.14
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	11	4.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	7	4.04
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	7	3.97
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	17	3.96
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	19	3.96
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	2	3.94
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	3	3.92
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	5	3.91
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	14	3.85
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	19	3.83
(1,24)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:SER:N	5	3.79
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1	3.73
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	7	3.73
(1,16)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:ARG:N	21	3.72
(1,16)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:ARG:N	23	3.69
(1,25)	1:19:A:SER:C	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	5	3.62
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	18	3.56
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	25	3.49
(1,16)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:ARG:N	16	3.47
(1,35)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	12	3.46
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	22	3.46
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	6	3.45
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	21	3.44
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	16	3.4
(1,10)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:TRP:N	14	3.37
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	21	3.35
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	20	3.3
(1,5)	1:7:A:LEU:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	3	3.24
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	5	3.21
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	18	3.21
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	3	3.1
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	17	3.08
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	5	3.07
(1,24)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:SER:N	17	3.06
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	24	3.02
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	18	3.01
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	8	2.95
(1,24)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:SER:N	23	2.92
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	7	2.92
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	14	2.9
(1,45)	1:36:A:ARG:C	1:37:A:PRO:N	1:37:A:PRO:CA	1:37:A:PRO:C	22	2.85
(1,25)	1:19:A:SER:C	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	23	2.79
(1,37)	1:27:A:HIS:C	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1	2.77
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	11	2.74
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	8	2.69
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	22	2.62
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	24	2.6
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	15	2.56
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	24	2.54
(1,25)	1:19:A:SER:C	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	13	2.33
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	4	2.26
(1,45)	1:36:A:ARG:C	1:37:A:PRO:N	1:37:A:PRO:CA	1:37:A:PRO:C	1	2.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	23	2.18
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	9	2.17
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	13	2.17
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	2	2.06
(1,5)	1:7:A:LEU:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	25	2.0
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	16	1.98
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	3	1.97
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	17	1.97
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	23	1.95
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	23	1.9
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	7	1.88
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	20	1.87
(1,5)	1:7:A:LEU:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	16	1.86
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	16	1.83
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	9	1.83
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	5	1.82
(1,2)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	13	1.74
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	14	1.72
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	10	1.71
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	21	1.7
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	2	1.66
(1,5)	1:7:A:LEU:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	7	1.66
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	8	1.64
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	1	1.63
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	23	1.61
(1,24)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:SER:N	16	1.6
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	4	1.6
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	1	1.6
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	13	1.6
(1,1)	1:5:A:GLU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	13	1.6
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	23	1.59
(1,20)	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	1:16:A:SER:N	6	1.57
(1,5)	1:7:A:LEU:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	4	1.56
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	9	1.54
(1,5)	1:7:A:LEU:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	15	1.52
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	11	1.51
(1,46)	1:37:A:PRO:N	1:37:A:PRO:CA	1:37:A:PRO:C	1:38:A:SER:N	9	1.5
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	16	1.5
(1,24)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:SER:N	19	1.5
(1,4)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:PRO:N	12	1.49
(1,45)	1:36:A:ARG:C	1:37:A:PRO:N	1:37:A:PRO:CA	1:37:A:PRO:C	8	1.44
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	19	1.41
(1,5)	1:7:A:LEU:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	18	1.4
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	12	1.39
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	17	1.38
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	13	1.37
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	25	1.37
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	21	1.37
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	14	1.36
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	18	1.34
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	12	1.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	22	1.34
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	13	1.32
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	19	1.31
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	10	1.31
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	6	1.29
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	15	1.28
(1,19)	1:14:A:ARG:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	12	1.26
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	6	1.25
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	20	1.24
(1,45)	1:36:A:ARG:C	1:37:A:PRO:N	1:37:A:PRO:CA	1:37:A:PRO:C	7	1.23
(1,44)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:PRO:N	15	1.23
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	21	1.23
(1,1)	1:5:A:GLU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	15	1.23
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	3	1.22
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	23	1.2
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	19	1.19
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	2	1.19
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	12	1.19
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	20	1.18
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	17	1.17
(1,24)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:SER:N	8	1.16
(1,14)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:LYS:N	1	1.16
(1,1)	1:5:A:GLU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1	1.15
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	2	1.13
(1,23)	1:17:A:ARG:C	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	19	1.1
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	14	1.09
(1,34)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	24	1.09
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	18	1.07
(1,1)	1:5:A:GLU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	20	1.07
(1,22)	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1:18:A:SER:N	1	1.06
(1,6)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	19	1.06
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	12	1.05
(1,9)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	22	1.05
(1,36)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ASN:N	17	1.04
(1,1)	1:5:A:GLU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	17	1.01