



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 06:27 AM UTC

PDB ID : 5JN6 / pdb_00005jn6
BMRB ID : 30070
Title : The NMR Solution Structure of RPA3313
Authors : Catazaro, J.; Lowe, A.J.; Powers, R.; Structural Genomics Consortium (SGC)
Deposited on : 2016-04-29

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

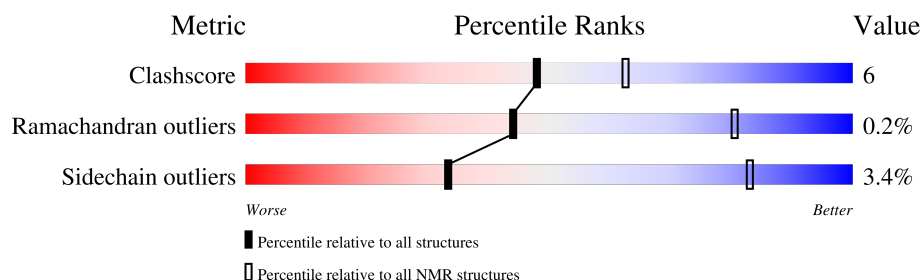
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	91	

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:20, A:27-A:55 (46)	0.70	1

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1004 atoms, of which 481 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1004	320	481	92	109	2	

There are 21 discrepancies between the modelled and reference sequences:

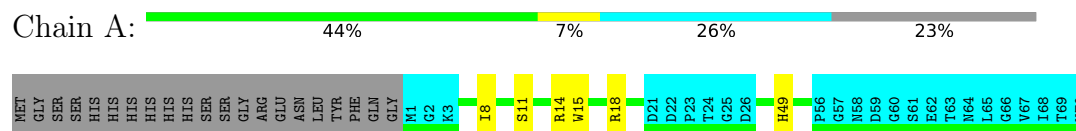
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q6N4M4
A	-19	GLY	-	expression tag	UNP Q6N4M4
A	-18	SER	-	expression tag	UNP Q6N4M4
A	-17	SER	-	expression tag	UNP Q6N4M4
A	-16	HIS	-	expression tag	UNP Q6N4M4
A	-15	HIS	-	expression tag	UNP Q6N4M4
A	-14	HIS	-	expression tag	UNP Q6N4M4
A	-13	HIS	-	expression tag	UNP Q6N4M4
A	-12	HIS	-	expression tag	UNP Q6N4M4
A	-11	HIS	-	expression tag	UNP Q6N4M4
A	-10	SER	-	expression tag	UNP Q6N4M4
A	-9	SER	-	expression tag	UNP Q6N4M4
A	-8	GLY	-	expression tag	UNP Q6N4M4
A	-7	ARG	-	expression tag	UNP Q6N4M4
A	-6	GLU	-	expression tag	UNP Q6N4M4
A	-5	ASN	-	expression tag	UNP Q6N4M4
A	-4	LEU	-	expression tag	UNP Q6N4M4
A	-3	TYR	-	expression tag	UNP Q6N4M4
A	-2	PHE	-	expression tag	UNP Q6N4M4
A	-1	GLN	-	expression tag	UNP Q6N4M4
A	0	GLY	-	expression tag	UNP Q6N4M4

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Uncharacterized protein

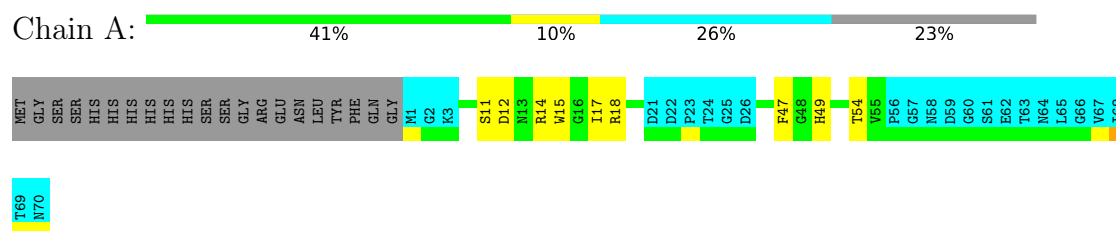


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

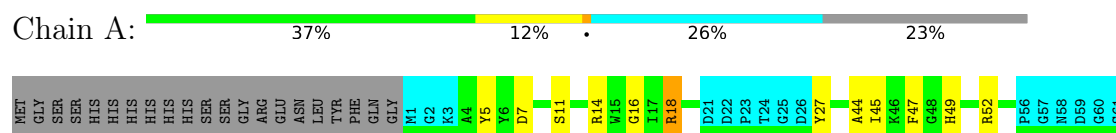
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Uncharacterized protein



4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein



E62
T63
N64
L65
G66
V67
I68
T69
N70

4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein

Chain A:  44% 5% 26% 23%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 G2 K3 I8 S11 R14 V15 G16 I17 D21 D22 P23 T24 G25 D26 A41 P56 G57 N58 D59 G60 S61 E62 T63 N64 L65 G66 V67 I68 T69 N70

4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

Chain A:  45% 5% 26% 23%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 G2 K3 S11 R14 D21 D22 P23 T24 G25 D26 A44 F47 G48 H49 P56 G57 N58 D59 G60 S61 E62 T63 N64 L65 G66 V67 I68 T69 N70

4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein

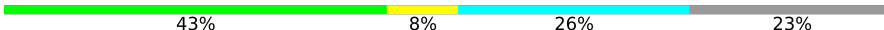
Chain A:  40% 10% 26% 23%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 G2 K3 A4 Y5 Y6 G10 S11 R14 W15 R18 D21 D22 P23 T24 G25 D26 Y27 A44 H49 P56 G57 N58 D59 G60 S61 E62 T63 N64 L65 G66 V67 I68 T69 N70

V67
I68
T69
N70

4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein

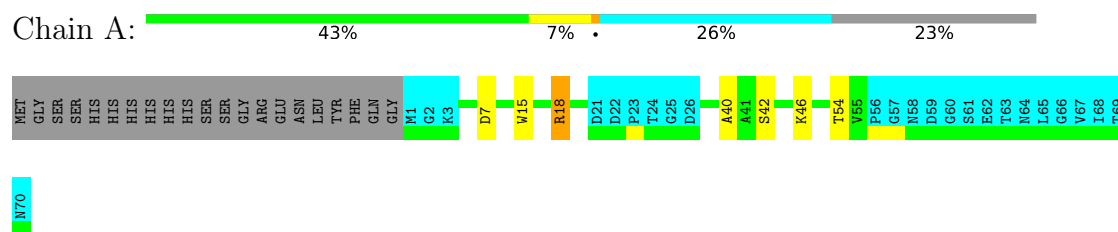
Chain A:  43% 8% 26% 23%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 G2 K3 Y6 S11 R14 H19 D20 D21 D22 P23 T24 G25 D26 F34 S42 K46 P56 G57 N58 D59 G60 S61 E62 T63 N64 L65 G66 V67 I68 T69

N70

4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



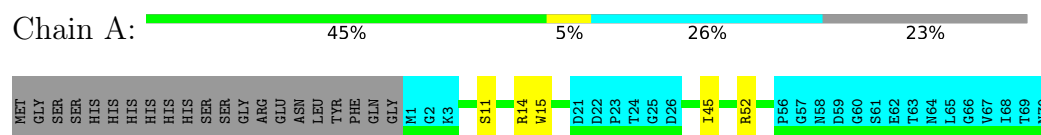
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



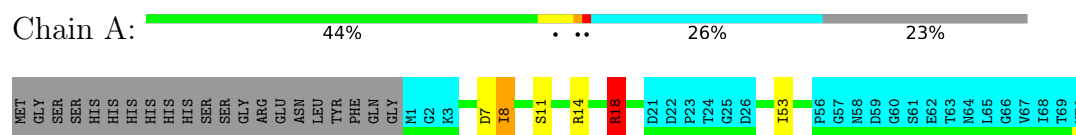
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



4.2.10 Score per residue for model 10

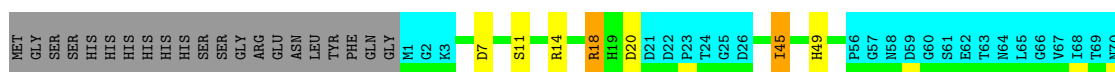
- Molecule 1: Uncharacterized protein



4.2.11 Score per residue for model 11

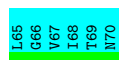
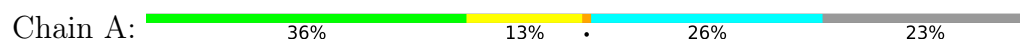
- Molecule 1: Uncharacterized protein





4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein



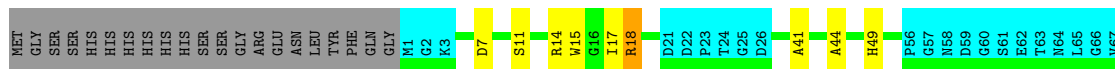
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein



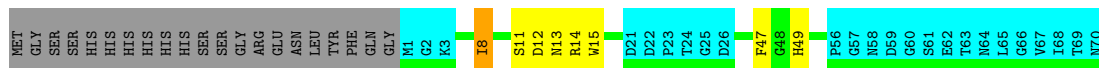
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



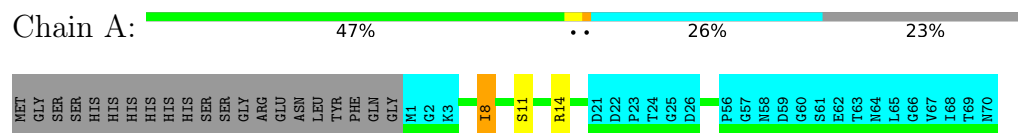
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



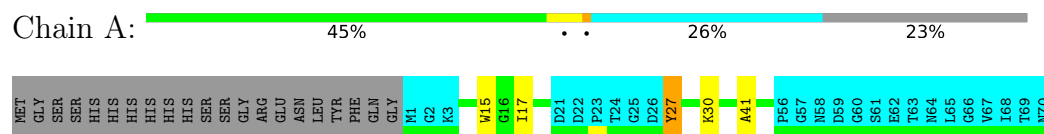
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein



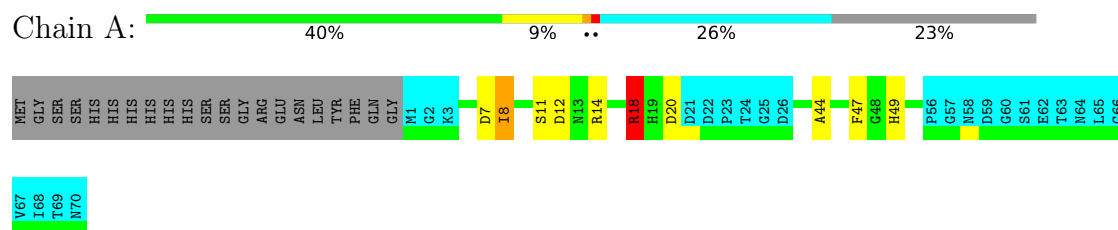
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein



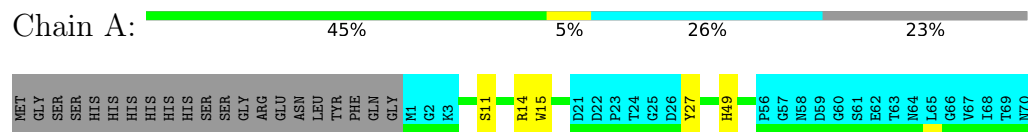
4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein



4.2.19 Score per residue for model 19

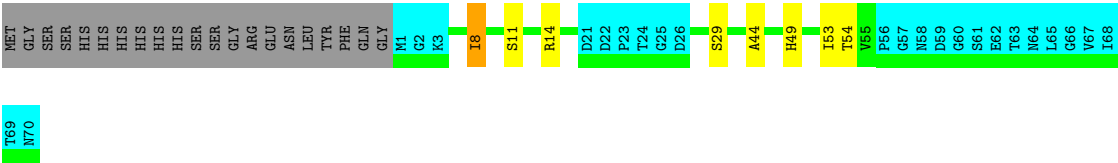
- Molecule 1: Uncharacterized protein



4.2.20 Score per residue for model 20

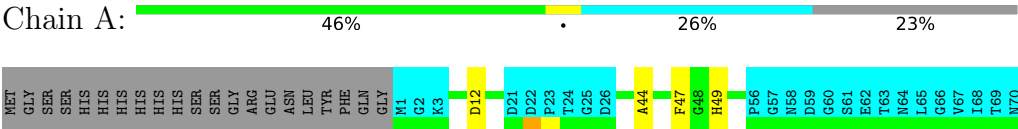
- Molecule 1: Uncharacterized protein





4.2.21 Score per residue for model 21

- Molecule 1: Uncharacterized protein



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 21 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
X-PLOR NIH	refinement	2.41.1

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	736
Number of shifts mapped to atoms	736
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.3±0.5
All	All	0	6

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	18	ARG	Sidechain	6

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	357	333	333	4±2
All	All	7497	6993	6993	85

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:SER:HB3	1:A:14:ARG:O	0.71	1.86	11	2
1:A:44:ALA:HA	1:A:49:HIS:CG	0.65	2.25	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:ASP:HB3	1:A:18:ARG:NH1	0.63	2.09	2	3
1:A:11:SER:HB2	1:A:14:ARG:O	0.62	1.94	16	14
1:A:15:TRP:CH2	1:A:41:ALA:HB2	0.59	2.32	3	3
1:A:7:ASP:HB3	1:A:18:ARG:CZ	0.59	2.28	2	2
1:A:15:TRP:CZ3	1:A:17:ILE:HD11	0.58	2.33	3	2
1:A:12:ASP:HA	1:A:49:HIS:CE1	0.58	2.34	21	3
1:A:47:PHE:HB3	1:A:49:HIS:CD2	0.57	2.34	18	5
1:A:8:ILE:HD13	1:A:8:ILE:H	0.54	1.62	18	7
1:A:42:SER:O	1:A:46:LYS:HG3	0.54	2.03	6	2
1:A:7:ASP:O	1:A:18:ARG:HB3	0.53	2.04	7	4
1:A:10:GLY:HA2	1:A:15:TRP:CZ3	0.51	2.40	5	1
1:A:13:ASN:OD1	1:A:14:ARG:HG2	0.50	2.07	12	1
1:A:5:TYR:HB2	1:A:27:TYR:CE2	0.50	2.41	5	1
1:A:12:ASP:HA	1:A:49:HIS:NE2	0.49	2.22	15	1
1:A:44:ALA:HA	1:A:49:HIS:ND1	0.49	2.23	4	6
1:A:47:PHE:HB3	1:A:49:HIS:CE1	0.48	2.44	12	2
1:A:5:TYR:CD1	1:A:27:TYR:HB2	0.47	2.45	12	1
1:A:18:ARG:NH1	1:A:20:ASP:HA	0.46	2.26	11	1
1:A:16:GLY:HA2	1:A:52:ARG:O	0.46	2.11	2	2
1:A:15:TRP:NE1	1:A:40:ALA:HB1	0.46	2.25	7	1
1:A:5:TYR:CE1	1:A:27:TYR:HB3	0.46	2.46	2	1
1:A:18:ARG:HA	1:A:54:THR:O	0.45	2.11	1	1
1:A:6:TYR:CB	1:A:19:HIS:HA	0.44	2.42	6	1
1:A:13:ASN:O	1:A:14:ARG:HD2	0.44	2.12	15	1
1:A:27:TYR:CE2	1:A:30:LYS:HA	0.44	2.48	17	1
1:A:15:TRP:HB3	1:A:49:HIS:CD2	0.44	2.47	19	1
1:A:18:ARG:HG2	1:A:18:ARG:HH11	0.44	1.73	10	2
1:A:15:TRP:CH2	1:A:17:ILE:HD11	0.44	2.48	17	1
1:A:7:ASP:O	1:A:18:ARG:HD3	0.43	2.13	18	2
1:A:18:ARG:HH11	1:A:18:ARG:CG	0.43	2.26	10	1
1:A:10:GLY:HA2	1:A:15:TRP:CE3	0.43	2.48	5	1
1:A:15:TRP:CZ2	1:A:17:ILE:HD11	0.42	2.48	12	2
1:A:45:ILE:O	1:A:45:ILE:HD13	0.42	2.15	11	1
1:A:6:TYR:OH	1:A:34:PHE:HA	0.41	2.15	6	1
1:A:18:ARG:HH12	1:A:20:ASP:CG	0.40	2.25	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	46/91 (51%)	45±1 (98±2%)	1±1 (1±2%)	0±0 (0±1%)	44 80
All	All	966/1911 (51%)	950 (98%)	14 (1%)	2 (0%)	44 80

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

Mol	Chain	Res	Type	Models (Total)
1	A	12	ASP	1
1	A	29	SER	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	34/71 (48%)	33±1 (97±3%)	1±1 (3±3%)	33 83
All	All	714/1491 (48%)	690 (97%)	24 (3%)	33 83

All 10 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	8	ILE	7
1	A	45	ILE	3
1	A	15	TRP	3
1	A	18	ARG	3
1	A	53	ILE	2
1	A	27	TYR	2
1	A	52	ARG	1
1	A	49	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	12	ASP	1
1	A	54	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	736
Number of shifts mapped to atoms	736
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	68	2.52 ± 0.08	Should be checked
$^{13}\text{C}_\beta$	60	2.81 ± 0.10	Should be checked
$^{13}\text{C}'$	67	2.67 ± 0.12	Should be applied
^{15}N	68	-0.58 ± 0.38	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 502 atoms were assigned a chemical shift out of a possible 596. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	231/233 (99%)	94/95 (99%)	91/92 (99%)	46/46 (100%)
Sidechain	246/290 (85%)	169/189 (89%)	77/88 (88%)	0/13 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	25/73 (34%)	25/36 (69%)	0/34 (0%)	0/3 (0%)
Overall	502/596 (84%)	288/320 (90%)	168/214 (79%)	46/62 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 715 atoms were assigned a chemical shift out of a possible 859. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	344/354 (97%)	141/146 (97%)	135/140 (96%)	68/68 (100%)
Sidechain	346/432 (80%)	235/279 (84%)	111/136 (82%)	0/17 (0%)
Aromatic	25/73 (34%)	25/36 (69%)	0/34 (0%)	0/3 (0%)
Overall	715/859 (83%)	401/461 (87%)	246/310 (79%)	68/88 (77%)

7.1.4 Statistically unusual chemical shifts ⓘ

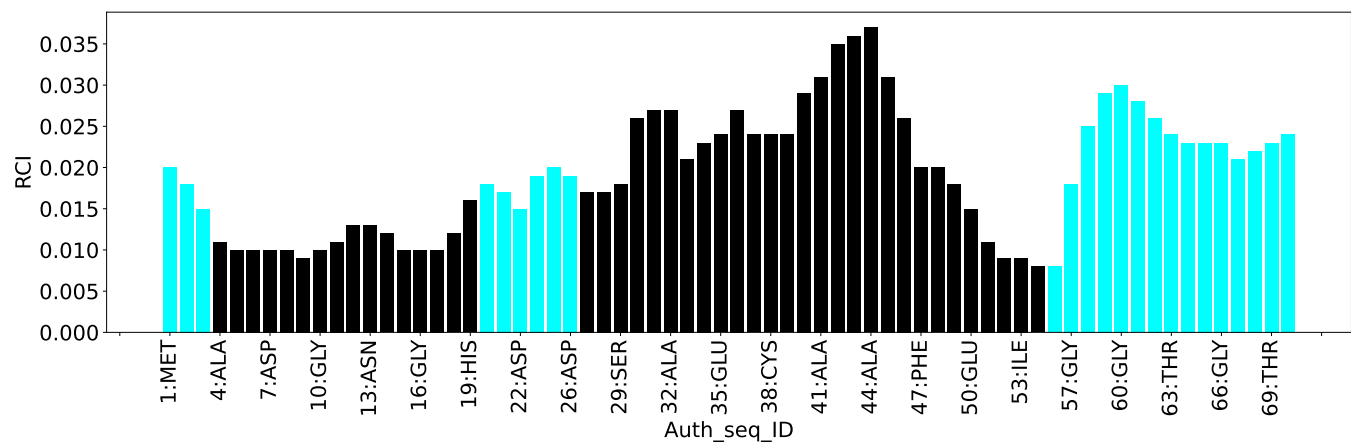
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	54	THR	HG1	6.85	0.08 – 2.19	27.1
1	A	24	THR	HG1	6.35	0.08 – 2.19	24.7
1	A	63	THR	HG1	5.00	0.08 – 2.19	18.3
1	A	69	THR	HG1	3.80	0.08 – 2.19	12.6
1	A	22	ASP	CA	43.35	44.71 – 64.67	-5.7
1	A	1	MET	CE	26.30	8.39 – 25.85	5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	912
Intra-residue ($ i-j =0$)	256
Sequential ($ i-j =1$)	269
Medium range ($ i-j >1$ and $ i-j <5$)	226
Long range ($ i-j \geq 5$)	95
Inter-chain	0
Hydrogen bond restraints	66
Disulfide bond restraints	0
Total dihedral-angle restraints	102
Number of unmapped restraints	0
Number of restraints per residue	11.1
Number of long range restraints per residue ¹	1.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	15.9	0.2
0.2-0.5 (Medium)	18.3	0.5
>0.5 (Large)	8.1	2.12

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)	7.8	6.87
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

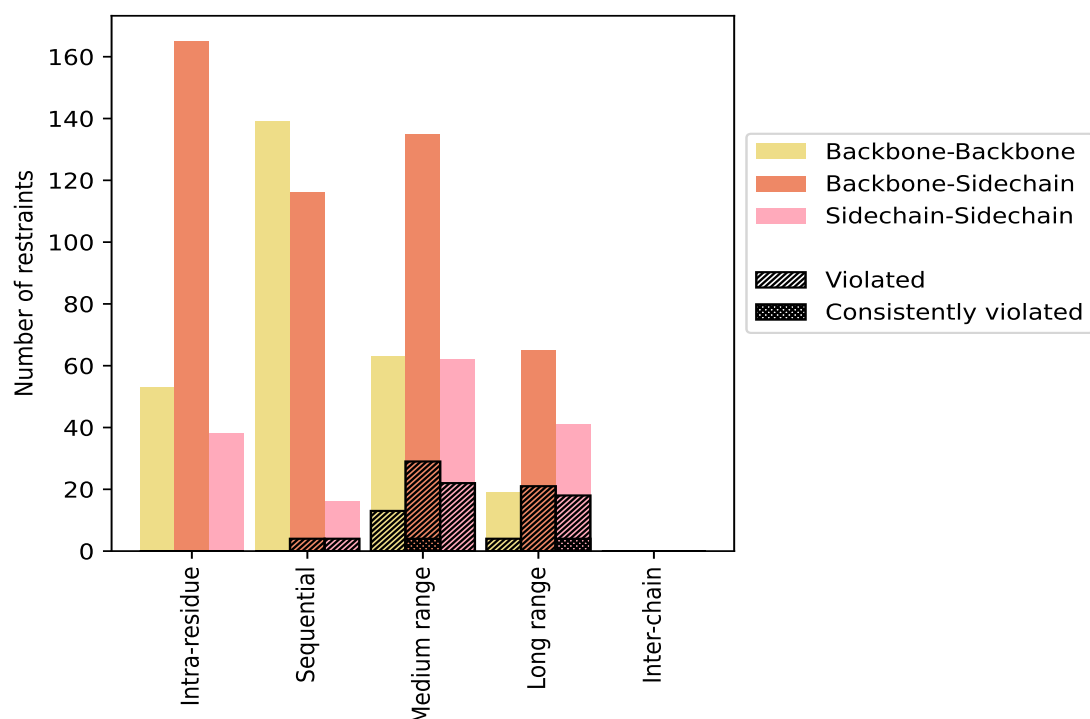
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	256	28.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	53	5.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	165	18.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	38	4.2	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	269	29.5	7	2.6	0.8	0	0.0	0.0
Backbone-Backbone	139	15.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	116	12.7	4	3.4	0.4	0	0.0	0.0
Sidechain-Sidechain	14	1.5	3	21.4	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	226	24.8	61	27.0	6.7	4	1.8	0.4
Backbone-Backbone	63	6.9	13	20.6	1.4	0	0.0	0.0
Backbone-Sidechain	103	11.3	28	27.2	3.1	4	3.9	0.4
Sidechain-Sidechain	60	6.6	20	33.3	2.2	0	0.0	0.0
Long range ($i-j \geq 5$)	95	10.4	36	37.9	3.9	4	4.2	0.4
Backbone-Backbone	19	2.1	4	21.1	0.4	0	0.0	0.0
Backbone-Sidechain	41	4.5	17	41.5	1.9	0	0.0	0.0
Sidechain-Sidechain	35	3.8	15	42.9	1.6	4	11.4	0.4
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	66	7.2	11	16.7	1.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	912	100.0	115	12.6	12.6	8	0.9	0.9
Backbone-Backbone	274	30.0	17	6.2	1.9	0	0.0	0.0
Backbone-Sidechain	481	52.7	54	11.2	5.9	4	0.8	0.4
Sidechain-Sidechain	157	17.2	44	28.0	4.8	4	2.5	0.4

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	0	3	24	19	0	46	0.35	1.57	0.33	0.24
2	0	2	24	21	0	47	0.39	1.79	0.38	0.23
3	0	3	24	24	0	51	0.35	1.91	0.38	0.22
4	0	2	21	19	0	42	0.42	1.96	0.45	0.26
5	0	4	22	17	0	43	0.39	1.81	0.39	0.24
6	0	2	26	20	0	48	0.33	1.9	0.36	0.21
7	0	4	21	14	0	39	0.3	1.32	0.26	0.21
8	0	2	24	18	0	44	0.36	1.59	0.36	0.22
9	0	4	21	17	0	42	0.36	1.23	0.31	0.24
10	0	2	18	20	0	40	0.43	1.61	0.43	0.24

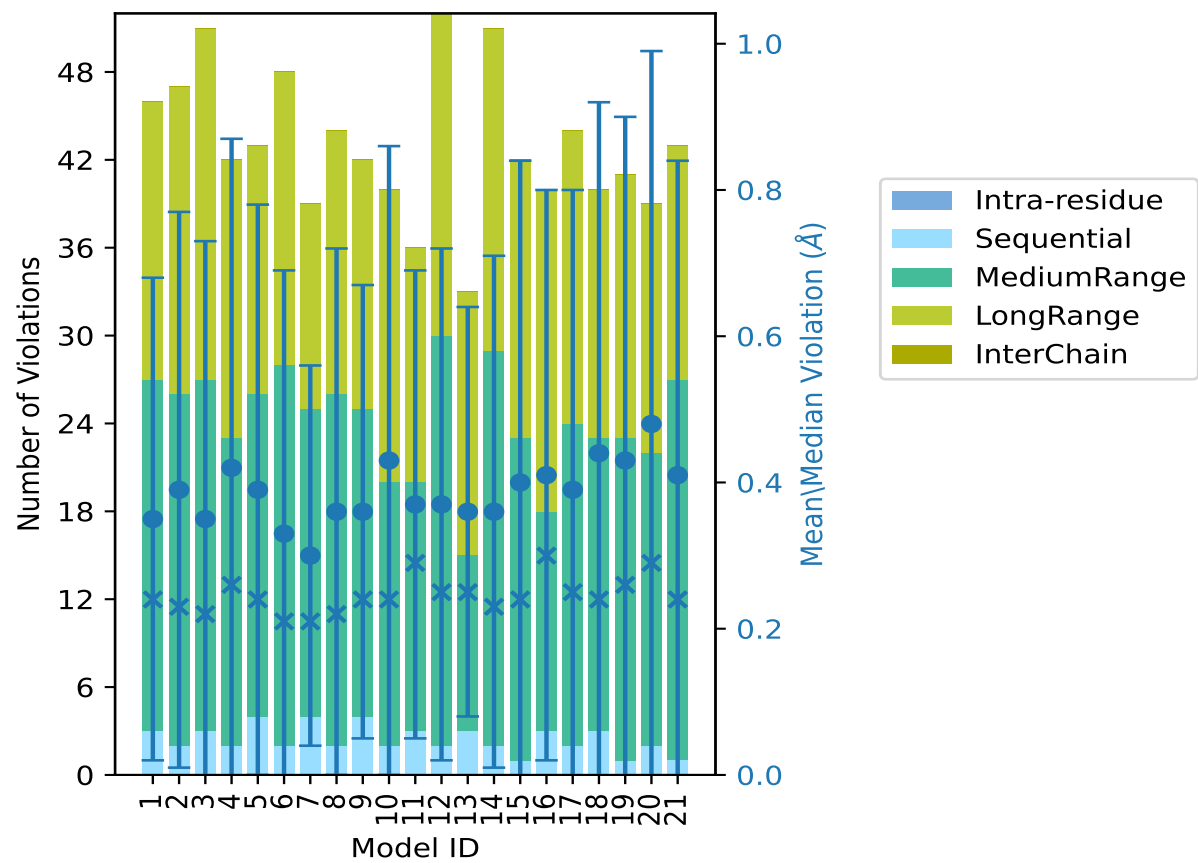
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	3	17	16	0	36	0.37	1.85	0.32	0.29
12	0	2	28	22	0	52	0.37	1.58	0.35	0.25
13	0	3	12	18	0	33	0.36	1.19	0.28	0.25
14	0	2	27	22	0	51	0.36	1.73	0.35	0.23
15	0	1	22	19	0	42	0.4	2.06	0.44	0.24
16	0	3	15	22	0	40	0.41	1.82	0.39	0.3
17	0	2	22	20	0	44	0.39	1.77	0.41	0.25
18	0	3	20	17	0	40	0.44	2.09	0.48	0.24
19	0	1	22	18	0	41	0.43	1.99	0.47	0.26
20	0	2	20	17	0	39	0.48	2.12	0.51	0.29
21	0	1	26	16	0	43	0.41	2.06	0.43	0.24

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

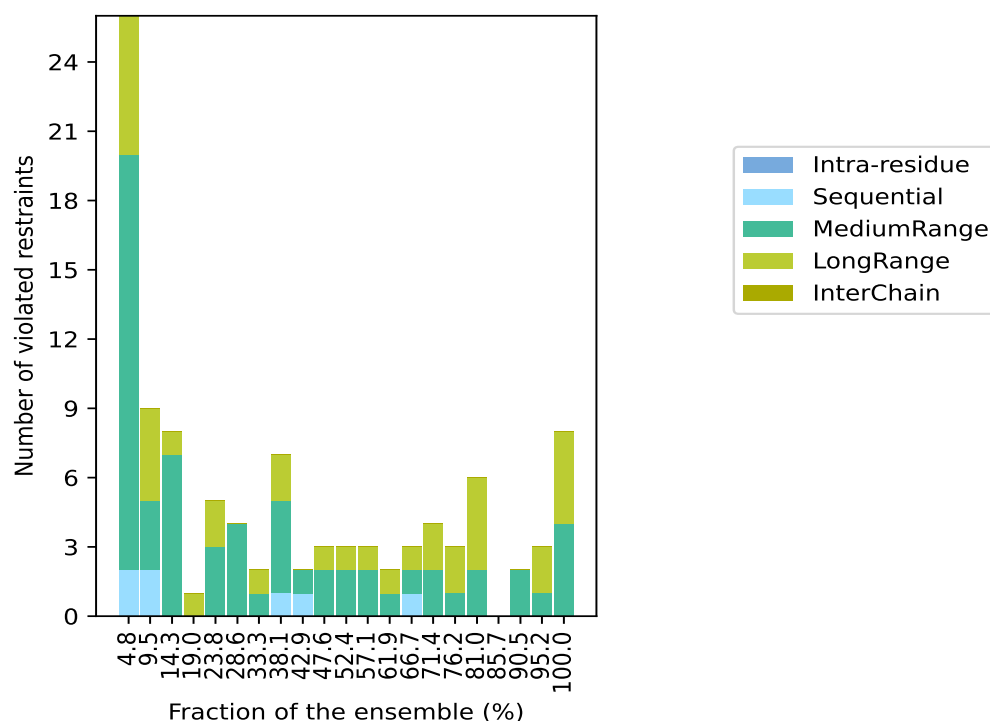
9.3 Distance violation statistics for the ensemble [i](#)

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, 742(IR:256, SQ:262, MR:165, LR:59, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	2	18	6	0	26	1	4.8
0	2	3	4	0	9	2	9.5
0	0	7	1	0	8	3	14.3
0	0	0	1	0	1	4	19.0
0	0	3	2	0	5	5	23.8
0	0	4	0	0	4	6	28.6
0	0	1	1	0	2	7	33.3
0	1	4	2	0	7	8	38.1
0	1	1	0	0	2	9	42.9
0	0	2	1	0	3	10	47.6
0	0	2	1	0	3	11	52.4
0	0	2	1	0	3	12	57.1
0	0	1	1	0	2	13	61.9
0	1	1	1	0	3	14	66.7
0	0	2	2	0	4	15	71.4
0	0	1	2	0	3	16	76.2
0	0	2	4	0	6	17	81.0
0	0	0	0	0	0	18	85.7
0	0	2	0	0	2	19	90.5
0	0	1	2	0	3	20	95.2
0	0	4	4	0	8	21	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

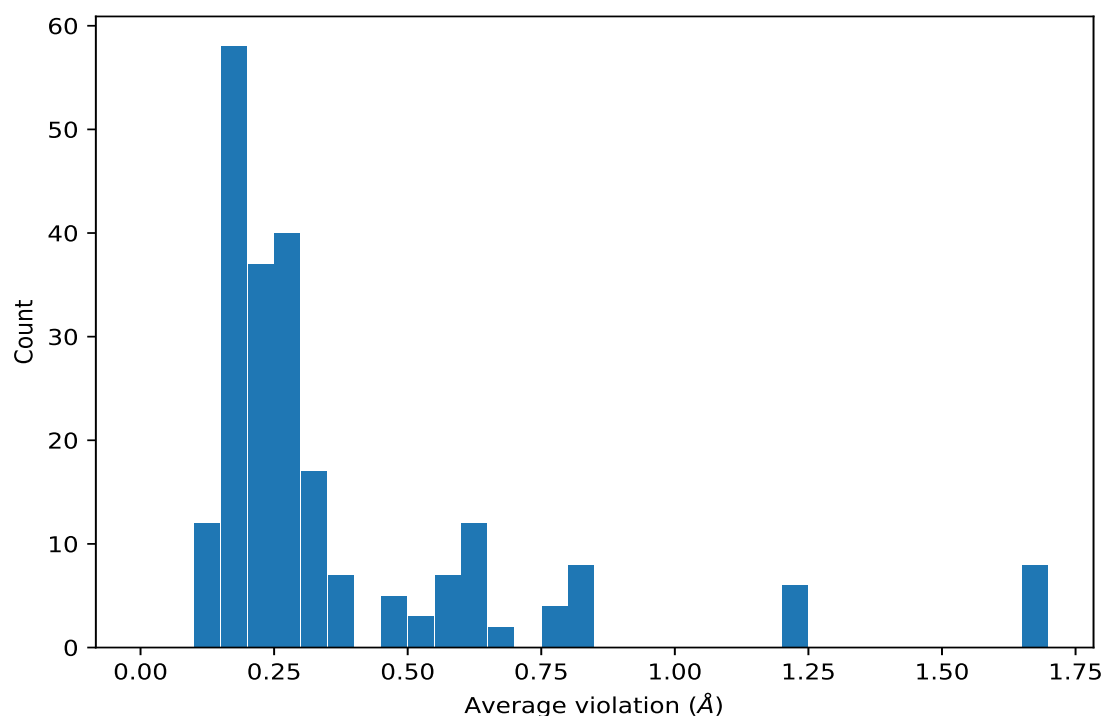
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	21	1.65	0.44	1.79
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	21	1.65	0.44	1.79
(1,225)	1:17:A:ILE:HG21	1:38:A:CYS:HB3	21	1.65	0.44	1.79
(1,225)	1:17:A:ILE:HG23	1:38:A:CYS:HB3	21	1.65	0.44	1.79
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	21	1.65	0.44	1.79
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	21	1.65	0.44	1.79
(1,226)	1:17:A:ILE:HG21	1:38:A:CYS:HB3	21	1.65	0.44	1.79
(1,226)	1:17:A:ILE:HG23	1:38:A:CYS:HB3	21	1.65	0.44	1.79
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	21	0.33	0.08	0.33
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	21	0.33	0.08	0.33
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	21	0.28	0.05	0.28
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	21	0.28	0.05	0.28
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	21	0.28	0.05	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	21	0.28	0.05	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	21	0.28	0.05	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	21	0.28	0.05	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	21	0.28	0.05	0.28
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	21	0.28	0.05	0.28
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	21	0.28	0.05	0.28
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	21	0.27	0.05	0.26
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	21	0.27	0.05	0.26
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	21	0.27	0.05	0.26
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	21	0.27	0.07	0.28
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	21	0.27	0.07	0.28
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	21	0.25	0.11	0.23
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	21	0.25	0.11	0.23
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	21	0.25	0.11	0.23
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	21	0.25	0.11	0.23
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	21	0.19	0.05	0.18
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB2	20	1.21	0.34	1.23
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB1	20	1.21	0.34	1.23
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB2	20	1.21	0.34	1.23
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB3	20	1.21	0.34	1.23
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB3	20	1.21	0.34	1.23
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB1	20	1.21	0.34	1.23
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	20	0.61	0.25	0.6
(1,231)	1:17:A:ILE:HG21	1:54:A:THR:HA	20	0.61	0.25	0.6
(1,231)	1:17:A:ILE:HG22	1:54:A:THR:HA	20	0.61	0.25	0.6
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	20	0.3	0.08	0.29
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	20	0.3	0.08	0.29
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	20	0.3	0.08	0.29
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	20	0.3	0.08	0.29
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	19	0.21	0.04	0.21
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	19	0.21	0.04	0.21
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	19	0.21	0.08	0.2
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	19	0.21	0.08	0.2
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG12	17	0.83	0.39	0.92
(1,535)	1:40:A:ALA:HB3	1:17:A:ILE:HG12	17	0.83	0.39	0.92
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG13	17	0.83	0.39	0.92
(1,535)	1:40:A:ALA:HB2	1:17:A:ILE:HG12	17	0.83	0.39	0.92
(1,535)	1:40:A:ALA:HB2	1:17:A:ILE:HG13	17	0.83	0.39	0.92
(1,535)	1:40:A:ALA:HB3	1:17:A:ILE:HG13	17	0.83	0.39	0.92
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	17	0.68	0.24	0.67
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD1	17	0.68	0.24	0.67
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG23	17	0.62	0.26	0.66
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG21	17	0.62	0.26	0.66
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG22	17	0.62	0.26	0.66
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG13	17	0.62	0.26	0.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG12	17	0.62	0.26	0.66
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG22	17	0.46	0.28	0.39
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG23	17	0.46	0.28	0.39
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG1	17	0.46	0.28	0.39
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG21	17	0.46	0.28	0.39
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	17	0.28	0.09	0.26
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	17	0.15	0.04	0.14
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	17	0.15	0.04	0.14
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG23	16	0.63	0.51	0.4
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG21	16	0.63	0.51	0.4
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG22	16	0.63	0.51	0.4
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG13	16	0.63	0.51	0.4
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	16	0.57	0.08	0.6
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG13	16	0.57	0.08	0.6
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	16	0.2	0.08	0.18
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	16	0.2	0.08	0.18
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG13	15	0.53	0.17	0.58
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	15	0.53	0.17	0.58
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	15	0.19	0.06	0.18
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	15	0.19	0.06	0.18
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	15	0.16	0.03	0.15
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	15	0.16	0.03	0.15
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	15	0.16	0.03	0.15
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	15	0.16	0.03	0.15
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	15	0.16	0.03	0.15
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	15	0.16	0.03	0.15
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	15	0.16	0.03	0.15
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	15	0.16	0.03	0.15
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	14	0.28	0.08	0.29
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	14	0.28	0.08	0.29
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	14	0.26	0.06	0.29
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	14	0.22	0.06	0.21
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	14	0.19	0.06	0.18
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	14	0.19	0.06	0.18
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	13	0.19	0.06	0.17
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	13	0.15	0.04	0.14
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	12	0.25	0.08	0.25
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	12	0.25	0.08	0.25
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	12	0.25	0.14	0.2
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	12	0.25	0.14	0.2
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	12	0.17	0.03	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	12	0.17	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	12	0.17	0.03	0.16
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	11	0.23	0.1	0.24
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	11	0.23	0.1	0.24
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	11	0.23	0.08	0.21
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	11	0.23	0.08	0.21
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	11	0.22	0.05	0.23
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	11	0.22	0.05	0.23
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	10	0.3	0.16	0.24
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	10	0.3	0.16	0.24
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	10	0.2	0.06	0.21
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	10	0.2	0.06	0.21
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	10	0.2	0.06	0.21
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	10	0.17	0.04	0.16
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	10	0.16	0.04	0.15
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	9	0.33	0.13	0.29
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	9	0.33	0.13	0.29
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	9	0.33	0.13	0.29
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	9	0.33	0.13	0.29
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	9	0.13	0.03	0.12
(1,738)	1:54:A:THR:HG21	1:52:A:ARG:HE	8	0.78	0.24	0.8
(1,738)	1:54:A:THR:HG22	1:52:A:ARG:HE	8	0.78	0.24	0.8
(1,738)	1:54:A:THR:HG1	1:52:A:ARG:HE	8	0.78	0.24	0.8
(1,738)	1:54:A:THR:HG23	1:52:A:ARG:HE	8	0.78	0.24	0.8
(1,227)	1:17:A:ILE:HG12	1:41:A:ALA:HA	8	0.29	0.1	0.27
(1,227)	1:17:A:ILE:HG13	1:41:A:ALA:HA	8	0.29	0.1	0.27
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG12	8	0.29	0.1	0.27
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG13	8	0.29	0.1	0.27
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	8	0.2	0.08	0.18
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	8	0.2	0.08	0.18
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	8	0.2	0.08	0.18
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	8	0.2	0.08	0.18
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	8	0.2	0.08	0.18
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	8	0.2	0.08	0.18
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	8	0.19	0.08	0.16
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	8	0.18	0.03	0.18
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	8	0.18	0.03	0.18
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	8	0.16	0.03	0.15
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	8	0.16	0.03	0.15
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	8	0.16	0.03	0.15
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	8	0.16	0.03	0.15
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG21	7	0.55	0.5	0.15
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG22	7	0.55	0.5	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG1	7	0.55	0.5	0.15
(2,20)	1:18:A:ARG:HH21	1:7:A:ASP:OD2	7	0.47	0.08	0.51
(2,18)	1:18:A:ARG:HH12	1:20:A:ASP:OD2	7	0.21	0.05	0.22
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB2	7	0.16	0.05	0.16
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB3	7	0.16	0.05	0.16
(1,134)	1:11:A:SER:HB2	1:15:A:TRP:HD1	6	0.38	0.15	0.38
(1,134)	1:11:A:SER:HB3	1:15:A:TRP:HD1	6	0.38	0.15	0.38
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD11	6	0.38	0.13	0.42
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD12	6	0.38	0.13	0.42
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD13	6	0.38	0.13	0.42
(1,801)	1:63:A:THR:H	1:60:A:GLY:H	6	0.24	0.08	0.22
(1,840)	1:69:A:THR:HB	1:67:A:VAL:HB	6	0.16	0.06	0.16
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD1	5	0.36	0.06	0.35
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD2	5	0.36	0.06	0.35
(1,148)	1:12:A:ASP:HA	1:49:A:HIS:HA	5	0.33	0.22	0.24
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE1	5	0.28	0.1	0.29
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE2	5	0.28	0.1	0.29
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE1	5	0.28	0.1	0.29
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE2	5	0.28	0.1	0.29
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ1	5	0.23	0.12	0.17
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ2	5	0.23	0.12	0.17
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ3	5	0.23	0.12	0.17
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ1	5	0.23	0.12	0.17
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ2	5	0.23	0.12	0.17
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ3	5	0.23	0.12	0.17
(1,750)	1:55:A:VAL:H	1:53:A:ILE:H	5	0.14	0.05	0.12
(1,547)	1:41:A:ALA:HB1	1:15:A:TRP:HD1	4	0.22	0.04	0.22
(1,547)	1:41:A:ALA:HB2	1:15:A:TRP:HD1	4	0.22	0.04	0.22
(1,547)	1:41:A:ALA:HB3	1:15:A:TRP:HD1	4	0.22	0.04	0.22
(1,421)	1:34:A:PHE:HA	1:30:A:LYS:HG2	3	0.3	0.01	0.3
(1,421)	1:34:A:PHE:HA	1:30:A:LYS:HG3	3	0.3	0.01	0.3
(1,290)	1:24:A:THR:HA	1:26:A:ASP:HB2	3	0.18	0.03	0.2
(1,290)	1:24:A:THR:HA	1:26:A:ASP:HB3	3	0.18	0.03	0.2
(1,146)	1:12:A:ASP:HB2	1:15:A:TRP:HB2	3	0.18	0.03	0.16
(1,146)	1:12:A:ASP:HB2	1:15:A:TRP:HB3	3	0.18	0.03	0.16
(1,146)	1:12:A:ASP:HB3	1:15:A:TRP:HB2	3	0.18	0.03	0.16
(1,146)	1:12:A:ASP:HB3	1:15:A:TRP:HB3	3	0.18	0.03	0.16
(1,184)	1:15:A:TRP:HB2	1:12:A:ASP:HB2	3	0.18	0.03	0.16
(1,184)	1:15:A:TRP:HB2	1:12:A:ASP:HB3	3	0.18	0.03	0.16
(1,184)	1:15:A:TRP:HB3	1:12:A:ASP:HB2	3	0.18	0.03	0.16
(1,184)	1:15:A:TRP:HB3	1:12:A:ASP:HB3	3	0.18	0.03	0.16
(1,676)	1:49:A:HIS:HA	1:45:A:ILE:HA	3	0.17	0.04	0.17

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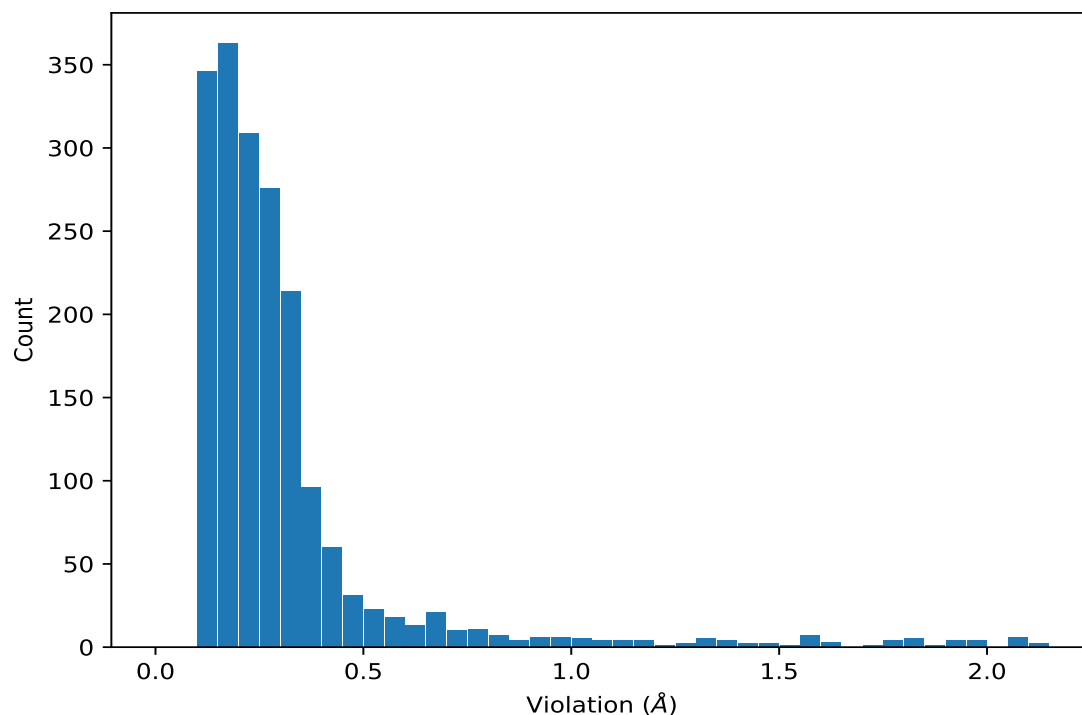
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,30)	1:4:A:ALA:HB1	1:34:A:PHE:HD1	3	0.17	0.06	0.15
(1,30)	1:4:A:ALA:HB1	1:34:A:PHE:HD2	3	0.17	0.06	0.15
(1,30)	1:4:A:ALA:HB2	1:34:A:PHE:HD1	3	0.17	0.06	0.15
(1,30)	1:4:A:ALA:HB2	1:34:A:PHE:HD2	3	0.17	0.06	0.15
(1,30)	1:4:A:ALA:HB3	1:34:A:PHE:HD1	3	0.17	0.06	0.15
(1,30)	1:4:A:ALA:HB3	1:34:A:PHE:HD2	3	0.17	0.06	0.15
(2,24)	1:20:A:ASP:H	1:5:A:TYR:O	3	0.16	0.05	0.15
(1,736)	1:54:A:THR:HB	1:52:A:ARG:HB2	3	0.16	0.04	0.14
(1,736)	1:54:A:THR:HB	1:52:A:ARG:HB3	3	0.16	0.04	0.14
(1,574)	1:42:A:SER:HB2	1:46:A:LYS:HE2	3	0.14	0.01	0.15
(1,574)	1:42:A:SER:HB2	1:46:A:LYS:HE3	3	0.14	0.01	0.15
(1,574)	1:42:A:SER:HB3	1:46:A:LYS:HE2	3	0.14	0.01	0.15
(1,574)	1:42:A:SER:HB3	1:46:A:LYS:HE3	3	0.14	0.01	0.15
(2,6)	1:14:A:ARG:HE	1:50:A:GLU:OE1	3	0.12	0.01	0.13
(1,216)	1:16:A:GLY:HA2	1:53:A:ILE:HG22	2	0.84	0.18	0.84
(1,216)	1:16:A:GLY:HA2	1:53:A:ILE:HG21	2	0.84	0.18	0.84
(1,203)	1:16:A:GLY:HA2	1:8:A:ILE:HB	2	0.56	0.01	0.56
(1,203)	1:16:A:GLY:HA3	1:8:A:ILE:HB	2	0.56	0.01	0.56
(1,806)	1:64:A:ASN:HA	1:63:A:THR:HG1	2	0.54	0.21	0.54
(1,261)	1:20:A:ASP:HB2	1:18:A:ARG:HE	2	0.3	0.02	0.3
(1,261)	1:20:A:ASP:HB3	1:18:A:ARG:HE	2	0.3	0.02	0.3
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ1	2	0.29	0.09	0.29
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ2	2	0.29	0.09	0.29
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ3	2	0.29	0.09	0.29
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ1	2	0.29	0.09	0.29
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ2	2	0.29	0.09	0.29
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ3	2	0.29	0.09	0.29
(1,117)	1:10:A:GLY:HA2	1:16:A:GLY:HA2	2	0.2	0.04	0.2
(1,117)	1:10:A:GLY:HA2	1:16:A:GLY:HA3	2	0.2	0.04	0.2
(1,117)	1:10:A:GLY:HA3	1:16:A:GLY:HA2	2	0.2	0.04	0.2
(1,117)	1:10:A:GLY:HA3	1:16:A:GLY:HA3	2	0.2	0.04	0.2
(1,12)	1:3:A:LYS:HB2	1:2:A:GLY:H	2	0.18	0.08	0.18
(1,12)	1:3:A:LYS:HB3	1:2:A:GLY:H	2	0.18	0.08	0.18
(1,384)	1:32:A:ALA:HB1	1:28:A:SER:HA	2	0.16	0.01	0.16
(1,384)	1:32:A:ALA:HB2	1:28:A:SER:HA	2	0.16	0.01	0.16
(1,384)	1:32:A:ALA:HB3	1:28:A:SER:HA	2	0.16	0.01	0.16
(2,16)	1:18:A:ARG:H	1:7:A:ASP:O	2	0.15	0.0	0.15
(2,60)	1:50:A:GLU:H	1:13:A:ASN:O	2	0.14	0.01	0.14
(1,42)	1:5:A:TYR:HB2	1:30:A:LYS:HG2	2	0.12	0.01	0.12
(1,42)	1:5:A:TYR:HB2	1:30:A:LYS:HG3	2	0.12	0.01	0.12
(1,42)	1:5:A:TYR:HB3	1:30:A:LYS:HG2	2	0.12	0.01	0.12
(1,42)	1:5:A:TYR:HB3	1:30:A:LYS:HG3	2	0.12	0.01	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	20	2.12
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	20	2.12
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	18	2.09
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	18	2.09
(1,226)	1:17:A:ILE:HG21	1:38:A:CYS:HB3	15	2.06
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	21	2.06
(1,225)	1:17:A:ILE:HG21	1:38:A:CYS:HB3	15	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	21	2.06
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	19	1.99
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	19	1.99
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	4	1.96
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	4	1.96
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	3	1.91
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	3	1.91
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	6	1.9
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	6	1.9
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB2	11	1.85
(1,226)	1:17:A:ILE:HG23	1:38:A:CYS:HB3	16	1.82
(1,225)	1:17:A:ILE:HG23	1:38:A:CYS:HB3	16	1.82
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	5	1.81
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	5	1.81
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG21	20	1.8
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	2	1.79
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	2	1.79
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	17	1.77
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	17	1.77
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB2	14	1.73
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG21	18	1.63
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	10	1.61
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	10	1.61
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB1	17	1.59
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	8	1.59
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	8	1.59
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	12	1.58
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	12	1.58
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	1	1.57
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	1	1.57
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB2	19	1.53
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG12	19	1.48
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB1	12	1.46
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB1	10	1.43
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG21	4	1.43
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	14	1.38
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	14	1.38
(1,535)	1:40:A:ALA:HB2	1:17:A:ILE:HG12	17	1.35
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB2	20	1.35
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB2	3	1.33
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB3	8	1.33
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG23	10	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:17:A:ILE:HG21	1:38:A:CYS:HB3	7	1.32
(1,225)	1:17:A:ILE:HG21	1:38:A:CYS:HB3	7	1.32
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB1	2	1.27
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG12	5	1.25
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG12	9	1.23
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB3	13	1.19
(1,535)	1:40:A:ALA:HB2	1:17:A:ILE:HG12	10	1.17
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB3	4	1.16
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB2	1	1.15
(1,226)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	9	1.14
(1,225)	1:17:A:ILE:HG13	1:38:A:CYS:HB3	9	1.14
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	20	1.13
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	18	1.13
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG12	21	1.09
(1,738)	1:54:A:THR:HG22	1:52:A:ARG:HE	16	1.05
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG12	8	1.05
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD1	13	1.05
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB1	15	1.03
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB2	21	1.03
(1,216)	1:16:A:GLY:HA2	1:53:A:ILE:HG21	15	1.02
(1,738)	1:54:A:THR:HG23	1:52:A:ARG:HE	10	1.01
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG1	13	1.01
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	15	0.98
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB1	9	0.98
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG23	9	0.96
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG12	2	0.95
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG21	11	0.95
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	12	0.95
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG12	18	0.94
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD1	10	0.93
(1,535)	1:40:A:ALA:HB3	1:17:A:ILE:HG12	12	0.92
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG22	14	0.92
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG23	12	0.91
(1,738)	1:54:A:THR:HG21	1:52:A:ARG:HE	14	0.9
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	3	0.88
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	14	0.88
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG23	15	0.85
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG23	1	0.85
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB1	5	0.84
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG13	8	0.83
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG22	5	0.83
(1,738)	1:54:A:THR:HG23	1:52:A:ARG:HE	21	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG23	17	0.82
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	4	0.82
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG21	10	0.8
(1,738)	1:54:A:THR:HG21	1:52:A:ARG:HE	2	0.79
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	20	0.79
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG13	9	0.79
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG23	16	0.78
(1,738)	1:54:A:THR:HG22	1:52:A:ARG:HE	4	0.77
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB1	18	0.77
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	11	0.77
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	3	0.76
(1,148)	1:12:A:ASP:HA	1:49:A:HIS:HA	16	0.76
(1,806)	1:64:A:ASN:HA	1:63:A:THR:HG1	1	0.75
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	19	0.75
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG22	6	0.74
(1,231)	1:17:A:ILE:HG21	1:54:A:THR:HA	6	0.74
(1,231)	1:17:A:ILE:HG21	1:54:A:THR:HA	18	0.74
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG13	4	0.73
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG23	21	0.73
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	19	0.73
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	13	0.71
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	13	0.71
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	16	0.71
(1,83)	1:8:A:ILE:HG12	1:10:A:GLY:HA2	9	0.7
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG22	19	0.69
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG13	4	0.69
(1,535)	1:40:A:ALA:HB2	1:17:A:ILE:HG13	11	0.68
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	15	0.68
(1,231)	1:17:A:ILE:HG22	1:54:A:THR:HA	13	0.68
(1,228)	1:17:A:ILE:HG13	1:44:A:ALA:HB3	16	0.68
(1,738)	1:54:A:THR:HG21	1:52:A:ARG:HE	12	0.67
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG13	2	0.67
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	19	0.67
(1,216)	1:16:A:GLY:HA2	1:53:A:ILE:HG22	9	0.67
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	11	0.67
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	11	0.67
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	11	0.67
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	11	0.67
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	20	0.67
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG23	4	0.66
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD1	2	0.66
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG13	11	0.65
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG13	14	0.65
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	17	0.65
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	2	0.63
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD1	6	0.63
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	18	0.62
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	1	0.62
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG13	13	0.62
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	5	0.62
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG13	10	0.61
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	8	0.61
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG13	20	0.61
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG12	1	0.6
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	14	0.6
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	14	0.6
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG22	20	0.6
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG22	11	0.59
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG13	12	0.58
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG22	3	0.58
(1,203)	1:16:A:GLY:HA2	1:8:A:ILE:HB	8	0.58
(1,203)	1:16:A:GLY:HA3	1:8:A:ILE:HB	8	0.58
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	9	0.58
(1,134)	1:11:A:SER:HB2	1:15:A:TRP:HD1	5	0.58
(1,134)	1:11:A:SER:HB3	1:15:A:TRP:HD1	5	0.58
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	3	0.57
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	14	0.57
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	7	0.56
(1,228)	1:17:A:ILE:HG12	1:44:A:ALA:HB1	6	0.56
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	6	0.56
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	1	0.55
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	1	0.55
(1,203)	1:16:A:GLY:HA2	1:8:A:ILE:HB	21	0.55
(1,203)	1:16:A:GLY:HA3	1:8:A:ILE:HB	21	0.55
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	10	0.55
(2,20)	1:18:A:ARG:HH21	1:7:A:ASP:OD2	7	0.54
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	2	0.54
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	21	0.53
(2,20)	1:18:A:ARG:HH21	1:7:A:ASP:OD2	5	0.52
(2,20)	1:18:A:ARG:HH21	1:7:A:ASP:OD2	18	0.52
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	9	0.52
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	9	0.52
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	12	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:18:A:ARG:HH21	1:7:A:ASP:OD2	2	0.51
(2,20)	1:18:A:ARG:HH21	1:7:A:ASP:OD2	14	0.51
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG13	5	0.51
(1,231)	1:17:A:ILE:HG22	1:54:A:THR:HA	16	0.51
(1,134)	1:11:A:SER:HB2	1:15:A:TRP:HD1	4	0.51
(1,134)	1:11:A:SER:HB3	1:15:A:TRP:HD1	4	0.51
(1,737)	1:54:A:THR:HG1	1:52:A:ARG:HD3	12	0.5
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG13	15	0.5
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	16	0.5
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	16	0.5
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	16	0.5
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	16	0.5
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD11	18	0.5
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD12	18	0.5
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD13	18	0.5
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	15	0.49
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG13	8	0.48
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	21	0.48
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	21	0.48
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG23	5	0.48
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD11	3	0.48
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD12	3	0.48
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD13	3	0.48
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	2	0.48
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	2	0.48
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	2	0.48
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	2	0.48
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG12	12	0.47
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG21	7	0.47
(1,227)	1:17:A:ILE:HG12	1:41:A:ALA:HA	12	0.47
(1,535)	1:40:A:ALA:HB2	1:17:A:ILE:HG13	20	0.46
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	2	0.46
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	2	0.46
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	3	0.46
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	3	0.46
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG23	1	0.46
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	16	0.45
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	16	0.45
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE1	6	0.45
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE2	6	0.45
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE1	6	0.45
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE2	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	21	0.45
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	21	0.45
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	21	0.45
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	21	0.45
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	18	0.44
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	18	0.44
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	1	0.44
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD1	17	0.44
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD2	17	0.44
(1,134)	1:11:A:SER:HB2	1:15:A:TRP:HD1	16	0.44
(1,134)	1:11:A:SER:HB3	1:15:A:TRP:HD1	16	0.44
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD1	15	0.44
(1,226)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	11	0.43
(1,225)	1:17:A:ILE:HG12	1:38:A:CYS:HB3	11	0.43
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	5	0.43
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD11	15	0.43
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD12	15	0.43
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD13	15	0.43
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	17	0.43
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	16	0.42
(1,535)	1:40:A:ALA:HB2	1:17:A:ILE:HG12	21	0.42
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	8	0.42
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	8	0.42
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	16	0.42
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	7	0.42
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	7	0.42
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	21	0.42
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	21	0.42
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG21	3	0.42
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD1	16	0.42
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD2	16	0.42
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	10	0.41
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	10	0.41
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG21	16	0.41
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	10	0.41
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	10	0.41
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	10	0.41
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	10	0.41
(1,199)	1:15:A:TRP:HA	1:17:A:ILE:HG12	7	0.41
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	5	0.4
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	5	0.4
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ1	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ2	5	0.4
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ3	5	0.4
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ1	5	0.4
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ2	5	0.4
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ3	5	0.4
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	19	0.4
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	19	0.4
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	11	0.4
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	11	0.4
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG23	2	0.4
(1,231)	1:17:A:ILE:HG21	1:54:A:THR:HA	8	0.4
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD11	19	0.4
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD12	19	0.4
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD13	19	0.4
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	16	0.4
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	16	0.4
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	16	0.4
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	16	0.4
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	7	0.4
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	7	0.4
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	7	0.4
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	7	0.4
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	18	0.39
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	18	0.39
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	1	0.39
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	1	0.39
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG1	17	0.39
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG22	19	0.39
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG21	8	0.39
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG23	15	0.39
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	21	0.39
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	15	0.39
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	15	0.39
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	13	0.39
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	13	0.39
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	13	0.39
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	13	0.39
(1,801)	1:63:A:THR:H	1:60:A:GLY:H	21	0.38
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	17	0.38
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ1	20	0.38
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ2	20	0.38
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ3	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ1	20	0.38
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ2	20	0.38
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ3	20	0.38
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG12	19	0.38
(1,227)	1:17:A:ILE:HG12	1:41:A:ALA:HA	19	0.38
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	14	0.38
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	14	0.38
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	14	0.38
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	14	0.38
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	4	0.38
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	5	0.37
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	5	0.37
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	5	0.37
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	6	0.37
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	6	0.37
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	2	0.37
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	2	0.37
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG22	14	0.37
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG23	21	0.37
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	20	0.37
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	20	0.37
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD11	16	0.37
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD12	16	0.37
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD13	16	0.37
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	13	0.37
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	13	0.37
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	13	0.37
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	13	0.37
(2,20)	1:18:A:ARG:HH21	1:7:A:ASP:OD2	11	0.36
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	17	0.36
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	21	0.36
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	2	0.36
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	2	0.36
(1,535)	1:40:A:ALA:HB3	1:17:A:ILE:HG12	3	0.36
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	1	0.36
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	1	0.36
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	21	0.36
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	21	0.36
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	9	0.36
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	9	0.36
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	9	0.36
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	8	0.36
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	8	0.36
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	8	0.36
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	8	0.36
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	9	0.36
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	9	0.36
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	9	0.36
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	9	0.36
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	7	0.35
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	7	0.35
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	20	0.35
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	20	0.35
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	2	0.35
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	2	0.35
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	2	0.35
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	2	0.35
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	2	0.35
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	2	0.35
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	2	0.35
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	2	0.35
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	2	0.35
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	9	0.35
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	9	0.35
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	9	0.35
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	17	0.35
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	17	0.35
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	11	0.35
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	11	0.35
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	20	0.35
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	20	0.35
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD1	12	0.35
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD2	12	0.35
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	14	0.35
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	14	0.35
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	1	0.34
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	1	0.34
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	1	0.34
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	1	0.34
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	1	0.34
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	1	0.34
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	1	0.34
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	1	0.34
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	17	0.34
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	17	0.34
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	17	0.34
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	21	0.34
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	21	0.34
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG1	3	0.34
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	19	0.34
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	19	0.34
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	8	0.34
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	8	0.34
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	8	0.34
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	8	0.34
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	3	0.34
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	3	0.34
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	3	0.34
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	3	0.34
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	10	0.34
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	10	0.34
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	10	0.34
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	10	0.34
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	16	0.34
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	16	0.34
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	16	0.34
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	16	0.34
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	12	0.34
(1,51)	1:6:A:TYR:HA	1:8:A:ILE:HG21	6	0.34
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	12	0.34
(1,806)	1:64:A:ASN:HA	1:63:A:THR:HG1	3	0.33
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	11	0.33
(1,739)	1:54:A:THR:HG23	1:52:A:ARG:HG3	20	0.33
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	21	0.33
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	21	0.33
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	6	0.33
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	6	0.33
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	11	0.33
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	11	0.33
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	14	0.33
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	14	0.33
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	13	0.33
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	13	0.33
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	13	0.33
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	13	0.33
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	13	0.33
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	13	0.33
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	13	0.33
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	13	0.33
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ1	8	0.33
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ2	8	0.33
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ3	8	0.33
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ1	8	0.33
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ2	8	0.33
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ3	8	0.33
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	9	0.33
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	9	0.33
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	16	0.33
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	16	0.33
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	12	0.32
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	15	0.32
(2,20)	1:18:A:ARG:HH21	1:7:A:ASP:OD2	10	0.32
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	19	0.32
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	14	0.32
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	14	0.32
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	14	0.32
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	14	0.32
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	14	0.32
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	14	0.32
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG13	3	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	11	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	11	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	11	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	11	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	11	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	11	0.32
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	11	0.32
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	11	0.32
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	11	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	16	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	16	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	16	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	16	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	16	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	16	0.32
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	16	0.32
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	16	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	17	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	17	0.32
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	17	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	17	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	17	0.32
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	17	0.32
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	17	0.32
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	17	0.32
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	17	0.32
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	6	0.32
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	6	0.32
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	6	0.32
(1,421)	1:34:A:PHE:HA	1:30:A:LYS:HG2	19	0.32
(1,421)	1:34:A:PHE:HA	1:30:A:LYS:HG3	19	0.32
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	4	0.32
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	4	0.32
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	19	0.32
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	19	0.32
(1,261)	1:20:A:ASP:HB2	1:18:A:ARG:HE	8	0.32
(1,261)	1:20:A:ASP:HB3	1:18:A:ARG:HE	8	0.32
(1,227)	1:17:A:ILE:HG13	1:41:A:ALA:HA	3	0.32
(1,134)	1:11:A:SER:HB2	1:15:A:TRP:HD1	15	0.32
(1,134)	1:11:A:SER:HB3	1:15:A:TRP:HD1	15	0.32
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	20	0.31
(1,801)	1:63:A:THR:H	1:60:A:GLY:H	2	0.31
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	12	0.31
(1,535)	1:40:A:ALA:HB3	1:17:A:ILE:HG13	14	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	6	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	6	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	6	0.31
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	6	0.31
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	6	0.31
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	6	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	6	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	6	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	6	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	7	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	7	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	7	0.31
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	7	0.31
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	7	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	7	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	7	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	7	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	20	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	20	0.31
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	20	0.31
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	20	0.31
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	20	0.31
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	20	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	20	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	20	0.31
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	20	0.31
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	1	0.31
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	1	0.31
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	1	0.31
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	11	0.31
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	11	0.31
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	11	0.31
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	2	0.31
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	2	0.31
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	5	0.31
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	5	0.31
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	18	0.31
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	18	0.31
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	3	0.31
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	3	0.31
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	20	0.31
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	20	0.31
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	20	0.31
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	20	0.31
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	18	0.31
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	18	0.31
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	18	0.31
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	18	0.31
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	17	0.31
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	17	0.31
(1,134)	1:11:A:SER:HB2	1:15:A:TRP:HD1	11	0.31
(1,134)	1:11:A:SER:HB3	1:15:A:TRP:HD1	11	0.31
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	7	0.3
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	8	0.3
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	20	0.3
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	12	0.3
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	12	0.3
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	12	0.3
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	12	0.3
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	12	0.3
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	12	0.3
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	12	0.3
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	12	0.3
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	12	0.3
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	12	0.3
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	12	0.3
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	19	0.3
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	19	0.3
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	19	0.3
(1,421)	1:34:A:PHE:HA	1:30:A:LYS:HG2	15	0.3
(1,421)	1:34:A:PHE:HA	1:30:A:LYS:HG3	15	0.3
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	10	0.3
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	10	0.3
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	18	0.3
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	18	0.3
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	14	0.3
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	14	0.3
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	3	0.3
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	3	0.3
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	17	0.3
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	17	0.3
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	7	0.3
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	7	0.3
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	7	0.3
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	7	0.3
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD1	5	0.3
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD2	5	0.3
(1,148)	1:12:A:ASP:HA	1:49:A:HIS:HA	3	0.3
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	6	0.3
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	6	0.3
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	11	0.29
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	16	0.29
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	20	0.29
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	13	0.29
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	13	0.29
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	13	0.29
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	13	0.29
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	13	0.29
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	13	0.29
(1,421)	1:34:A:PHE:HA	1:30:A:LYS:HG2	6	0.29
(1,421)	1:34:A:PHE:HA	1:30:A:LYS:HG3	6	0.29
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	17	0.29
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	17	0.29
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	17	0.29
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	1	0.29
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	1	0.29
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	14	0.29
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE1	4	0.29
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE2	4	0.29
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE1	4	0.29
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE2	4	0.29
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE1	19	0.29
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE2	19	0.29
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE1	19	0.29
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE2	19	0.29
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	5	0.29
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	5	0.29
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	5	0.29
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	5	0.29
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD1	3	0.29
(1,164)	1:13:A:ASN:HA	1:47:A:PHE:HD2	3	0.29
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	6	0.29
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	6	0.29
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	6	0.29
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	6	0.29
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	9	0.29
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	9	0.29
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	11	0.29
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	6	0.28
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	4	0.28
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB2	1	0.28
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB3	1	0.28
(1,547)	1:41:A:ALA:HB1	1:15:A:TRP:HD1	14	0.28
(1,547)	1:41:A:ALA:HB2	1:15:A:TRP:HD1	14	0.28
(1,547)	1:41:A:ALA:HB3	1:15:A:TRP:HD1	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	9	0.28
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	9	0.28
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	8	0.28
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	8	0.28
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	8	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	8	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	8	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	8	0.28
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	8	0.28
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	8	0.28
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	8	0.28
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	9	0.28
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	9	0.28
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	9	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	9	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	9	0.28
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	9	0.28
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	9	0.28
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	9	0.28
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	9	0.28
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	12	0.28
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	12	0.28
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	17	0.28
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	17	0.28
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	4	0.28
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	4	0.28
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	13	0.28
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	13	0.28
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	16	0.28
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	16	0.28
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	8	0.28
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	8	0.28
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	20	0.28
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	20	0.28
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	2	0.28
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	6	0.28
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	6	0.28
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	17	0.28
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	3	0.28
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	3	0.28
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	3	0.28
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	10	0.28
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	10	0.28
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	10	0.28
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	10	0.28
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	1	0.28
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	1	0.28
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	1	0.28
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	1	0.28
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	19	0.27
(2,18)	1:18:A:ARG:HH12	1:20:A:ASP:OD2	18	0.27
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	3	0.27
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	3	0.27
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG12	10	0.27
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG13	14	0.27
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG12	17	0.27
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	4	0.27
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	4	0.27
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	3	0.27
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	3	0.27
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	3	0.27
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	4	0.27
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	4	0.27
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	4	0.27
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	15	0.27
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	15	0.27
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	1	0.27
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	1	0.27
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	15	0.27
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	15	0.27
(1,261)	1:20:A:ASP:HB2	1:18:A:ARG:HE	2	0.27
(1,261)	1:20:A:ASP:HB3	1:18:A:ARG:HE	2	0.27
(1,227)	1:17:A:ILE:HG12	1:41:A:ALA:HA	10	0.27
(1,227)	1:17:A:ILE:HG13	1:41:A:ALA:HA	14	0.27
(1,227)	1:17:A:ILE:HG12	1:41:A:ALA:HA	17	0.27
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	5	0.27
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	5	0.27
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	12	0.27
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	12	0.27
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	12	0.27
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	12	0.27
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	20	0.27
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:8:A:ILE:HG21	1:6:A:TYR:H	6	0.27
(2,17)	1:18:A:ARG:NH1	1:20:A:ASP:OD2	18	0.26
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	2	0.26
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	6	0.26
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	4	0.26
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	4	0.26
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	4	0.26
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	4	0.26
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	4	0.26
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	4	0.26
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	9	0.26
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	9	0.26
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	9	0.26
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	9	0.26
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	9	0.26
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	9	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	10	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	10	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	10	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	10	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	10	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	10	0.26
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	10	0.26
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	10	0.26
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	10	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	14	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	14	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	14	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	14	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	14	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	14	0.26
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	14	0.26
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	14	0.26
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	14	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	15	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	15	0.26
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	15	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	15	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	15	0.26
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	15	0.26
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	15	0.26
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	15	0.26
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	12	0.26
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	12	0.26
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	12	0.26
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	16	0.26
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	16	0.26
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	16	0.26
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	18	0.26
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	18	0.26
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	18	0.26
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	20	0.26
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	20	0.26
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	20	0.26
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	4	0.26
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	4	0.26
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	12	0.26
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	12	0.26
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	19	0.26
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	19	0.26
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	8	0.26
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	8	0.26
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	9	0.26
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	9	0.26
(1,231)	1:17:A:ILE:HG22	1:54:A:THR:HA	11	0.26
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	1	0.26
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	1	0.26
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	20	0.26
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	20	0.26
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	20	0.26
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	20	0.26
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	4	0.26
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	4	0.26
(1,12)	1:3:A:LYS:HB2	1:2:A:GLY:H	18	0.26
(1,12)	1:3:A:LYS:HB3	1:2:A:GLY:H	18	0.26
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	13	0.25
(2,18)	1:18:A:ARG:HH12	1:20:A:ASP:OD2	3	0.25
(1,840)	1:69:A:THR:HB	1:67:A:VAL:HB	12	0.25
(1,780)	1:61:A:SER:H	1:59:A:ASP:H	9	0.25
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	6	0.25
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	13	0.25
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	2	0.25
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	1	0.25
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	1	0.25
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	4	0.25
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	4	0.25
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	10	0.25
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	10	0.25
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	7	0.25
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG13	1	0.25
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	5	0.25
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	5	0.25
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	5	0.25
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	5	0.25
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	5	0.25
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	5	0.25
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	5	0.25
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	5	0.25
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	5	0.25
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	19	0.25
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	19	0.25
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	19	0.25
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	19	0.25
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	19	0.25
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	19	0.25
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	19	0.25
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	19	0.25
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	19	0.25
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	7	0.25
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	7	0.25
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	7	0.25
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	12	0.25
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	12	0.25
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	17	0.25
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	17	0.25
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	21	0.25
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	21	0.25
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	5	0.25
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	5	0.25
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	5	0.25
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	19	0.25
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	19	0.25
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	19	0.25
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	21	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	21	0.25
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	12	0.25
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	12	0.25
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	12	0.25
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	14	0.25
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	14	0.25
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG23	2	0.25
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG21	13	0.25
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	9	0.25
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	19	0.25
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	19	0.25
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	19	0.25
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	19	0.25
(1,38)	1:5:A:TYR:HB3	1:19:A:HIS:HD2	1	0.25
(1,30)	1:4:A:ALA:HB1	1:34:A:PHE:HD1	17	0.25
(1,30)	1:4:A:ALA:HB1	1:34:A:PHE:HD2	17	0.25
(1,30)	1:4:A:ALA:HB2	1:34:A:PHE:HD1	17	0.25
(1,30)	1:4:A:ALA:HB2	1:34:A:PHE:HD2	17	0.25
(1,30)	1:4:A:ALA:HB3	1:34:A:PHE:HD1	17	0.25
(1,30)	1:4:A:ALA:HB3	1:34:A:PHE:HD2	17	0.25
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	11	0.24
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	15	0.24
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	15	0.24
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	17	0.24
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	21	0.24
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	21	0.24
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	12	0.24
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	12	0.24
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	18	0.24
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	18	0.24
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	18	0.24
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	18	0.24
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	18	0.24
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	18	0.24
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	18	0.24
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	18	0.24
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	18	0.24
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	21	0.24
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	21	0.24
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	21	0.24
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	21	0.24
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	21	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	21	0.24
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	21	0.24
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	21	0.24
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	21	0.24
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	14	0.24
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	14	0.24
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	14	0.24
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	18	0.24
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	18	0.24
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	7	0.24
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG22	5	0.24
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	12	0.24
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	12	0.24
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	1	0.24
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	1	0.24
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	1	0.24
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	1	0.24
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	11	0.24
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	11	0.24
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	11	0.24
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	11	0.24
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	4	0.24
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	4	0.24
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	4	0.24
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	4	0.24
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	5	0.24
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	5	0.24
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	5	0.24
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	5	0.24
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	17	0.24
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	17	0.24
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	17	0.24
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	17	0.24
(1,148)	1:12:A:ASP:HA	1:49:A:HIS:HA	17	0.24
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	15	0.24
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	15	0.24
(1,117)	1:10:A:GLY:HA2	1:16:A:GLY:HA2	1	0.24
(1,117)	1:10:A:GLY:HA2	1:16:A:GLY:HA3	1	0.24
(1,117)	1:10:A:GLY:HA3	1:16:A:GLY:HA2	1	0.24
(1,117)	1:10:A:GLY:HA3	1:16:A:GLY:HA3	1	0.24
(2,24)	1:20:A:ASP:H	1:5:A:TYR:O	9	0.23
(2,18)	1:18:A:ARG:HH12	1:20:A:ASP:OD2	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:63:A:THR:H	1:60:A:GLY:H	8	0.23
(1,750)	1:55:A:VAL:H	1:53:A:ILE:H	1	0.23
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	8	0.23
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	10	0.23
(1,738)	1:54:A:THR:HG1	1:52:A:ARG:HE	7	0.23
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	5	0.23
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	5	0.23
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	5	0.23
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	5	0.23
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	5	0.23
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	5	0.23
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	13	0.23
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	13	0.23
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	15	0.23
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	15	0.23
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	18	0.23
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	18	0.23
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	20	0.23
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	20	0.23
(1,547)	1:41:A:ALA:HB1	1:15:A:TRP:HD1	3	0.23
(1,547)	1:41:A:ALA:HB2	1:15:A:TRP:HD1	3	0.23
(1,547)	1:41:A:ALA:HB3	1:15:A:TRP:HD1	3	0.23
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG12	14	0.23
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	15	0.23
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	15	0.23
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	15	0.23
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	9	0.23
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	9	0.23
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	11	0.23
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	11	0.23
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	15	0.23
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	15	0.23
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	15	0.23
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	20	0.23
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	20	0.23
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	16	0.23
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	16	0.23
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	2	0.23
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	2	0.23
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	20	0.23
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	20	0.23
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	10	0.23
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	10	0.23
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	14	0.23
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	14	0.23
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	17	0.23
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	17	0.23
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	17	0.23
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	17	0.23
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	18	0.23
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	18	0.23
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	18	0.23
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	18	0.23
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	13	0.23
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	13	0.23
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	13	0.23
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	20	0.23
(2,18)	1:18:A:ARG:HH12	1:20:A:ASP:OD2	14	0.22
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	3	0.22
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	1	0.22
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	18	0.22
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	21	0.22
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	7	0.22
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	7	0.22
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	7	0.22
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	7	0.22
(1,676)	1:49:A:HIS:HA	1:45:A:ILE:HA	21	0.22
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	7	0.22
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	7	0.22
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	7	0.22
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	7	0.22
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	2	0.22
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	2	0.22
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	21	0.22
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	21	0.22
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	4	0.22
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	2	0.22
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	2	0.22
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	2	0.22
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	8	0.22
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	8	0.22
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	8	0.22
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	10	0.22
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	10	0.22
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	6	0.22
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	6	0.22
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	10	0.22
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	10	0.22
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	14	0.22
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	14	0.22
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	3	0.22
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	5	0.22
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	7	0.22
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	7	0.22
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	16	0.22
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	16	0.22
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG22	9	0.22
(1,184)	1:15:A:TRP:HB2	1:12:A:ASP:HB2	18	0.22
(1,184)	1:15:A:TRP:HB2	1:12:A:ASP:HB3	18	0.22
(1,184)	1:15:A:TRP:HB3	1:12:A:ASP:HB2	18	0.22
(1,184)	1:15:A:TRP:HB3	1:12:A:ASP:HB3	18	0.22
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	2	0.22
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	2	0.22
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	2	0.22
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	2	0.22
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	15	0.22
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	15	0.22
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	15	0.22
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	15	0.22
(1,146)	1:12:A:ASP:HB2	1:15:A:TRP:HB2	18	0.22
(1,146)	1:12:A:ASP:HB2	1:15:A:TRP:HB3	18	0.22
(1,146)	1:12:A:ASP:HB3	1:15:A:TRP:HB2	18	0.22
(1,146)	1:12:A:ASP:HB3	1:15:A:TRP:HB3	18	0.22
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	18	0.22
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	17	0.21
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	16	0.21
(1,810)	1:65:A:LEU:HD11	1:63:A:THR:H	19	0.21
(1,810)	1:65:A:LEU:HD12	1:63:A:THR:H	19	0.21
(1,810)	1:65:A:LEU:HD13	1:63:A:THR:H	19	0.21
(1,810)	1:65:A:LEU:HD21	1:63:A:THR:H	19	0.21
(1,810)	1:65:A:LEU:HD22	1:63:A:THR:H	19	0.21
(1,810)	1:65:A:LEU:HD23	1:63:A:THR:H	19	0.21
(1,736)	1:54:A:THR:HB	1:52:A:ARG:HB2	6	0.21
(1,736)	1:54:A:THR:HB	1:52:A:ARG:HB3	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	12	0.21
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	12	0.21
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	8	0.21
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	8	0.21
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG12	2	0.21
(1,547)	1:41:A:ALA:HB1	1:15:A:TRP:HD1	18	0.21
(1,547)	1:41:A:ALA:HB2	1:15:A:TRP:HD1	18	0.21
(1,547)	1:41:A:ALA:HB3	1:15:A:TRP:HD1	18	0.21
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	15	0.21
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	15	0.21
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	17	0.21
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	17	0.21
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	19	0.21
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	19	0.21
(1,501)	1:38:A:CYS:HA	1:17:A:ILE:HG13	6	0.21
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	1	0.21
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	1	0.21
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	16	0.21
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	16	0.21
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	6	0.21
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	6	0.21
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	6	0.21
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	8	0.21
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	8	0.21
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	8	0.21
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	1	0.21
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	1	0.21
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	3	0.21
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	3	0.21
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	4	0.21
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	8	0.21
(1,290)	1:24:A:THR:HA	1:26:A:ASP:HB2	12	0.21
(1,290)	1:24:A:THR:HA	1:26:A:ASP:HB3	12	0.21
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	20	0.21
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	20	0.21
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	20	0.21
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	20	0.21
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG22	1	0.21
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG21	18	0.21
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	15	0.21
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	15	0.21
(1,227)	1:17:A:ILE:HG12	1:41:A:ALA:HA	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	11	0.21
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	11	0.21
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB2	8	0.21
(1,178)	1:14:A:ARG:HD2	1:15:A:TRP:HB3	8	0.21
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB2	8	0.21
(1,178)	1:14:A:ARG:HD3	1:15:A:TRP:HB3	8	0.21
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	13	0.21
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	13	0.21
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	13	0.21
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	13	0.21
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	7	0.21
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	7	0.21
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	7	0.21
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	2	0.2
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	15	0.2
(1,840)	1:69:A:THR:HB	1:67:A:VAL:HB	7	0.2
(1,801)	1:63:A:THR:H	1:60:A:GLY:H	12	0.2
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	5	0.2
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	14	0.2
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	14	0.2
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	14	0.2
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	14	0.2
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	14	0.2
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	14	0.2
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	14	0.2
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	14	0.2
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	8	0.2
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ1	6	0.2
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ2	6	0.2
(1,586)	1:43:A:ASN:HB2	1:46:A:LYS:HZ3	6	0.2
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ1	6	0.2
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ2	6	0.2
(1,586)	1:43:A:ASN:HB3	1:46:A:LYS:HZ3	6	0.2
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	20	0.2
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	20	0.2
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	21	0.2
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	7	0.2
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	7	0.2
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	7	0.2
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	7	0.2
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	20	0.2
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:31:A:GLU:HA	1:35:A:GLU:HG2	13	0.2
(1,375)	1:31:A:GLU:HA	1:35:A:GLU:HG3	13	0.2
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	6	0.2
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE1	12	0.2
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE2	12	0.2
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE1	12	0.2
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE2	12	0.2
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	8	0.2
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	8	0.2
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	8	0.2
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	8	0.2
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	9	0.2
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	9	0.2
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	9	0.2
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	9	0.2
(1,290)	1:24:A:THR:HA	1:26:A:ASP:HB2	17	0.2
(1,290)	1:24:A:THR:HA	1:26:A:ASP:HB3	17	0.2
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	5	0.2
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	5	0.2
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	14	0.2
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	14	0.2
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	6	0.2
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	6	0.2
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	15	0.2
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	15	0.2
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	11	0.2
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	11	0.2
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG22	19	0.2
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG22	13	0.2
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	2	0.2
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	2	0.2
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	2	0.2
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	2	0.2
(1,148)	1:12:A:ASP:HA	1:49:A:HIS:HA	10	0.2
(1,86)	1:8:A:ILE:HG22	1:17:A:ILE:HD11	20	0.2
(2,18)	1:18:A:ARG:HH12	1:20:A:ASP:OD2	8	0.19
(1,840)	1:69:A:THR:HB	1:67:A:VAL:HB	21	0.19
(1,787)	1:62:A:GLU:HA	1:60:A:GLY:HA2	6	0.19
(1,787)	1:62:A:GLU:HA	1:60:A:GLY:HA3	6	0.19
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	21	0.19
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	21	0.19
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	21	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	21	0.19
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	21	0.19
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	21	0.19
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	21	0.19
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	21	0.19
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	1	0.19
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	1	0.19
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	17	0.19
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	17	0.19
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	17	0.19
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	17	0.19
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	1	0.19
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	1	0.19
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	9	0.19
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	9	0.19
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	2	0.19
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	2	0.19
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	16	0.19
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	16	0.19
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	5	0.19
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	5	0.19
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	14	0.19
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	14	0.19
(1,403)	1:33:A:ALA:HA	1:8:A:ILE:HG22	18	0.19
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	14	0.19
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	14	0.19
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	7	0.19
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	7	0.19
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	4	0.19
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	4	0.19
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	4	0.19
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	4	0.19
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG22	12	0.19
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG22	4	0.19
(1,257)	1:19:A:HIS:HB2	1:53:A:ILE:HG21	5	0.19
(1,236)	1:18:A:ARG:HA	1:8:A:ILE:HG21	2	0.19
(1,231)	1:17:A:ILE:HG23	1:54:A:THR:HA	10	0.19
(1,185)	1:15:A:TRP:HA	1:13:A:ASN:H	14	0.19
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	1	0.19
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	1	0.19
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	21	0.19
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	21	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	21	0.19
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	9	0.18
(1,801)	1:63:A:THR:H	1:60:A:GLY:H	4	0.18
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	14	0.18
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	17	0.18
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	8	0.18
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	8	0.18
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	8	0.18
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	8	0.18
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	11	0.18
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	11	0.18
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	11	0.18
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	11	0.18
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	8	0.18
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	8	0.18
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	8	0.18
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	8	0.18
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	11	0.18
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	11	0.18
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	11	0.18
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	11	0.18
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	6	0.18
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	6	0.18
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	3	0.18
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	18	0.18
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	6	0.18
(1,547)	1:41:A:ALA:HB1	1:15:A:TRP:HD1	9	0.18
(1,547)	1:41:A:ALA:HB2	1:15:A:TRP:HD1	9	0.18
(1,547)	1:41:A:ALA:HB3	1:15:A:TRP:HD1	9	0.18
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	3	0.18
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	3	0.18
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	3	0.18
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	3	0.18
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	3	0.18
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	3	0.18
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	3	0.18
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	3	0.18
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	3	0.18
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	19	0.18
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	19	0.18
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	19	0.18
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	12	0.18
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	12	0.18
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	18	0.18
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	18	0.18
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	11	0.18
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	11	0.18
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	3	0.18
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	3	0.18
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	16	0.18
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	16	0.18
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	17	0.18
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	17	0.18
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	10	0.18
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	17	0.18
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	5	0.18
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	5	0.18
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	5	0.18
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	5	0.18
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	1	0.18
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	1	0.18
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	1	0.18
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	2	0.18
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	7	0.18
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	1	0.17
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	14	0.17
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	7	0.17
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	7	0.17
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	2	0.17
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	2	0.17
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	2	0.17
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	2	0.17
(1,676)	1:49:A:HIS:HA	1:45:A:ILE:HA	2	0.17
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	2	0.17
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	2	0.17
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	2	0.17
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	2	0.17
(1,660)	1:48:A:GLY:HA2	1:44:A:ALA:HA	11	0.17
(1,660)	1:48:A:GLY:HA3	1:44:A:ALA:HA	11	0.17
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	5	0.17
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	5	0.17
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	9	0.17
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	11	0.17
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	11	0.17
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	5	0.17
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	5	0.17
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	12	0.17
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	12	0.17
(1,535)	1:40:A:ALA:HB1	1:17:A:ILE:HG13	6	0.17
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD1	16	0.17
(1,502)	1:38:A:CYS:HA	1:34:A:PHE:HD2	16	0.17
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB1	4	0.17
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB2	4	0.17
(1,491)	1:37:A:ALA:HB1	1:32:A:ALA:HB3	4	0.17
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB1	4	0.17
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB2	4	0.17
(1,491)	1:37:A:ALA:HB2	1:32:A:ALA:HB3	4	0.17
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB1	4	0.17
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB2	4	0.17
(1,491)	1:37:A:ALA:HB3	1:32:A:ALA:HB3	4	0.17
(1,490)	1:36:A:ALA:HB1	1:39:A:ALA:HA	21	0.17
(1,490)	1:36:A:ALA:HB2	1:39:A:ALA:HA	21	0.17
(1,490)	1:36:A:ALA:HB3	1:39:A:ALA:HA	21	0.17
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	3	0.17
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	3	0.17
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	3	0.17
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	3	0.17
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ1	7	0.17
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ2	7	0.17
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ3	7	0.17
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ1	7	0.17
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ2	7	0.17
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ3	7	0.17
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	13	0.17
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	13	0.17
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	18	0.17
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	21	0.17
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	8	0.17
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	8	0.17
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	4	0.17
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	4	0.17
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	6	0.17
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	6	0.17
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	6	0.17
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	7	0.17
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	7	0.17
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	7	0.17
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	7	0.17
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	15	0.17
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	15	0.17
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	15	0.17
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	15	0.17
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	8	0.17
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	8	0.17
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	8	0.17
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	18	0.17
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	18	0.17
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	18	0.17
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	8	0.17
(1,813)	1:65:A:LEU:HA	1:64:A:ASN:HD21	18	0.16
(1,813)	1:65:A:LEU:HA	1:64:A:ASN:HD22	18	0.16
(1,801)	1:63:A:THR:H	1:60:A:GLY:H	3	0.16
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	9	0.16
(1,750)	1:55:A:VAL:H	1:53:A:ILE:H	18	0.16
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	6	0.16
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	7	0.16
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB2	3	0.16
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB3	3	0.16
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB2	8	0.16
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB3	8	0.16
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB2	15	0.16
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB3	15	0.16
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	17	0.16
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	17	0.16
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	17	0.16
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	17	0.16
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	17	0.16
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	17	0.16
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	17	0.16
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	17	0.16
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	4	0.16
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	4	0.16
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	14	0.16
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	14	0.16
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	19	0.16
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	5	0.16
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	6	0.16
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	6	0.16
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	10	0.16
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	10	0.16
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	13	0.16
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	13	0.16
(1,384)	1:32:A:ALA:HB1	1:28:A:SER:HA	6	0.16
(1,384)	1:32:A:ALA:HB2	1:28:A:SER:HA	6	0.16
(1,384)	1:32:A:ALA:HB3	1:28:A:SER:HA	6	0.16
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	4	0.16
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	4	0.16
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	7	0.16
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	7	0.16
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	14	0.16
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	14	0.16
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	1	0.16
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE1	13	0.16
(1,349)	1:30:A:LYS:HG2	1:27:A:TYR:HE2	13	0.16
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE1	13	0.16
(1,349)	1:30:A:LYS:HG3	1:27:A:TYR:HE2	13	0.16
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	2	0.16
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	2	0.16
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	16	0.16
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	16	0.16
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	3	0.16
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	3	0.16
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	16	0.16
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	16	0.16
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	21	0.16
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	21	0.16
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	21	0.16
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	21	0.16
(1,184)	1:15:A:TRP:HB2	1:12:A:ASP:HB2	12	0.16
(1,184)	1:15:A:TRP:HB2	1:12:A:ASP:HB3	12	0.16
(1,184)	1:15:A:TRP:HB3	1:12:A:ASP:HB2	12	0.16
(1,184)	1:15:A:TRP:HB3	1:12:A:ASP:HB3	12	0.16
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB2	14	0.16
(1,163)	1:13:A:ASN:HB2	1:15:A:TRP:HB3	14	0.16
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB2	14	0.16
(1,163)	1:13:A:ASN:HB3	1:15:A:TRP:HB3	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	3	0.16
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	3	0.16
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	13	0.16
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	13	0.16
(1,146)	1:12:A:ASP:HB2	1:15:A:TRP:HB2	12	0.16
(1,146)	1:12:A:ASP:HB2	1:15:A:TRP:HB3	12	0.16
(1,146)	1:12:A:ASP:HB3	1:15:A:TRP:HB2	12	0.16
(1,146)	1:12:A:ASP:HB3	1:15:A:TRP:HB3	12	0.16
(1,117)	1:10:A:GLY:HA2	1:16:A:GLY:HA2	11	0.16
(1,117)	1:10:A:GLY:HA2	1:16:A:GLY:HA3	11	0.16
(1,117)	1:10:A:GLY:HA3	1:16:A:GLY:HA2	11	0.16
(1,117)	1:10:A:GLY:HA3	1:16:A:GLY:HA3	11	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	4	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	4	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	4	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	6	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	6	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	6	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	11	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	11	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	11	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	16	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	16	0.16
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	16	0.16
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	1	0.16
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	13	0.16
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	17	0.16
(1,41)	1:5:A:TYR:HB2	1:27:A:TYR:HA	5	0.16
(1,41)	1:5:A:TYR:HB3	1:27:A:TYR:HA	5	0.16
(1,40)	1:5:A:TYR:HB2	1:27:A:TYR:HA	5	0.16
(1,40)	1:5:A:TYR:HB3	1:27:A:TYR:HA	5	0.16
(2,60)	1:50:A:GLU:H	1:13:A:ASN:O	4	0.15
(2,24)	1:20:A:ASP:H	1:5:A:TYR:O	3	0.15
(2,18)	1:18:A:ARG:HH12	1:20:A:ASP:OD2	9	0.15
(2,16)	1:18:A:ARG:H	1:7:A:ASP:O	2	0.15
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	13	0.15
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	12	0.15
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	12	0.15
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	12	0.15
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	12	0.15
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	19	0.15
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	19	0.15
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	19	0.15
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	12	0.15
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	12	0.15
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	12	0.15
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	12	0.15
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	19	0.15
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	19	0.15
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	19	0.15
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	19	0.15
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	21	0.15
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	21	0.15
(1,574)	1:42:A:SER:HB2	1:46:A:LYS:HE2	5	0.15
(1,574)	1:42:A:SER:HB2	1:46:A:LYS:HE3	5	0.15
(1,574)	1:42:A:SER:HB3	1:46:A:LYS:HE2	5	0.15
(1,574)	1:42:A:SER:HB3	1:46:A:LYS:HE3	5	0.15
(1,574)	1:42:A:SER:HB2	1:46:A:LYS:HE2	19	0.15
(1,574)	1:42:A:SER:HB2	1:46:A:LYS:HE3	19	0.15
(1,574)	1:42:A:SER:HB3	1:46:A:LYS:HE2	19	0.15
(1,574)	1:42:A:SER:HB3	1:46:A:LYS:HE3	19	0.15
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	14	0.15
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	14	0.15
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	14	0.15
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	14	0.15
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	15	0.15
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	15	0.15
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	13	0.15
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	2	0.15
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	9	0.15
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	9	0.15
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	9	0.15
(1,384)	1:32:A:ALA:HB1	1:28:A:SER:HA	17	0.15
(1,384)	1:32:A:ALA:HB2	1:28:A:SER:HA	17	0.15
(1,384)	1:32:A:ALA:HB3	1:28:A:SER:HA	17	0.15
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	19	0.15
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	19	0.15
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	19	0.15
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	20	0.15
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	21	0.15
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	21	0.15
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	21	0.15
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	21	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	21	0.15
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	21	0.15
(1,184)	1:15:A:TRP:HB2	1:12:A:ASP:HB2	2	0.15
(1,184)	1:15:A:TRP:HB2	1:12:A:ASP:HB3	2	0.15
(1,184)	1:15:A:TRP:HB3	1:12:A:ASP:HB2	2	0.15
(1,184)	1:15:A:TRP:HB3	1:12:A:ASP:HB3	2	0.15
(1,148)	1:12:A:ASP:HA	1:49:A:HIS:HA	9	0.15
(1,146)	1:12:A:ASP:HB2	1:15:A:TRP:HB2	2	0.15
(1,146)	1:12:A:ASP:HB2	1:15:A:TRP:HB3	2	0.15
(1,146)	1:12:A:ASP:HB3	1:15:A:TRP:HB2	2	0.15
(1,146)	1:12:A:ASP:HB3	1:15:A:TRP:HB3	2	0.15
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	10	0.15
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	21	0.15
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG1	16	0.15
(1,30)	1:4:A:ALA:HB1	1:34:A:PHE:HD1	6	0.15
(1,30)	1:4:A:ALA:HB1	1:34:A:PHE:HD2	6	0.15
(1,30)	1:4:A:ALA:HB2	1:34:A:PHE:HD1	6	0.15
(1,30)	1:4:A:ALA:HB2	1:34:A:PHE:HD2	6	0.15
(1,30)	1:4:A:ALA:HB3	1:34:A:PHE:HD1	6	0.15
(1,30)	1:4:A:ALA:HB3	1:34:A:PHE:HD2	6	0.15
(2,16)	1:18:A:ARG:H	1:7:A:ASP:O	14	0.14
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	9	0.14
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	12	0.14
(1,736)	1:54:A:THR:HB	1:52:A:ARG:HB2	9	0.14
(1,736)	1:54:A:THR:HB	1:52:A:ARG:HB3	9	0.14
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	12	0.14
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	12	0.14
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	12	0.14
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	12	0.14
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	12	0.14
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	12	0.14
(1,709)	1:52:A:ARG:HD2	1:50:A:GLU:HG2	7	0.14
(1,709)	1:52:A:ARG:HD2	1:50:A:GLU:HG3	7	0.14
(1,709)	1:52:A:ARG:HD3	1:50:A:GLU:HG2	7	0.14
(1,709)	1:52:A:ARG:HD3	1:50:A:GLU:HG3	7	0.14
(1,700)	1:50:A:GLU:HG2	1:52:A:ARG:HD2	7	0.14
(1,700)	1:50:A:GLU:HG2	1:52:A:ARG:HD3	7	0.14
(1,700)	1:50:A:GLU:HG3	1:52:A:ARG:HD2	7	0.14
(1,700)	1:50:A:GLU:HG3	1:52:A:ARG:HD3	7	0.14
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	10	0.14
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	10	0.14
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	10	0.14
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	10	0.14
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	10	0.14
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	10	0.14
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	10	0.14
(1,641)	1:47:A:PHE:HB2	1:46:A:LYS:HE2	3	0.14
(1,641)	1:47:A:PHE:HB2	1:46:A:LYS:HE3	3	0.14
(1,641)	1:47:A:PHE:HB3	1:46:A:LYS:HE2	3	0.14
(1,641)	1:47:A:PHE:HB3	1:46:A:LYS:HE3	3	0.14
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	12	0.14
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	6	0.14
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	6	0.14
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	7	0.14
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	7	0.14
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	3	0.14
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	3	0.14
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	6	0.14
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	6	0.14
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	11	0.14
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	11	0.14
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	1	0.14
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	2	0.14
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	5	0.14
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	14	0.14
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	14	0.14
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	17	0.14
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	17	0.14
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	17	0.14
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	17	0.14
(1,290)	1:24:A:THR:HA	1:26:A:ASP:HB2	21	0.14
(1,290)	1:24:A:THR:HA	1:26:A:ASP:HB3	21	0.14
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	3	0.14
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	3	0.14
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	18	0.14
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	18	0.14
(1,208)	1:16:A:GLY:HA2	1:14:A:ARG:HE	19	0.14
(1,208)	1:16:A:GLY:HA3	1:14:A:ARG:HE	19	0.14
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	12	0.14
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	12	0.14
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	12	0.14
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	12	0.14
(1,134)	1:11:A:SER:HB2	1:15:A:TRP:HD1	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:11:A:SER:HB3	1:15:A:TRP:HD1	6	0.14
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	14	0.14
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	14	0.14
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	14	0.14
(1,74)	1:7:A:ASP:HA	1:19:A:HIS:HA	15	0.14
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG22	8	0.14
(2,60)	1:50:A:GLU:H	1:13:A:ASN:O	17	0.13
(2,18)	1:18:A:ARG:HH12	1:20:A:ASP:OD2	21	0.13
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	3	0.13
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	6	0.13
(2,6)	1:14:A:ARG:HE	1:50:A:GLU:OE1	3	0.13
(2,6)	1:14:A:ARG:HE	1:50:A:GLU:OE1	15	0.13
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	15	0.13
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	9	0.13
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	10	0.13
(1,742)	1:54:A:THR:HB	1:53:A:ILE:H	13	0.13
(1,708)	1:52:A:ARG:HB2	1:15:A:TRP:HA	16	0.13
(1,708)	1:52:A:ARG:HB3	1:15:A:TRP:HA	16	0.13
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	1	0.13
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	1	0.13
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	1	0.13
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	1	0.13
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	5	0.13
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	5	0.13
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	5	0.13
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	5	0.13
(1,676)	1:49:A:HIS:HA	1:45:A:ILE:HA	5	0.13
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	1	0.13
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	1	0.13
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	1	0.13
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	1	0.13
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	5	0.13
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	5	0.13
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	5	0.13
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	5	0.13
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	6	0.13
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	13	0.13
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	1	0.13
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	1	0.13
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	2	0.13
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	2	0.13
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	10	0.13
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	8	0.13
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	8	0.13
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	10	0.13
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	10	0.13
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	15	0.13
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	15	0.13
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ1	1	0.13
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ2	1	0.13
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ3	1	0.13
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ1	1	0.13
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ2	1	0.13
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ3	1	0.13
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	3	0.13
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	3	0.13
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	3	0.13
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	11	0.13
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	11	0.13
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	11	0.13
(1,402)	1:32:A:ALA:HB1	1:36:A:ALA:HA	12	0.13
(1,402)	1:32:A:ALA:HB2	1:36:A:ALA:HA	12	0.13
(1,402)	1:32:A:ALA:HB3	1:36:A:ALA:HA	12	0.13
(1,379)	1:31:A:GLU:HG2	1:35:A:GLU:HA	2	0.13
(1,379)	1:31:A:GLU:HG3	1:35:A:GLU:HA	2	0.13
(1,361)	1:30:A:LYS:HD2	1:34:A:PHE:H	4	0.13
(1,361)	1:30:A:LYS:HD3	1:34:A:PHE:H	4	0.13
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	11	0.13
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	15	0.13
(1,337)	1:29:A:SER:HB2	1:27:A:TYR:HE1	6	0.13
(1,337)	1:29:A:SER:HB2	1:27:A:TYR:HE2	6	0.13
(1,337)	1:29:A:SER:HB3	1:27:A:TYR:HE1	6	0.13
(1,337)	1:29:A:SER:HB3	1:27:A:TYR:HE2	6	0.13
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	2	0.13
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	2	0.13
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	2	0.13
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	2	0.13
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	15	0.13
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	15	0.13
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	15	0.13
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	15	0.13
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	15	0.13
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	18	0.13
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	18	0.13
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	18	0.13
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	18	0.13
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	7	0.13
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	7	0.13
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	10	0.13
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	10	0.13
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	12	0.13
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	12	0.13
(1,42)	1:5:A:TYR:HB2	1:30:A:LYS:HG2	12	0.13
(1,42)	1:5:A:TYR:HB2	1:30:A:LYS:HG3	12	0.13
(1,42)	1:5:A:TYR:HB3	1:30:A:LYS:HG2	12	0.13
(1,42)	1:5:A:TYR:HB3	1:30:A:LYS:HG3	12	0.13
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG1	6	0.13
(1,39)	1:5:A:TYR:HB3	1:24:A:THR:HG22	19	0.13
(2,12)	1:16:A:GLY:H	1:9:A:VAL:O	16	0.12
(1,840)	1:69:A:THR:HB	1:67:A:VAL:HB	17	0.12
(1,823)	1:66:A:GLY:HA2	1:68:A:ILE:HA	1	0.12
(1,823)	1:66:A:GLY:HA3	1:68:A:ILE:HA	1	0.12
(1,750)	1:55:A:VAL:H	1:53:A:ILE:H	14	0.12
(1,749)	1:55:A:VAL:H	1:17:A:ILE:HB	3	0.12
(1,736)	1:54:A:THR:HB	1:52:A:ARG:HB2	5	0.12
(1,736)	1:54:A:THR:HB	1:52:A:ARG:HB3	5	0.12
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB2	18	0.12
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB3	18	0.12
(1,726)	1:53:A:ILE:H	1:51:A:VAL:HA	14	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	1	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	1	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	1	0.12
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	1	0.12
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	1	0.12
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	1	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	3	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	3	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	3	0.12
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	3	0.12
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	3	0.12
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	3	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD11	7	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD12	7	0.12
(1,724)	1:52:A:ARG:HG2	1:53:A:ILE:HD13	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD11	7	0.12
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD12	7	0.12
(1,724)	1:52:A:ARG:HG3	1:53:A:ILE:HD13	7	0.12
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	3	0.12
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	3	0.12
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	3	0.12
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	3	0.12
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	4	0.12
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	4	0.12
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	4	0.12
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	4	0.12
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA2	20	0.12
(1,685)	1:50:A:GLU:HB2	1:48:A:GLY:HA3	20	0.12
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA2	20	0.12
(1,685)	1:50:A:GLU:HB3	1:48:A:GLY:HA3	20	0.12
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	3	0.12
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	3	0.12
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	3	0.12
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	3	0.12
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	4	0.12
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	4	0.12
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	4	0.12
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	4	0.12
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB2	20	0.12
(1,673)	1:48:A:GLY:HA2	1:50:A:GLU:HB3	20	0.12
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB2	20	0.12
(1,673)	1:48:A:GLY:HA3	1:50:A:GLU:HB3	20	0.12
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	10	0.12
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	10	0.12
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	20	0.12
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	20	0.12
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB2	20	0.12
(1,614)	1:45:A:ILE:HB	1:49:A:HIS:HB3	20	0.12
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	7	0.12
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	9	0.12
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	14	0.12
(1,590)	1:44:A:ALA:HA	1:40:A:ALA:HA	15	0.12
(1,574)	1:42:A:SER:HB2	1:46:A:LYS:HE2	1	0.12
(1,574)	1:42:A:SER:HB2	1:46:A:LYS:HE3	1	0.12
(1,574)	1:42:A:SER:HB3	1:46:A:LYS:HE2	1	0.12
(1,574)	1:42:A:SER:HB3	1:46:A:LYS:HE3	1	0.12
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	19	0.12
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	4	0.12
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	4	0.12
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	7	0.12
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	7	0.12
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	8	0.12
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	8	0.12
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	10	0.12
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	10	0.12
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	14	0.12
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	1	0.12
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	3	0.12
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	21	0.12
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	21	0.12
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB2	4	0.12
(1,326)	1:28:A:SER:HA	1:26:A:ASP:HB3	4	0.12
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	18	0.12
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	18	0.12
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB2	13	0.12
(1,275)	1:24:A:THR:HB	1:7:A:ASP:HB3	13	0.12
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG21	10	0.12
(1,270)	1:21:A:ASP:HB2	1:19:A:HIS:HA	1	0.12
(1,270)	1:21:A:ASP:HB3	1:19:A:HIS:HA	1	0.12
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	5	0.12
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	5	0.12
(1,42)	1:5:A:TYR:HB2	1:30:A:LYS:HG2	17	0.12
(1,42)	1:5:A:TYR:HB2	1:30:A:LYS:HG3	17	0.12
(1,42)	1:5:A:TYR:HB3	1:30:A:LYS:HG2	17	0.12
(1,42)	1:5:A:TYR:HB3	1:30:A:LYS:HG3	17	0.12
(2,64)	1:52:A:ARG:HH11	1:51:A:VAL:O	16	0.11
(2,26)	1:33:A:ALA:H	1:29:A:SER:O	14	0.11
(2,8)	1:14:A:ARG:HH21	1:50:A:GLU:OE1	7	0.11
(1,840)	1:69:A:THR:HB	1:67:A:VAL:HB	6	0.11
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB2	12	0.11
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB3	12	0.11
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB2	19	0.11
(1,735)	1:54:A:THR:HA	1:52:A:ARG:HB3	19	0.11
(1,698)	1:50:A:GLU:HA	1:52:A:ARG:H	15	0.11
(1,573)	1:42:A:SER:HB2	1:46:A:LYS:HA	4	0.11
(1,573)	1:42:A:SER:HB3	1:46:A:LYS:HA	4	0.11
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB2	17	0.11
(1,565)	1:42:A:SER:HA	1:38:A:CYS:HB3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,564)	1:41:A:ALA:HA	1:46:A:LYS:H	21	0.11
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	8	0.11
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	14	0.11
(1,488)	1:36:A:ALA:HB1	1:38:A:CYS:HG	21	0.11
(1,488)	1:36:A:ALA:HB2	1:38:A:CYS:HG	21	0.11
(1,488)	1:36:A:ALA:HB3	1:38:A:CYS:HG	21	0.11
(1,438)	1:35:A:GLU:HB2	1:31:A:GLU:H	2	0.11
(1,438)	1:35:A:GLU:HB3	1:31:A:GLU:H	2	0.11
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	9	0.11
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	9	0.11
(1,381)	1:31:A:GLU:HB2	1:36:A:ALA:H	10	0.11
(1,381)	1:31:A:GLU:HB3	1:36:A:ALA:H	10	0.11
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	9	0.11
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG2	5	0.11
(1,333)	1:28:A:SER:HB2	1:31:A:GLU:HG3	5	0.11
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG2	5	0.11
(1,333)	1:28:A:SER:HB3	1:31:A:GLU:HG3	5	0.11
(1,274)	1:21:A:ASP:H	1:24:A:THR:HG1	6	0.11
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	4	0.11
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	4	0.11
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	4	0.11
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	4	0.11
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB2	19	0.11
(1,201)	1:15:A:TRP:HB2	1:47:A:PHE:HB3	19	0.11
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB2	19	0.11
(1,201)	1:15:A:TRP:HB3	1:47:A:PHE:HB3	19	0.11
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD11	14	0.11
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD12	14	0.11
(1,198)	1:15:A:TRP:HA	1:17:A:ILE:HD13	14	0.11
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	11	0.11
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	11	0.11
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD21	16	0.11
(1,147)	1:12:A:ASP:H	1:43:A:ASN:HD22	16	0.11
(1,30)	1:4:A:ALA:HB1	1:34:A:PHE:HD1	19	0.11
(1,30)	1:4:A:ALA:HB1	1:34:A:PHE:HD2	19	0.11
(1,30)	1:4:A:ALA:HB2	1:34:A:PHE:HD1	19	0.11
(1,30)	1:4:A:ALA:HB2	1:34:A:PHE:HD2	19	0.11
(1,30)	1:4:A:ALA:HB3	1:34:A:PHE:HD1	19	0.11
(1,30)	1:4:A:ALA:HB3	1:34:A:PHE:HD2	19	0.11
(1,29)	1:4:A:ALA:HB1	1:30:A:LYS:HB2	3	0.11
(1,29)	1:4:A:ALA:HB1	1:30:A:LYS:HB3	3	0.11
(1,29)	1:4:A:ALA:HB2	1:30:A:LYS:HB2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:4:A:ALA:HB2	1:30:A:LYS:HB3	3	0.11
(1,29)	1:4:A:ALA:HB3	1:30:A:LYS:HB2	3	0.11
(1,29)	1:4:A:ALA:HB3	1:30:A:LYS:HB3	3	0.11
(1,12)	1:3:A:LYS:HB2	1:2:A:GLY:H	9	0.11
(1,12)	1:3:A:LYS:HB3	1:2:A:GLY:H	9	0.11
(2,24)	1:20:A:ASP:H	1:5:A:TYR:O	6	0.1
(2,6)	1:14:A:ARG:HE	1:50:A:GLU:OE1	12	0.1
(1,840)	1:69:A:THR:HB	1:67:A:VAL:HB	8	0.1
(1,767)	1:59:A:ASP:H	1:57:A:GLY:H	8	0.1
(1,750)	1:55:A:VAL:H	1:53:A:ILE:H	3	0.1
(1,750)	1:55:A:VAL:H	1:53:A:ILE:H	9	0.1
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB2	8	0.1
(1,657)	1:47:A:PHE:HA	1:49:A:HIS:HB3	8	0.1
(1,548)	1:41:A:ALA:HA	1:17:A:ILE:HG12	8	0.1
(1,518)	1:38:A:CYS:HA	1:42:A:SER:HA	12	0.1
(1,470)	1:35:A:GLU:HG2	1:40:A:ALA:H	9	0.1
(1,470)	1:35:A:GLU:HG3	1:40:A:ALA:H	9	0.1
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ1	20	0.1
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ2	20	0.1
(1,422)	1:34:A:PHE:HB2	1:30:A:LYS:HZ3	20	0.1
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ1	20	0.1
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ2	20	0.1
(1,422)	1:34:A:PHE:HB3	1:30:A:LYS:HZ3	20	0.1
(1,360)	1:30:A:LYS:HA	1:34:A:PHE:HZ	16	0.1
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB2	12	0.1
(1,289)	1:24:A:THR:H	1:26:A:ASP:HB3	12	0.1
(1,227)	1:17:A:ILE:HG12	1:41:A:ALA:HA	8	0.1
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB1	15	0.1
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB2	15	0.1
(1,106)	1:9:A:VAL:H	1:37:A:ALA:HB3	15	0.1

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

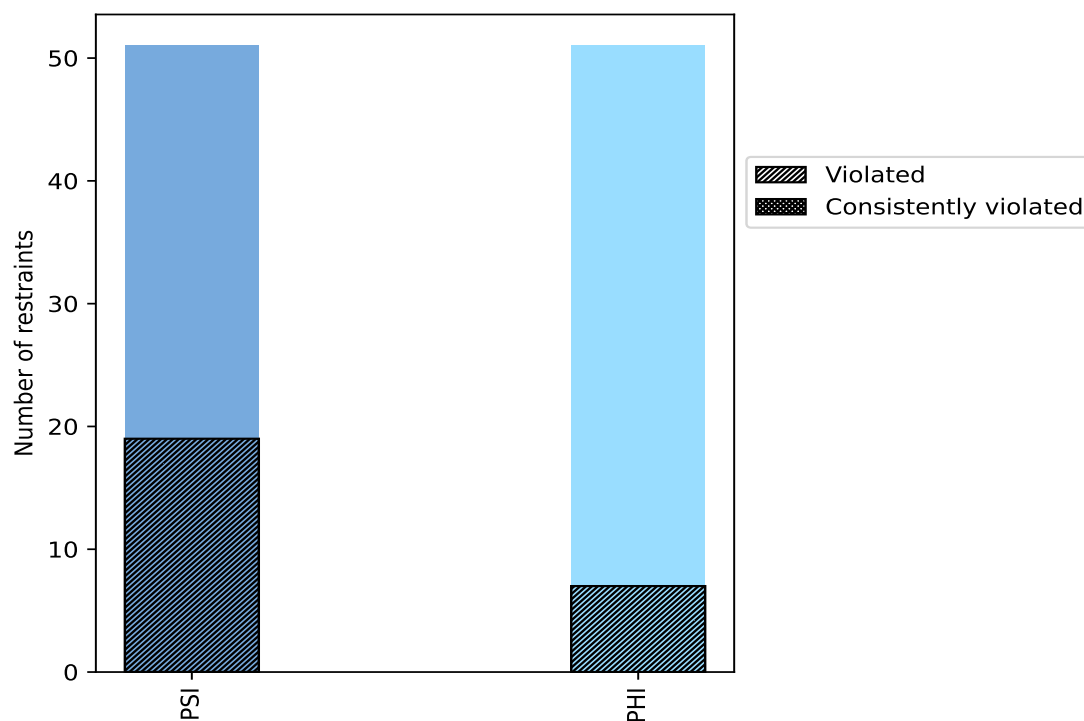
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	51	50.0	19	37.3	18.6	0	0.0	0.0
PHI	51	50.0	7	13.7	6.9	0	0.0	0.0
Total	102	100.0	26	25.5	25.5	0	0.0	0.0

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](#)



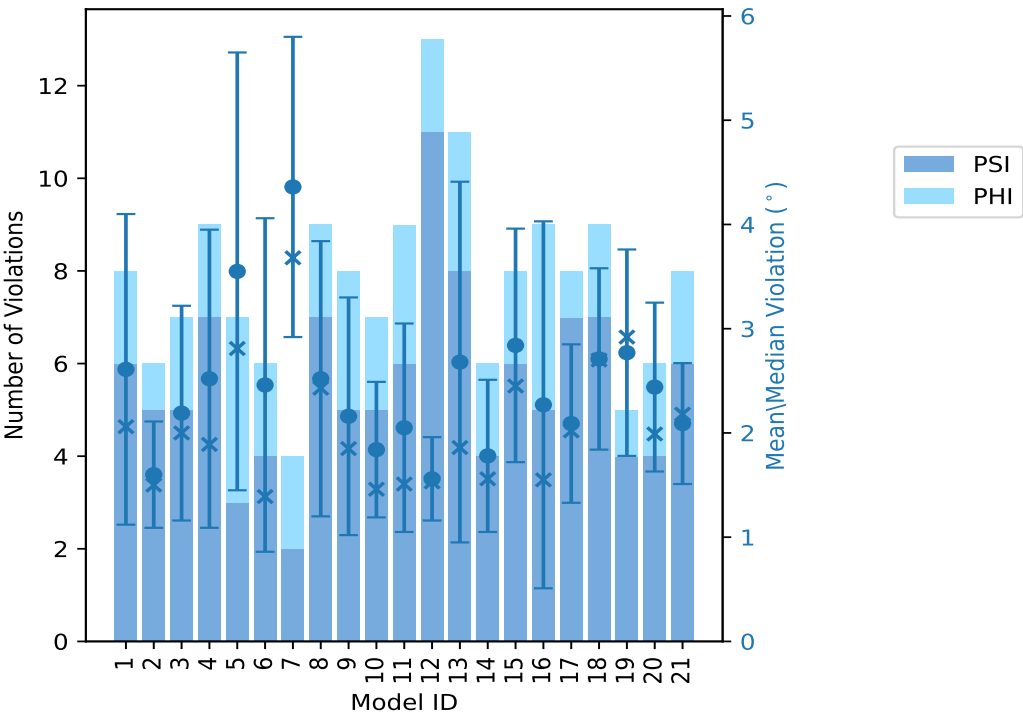
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	6	2	8	2.61	5.54	1.49	2.06
2	5	1	6	1.6	2.32	0.51	1.5
3	5	2	7	2.19	3.83	1.03	2.0
4	7	2	9	2.52	5.11	1.43	1.89
5	3	4	7	3.55	6.87	2.1	2.81
6	4	2	6	2.46	4.89	1.6	1.39
7	2	2	4	4.36	6.81	1.44	3.68
8	7	2	9	2.52	5.09	1.32	2.43
9	5	3	8	2.16	4.63	1.14	1.85
10	5	2	7	1.84	3.14	0.65	1.46
11	6	3	9	2.05	4.05	1.0	1.51
12	11	2	13	1.56	2.55	0.4	1.53
13	8	3	11	2.68	6.71	1.73	1.86
14	4	2	6	1.78	3.34	0.73	1.56
15	6	2	8	2.84	4.82	1.12	2.45
16	5	4	9	2.27	6.85	1.76	1.55
17	7	1	8	2.09	3.55	0.76	2.02
18	7	2	9	2.71	3.88	0.87	2.7
19	4	1	5	2.77	3.93	0.99	2.92
20	4	2	6	2.44	3.61	0.81	1.99
21	6	2	8	2.09	3.18	0.58	2.18

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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	
PSI	PHI	Total	Count ¹	%
5	2	7	1	4.8
4	1	5	2	9.5
2	1	3	3	14.3
0	0	0	4	19.0
1	0	1	5	23.8
0	0	0	6	28.6
0	0	0	7	33.3
1	0	1	8	38.1
0	1	1	9	42.9
1	1	2	10	47.6
1	0	1	11	52.4

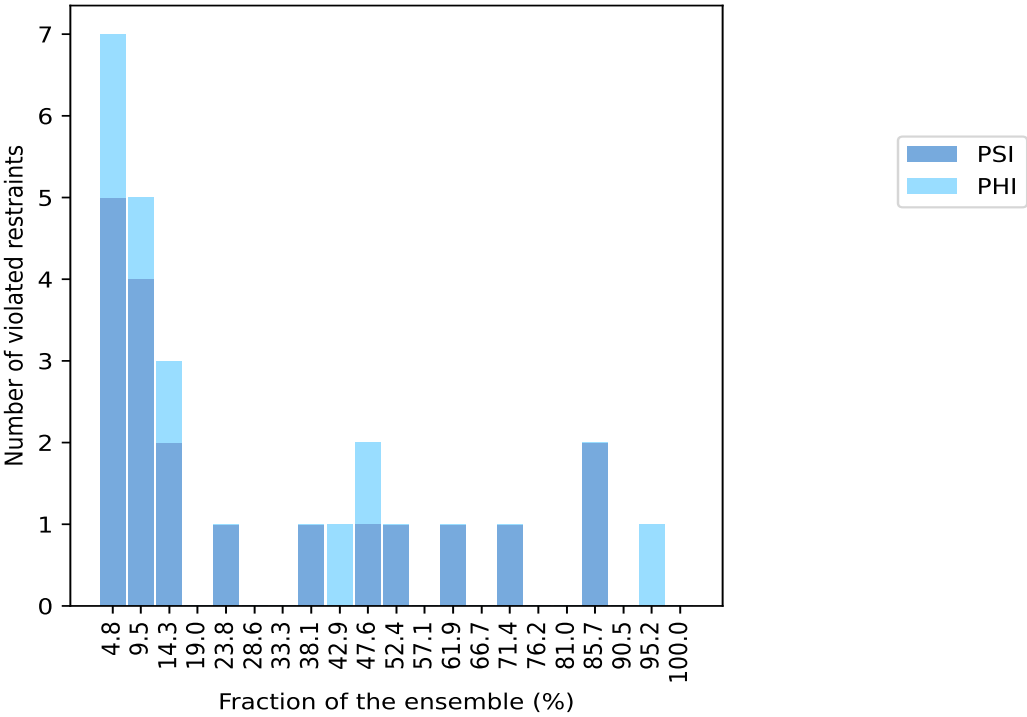
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	57.1
1	0	1	13	61.9
0	0	0	14	66.7
1	0	1	15	71.4
0	0	0	16	76.2
0	0	0	17	81.0
2	0	2	18	85.7
0	0	0	19	90.5
0	1	1	20	95.2
0	0	0	21	100.0

¹ Number of models with violations

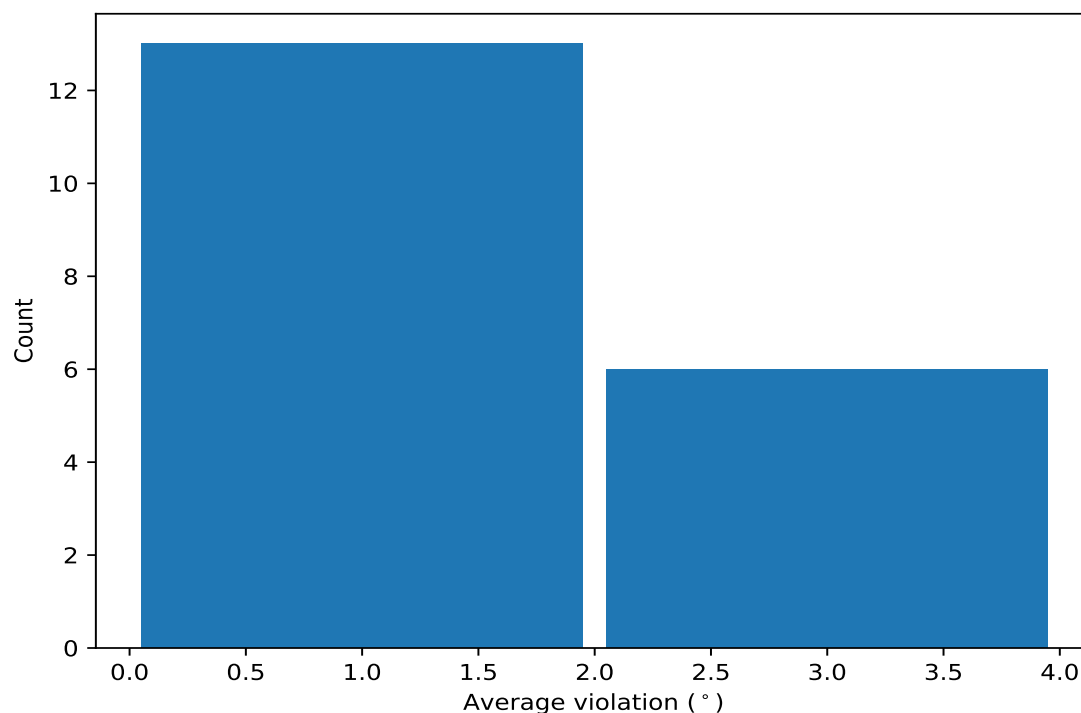
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	20	3.72	1.3	3.78
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	18	3.6	1.91	3.58
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	18	2.16	0.76	1.98
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	15	2.72	1.27	3.11
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	13	1.81	0.46	1.77
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	11	2.3	0.97	2.09
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	10	2.66	1.38	2.42
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	10	1.49	0.4	1.31
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	9	1.58	0.4	1.44
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	8	1.76	0.83	1.34
(1,40)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	5	1.79	0.44	1.77
(1,39)	1:23:A:PRO:C	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	3	1.91	0.73	1.88
(1,48)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:LYS:N	3	1.79	0.64	1.37

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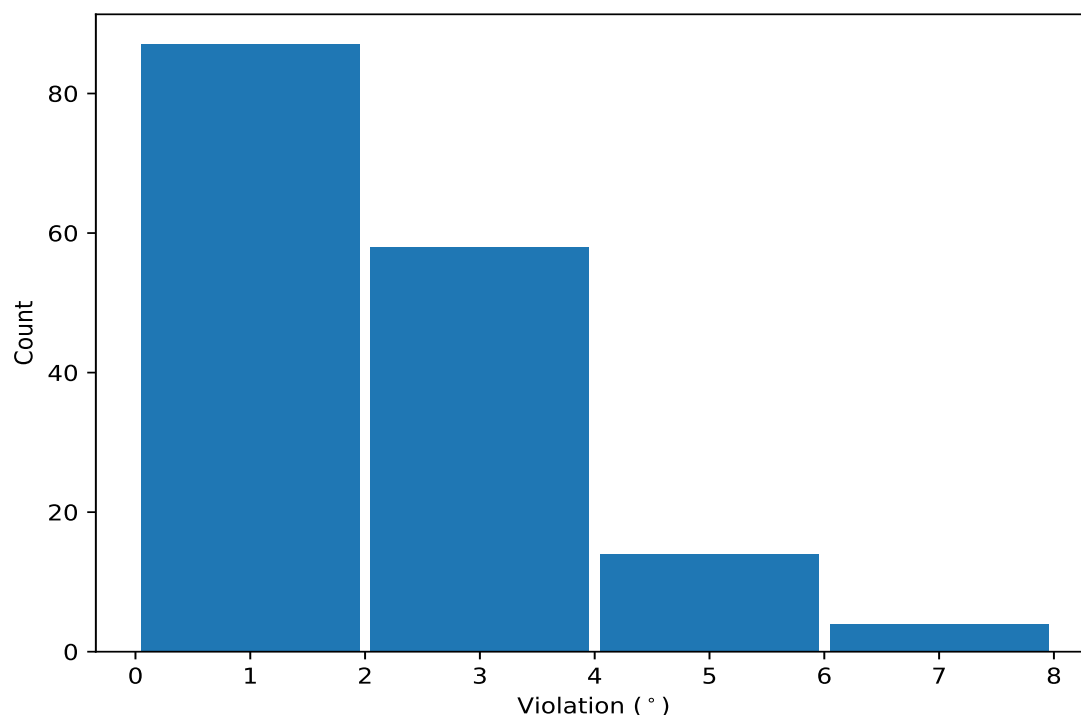
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,8)	1:6:A:TYR:N	1:6:A:TYR:CA	1:6:A:TYR:C	1:7:A:ASP:N	3	1.61	0.18	1.53
(1,17)	1:10:A:GLY:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	2	1.7	0.22	1.7
(1,10)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:ILE:N	2	1.57	0.02	1.57
(1,14)	1:9:A:VAL:N	1:9:A:VAL:CA	1:9:A:VAL:C	1:10:A:GLY:N	2	1.5	0.05	1.5
(1,96)	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	1:54:A:THR:N	2	1.33	0.02	1.33
(1,102)	1:56:A:PRO:N	1:56:A:PRO:CA	1:56:A:PRO:C	1:57:A:GLY:N	2	1.15	0.11	1.15

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	5	6.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	16	6.85
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	7	6.81
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	13	6.71
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	1	5.54
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	5	5.53
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	5	5.16
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	4	5.11
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	8	5.09
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	13	4.92
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	6	4.89
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	15	4.82
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	9	4.63
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	4	4.58
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	6	4.54
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1	4.46
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	8	4.26
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	11	4.05
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	7	3.98
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	15	3.93
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	19	3.93
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	18	3.88
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	13	3.86
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	3	3.83
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	18	3.79
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	15	3.74
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	11	3.67
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	19	3.65
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	3	3.61
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	20	3.61
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	17	3.55
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	20	3.52
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	16	3.48
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	4	3.44
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	7	3.38
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	9	3.35
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	14	3.34
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	7	3.26
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	13	3.22
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	18	3.22
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	21	3.18
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	18	3.16
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	10	3.14
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	8	3.11
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	19	2.92
(1,39)	1:23:A:PRO:C	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	5	2.81
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	1	2.77
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	18	2.7
(1,48)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:LYS:N	17	2.69
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	18	2.62
(1,40)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	4	2.57
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	15	2.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	12	2.55
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	17	2.55
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	8	2.44
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	8	2.43
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	21	2.43
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	21	2.37
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	15	2.34
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	2	2.32
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	21	2.32
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	1	2.27
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	10	2.22
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	2	2.21
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	3	2.17
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	10	2.14
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	19	2.14
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	15	2.11
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	11	2.11
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	17	2.09
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	18	2.06
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	20	2.06
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	21	2.04
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	13	2.01
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	3	2.0
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	12	2.0
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	17	1.95
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	20	1.92
(1,17)	1:10:A:GLY:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	16	1.92
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	15	1.91
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	4	1.89
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	18	1.88
(1,39)	1:23:A:PRO:C	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	9	1.88
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	9	1.86
(1,8)	1:6:A:TYR:N	1:6:A:TYR:CA	1:6:A:TYR:C	1:7:A:ASP:N	13	1.86
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	12	1.85
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	16	1.84
(1,40)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	1	1.84
(1,68)	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	1:40:A:ALA:N	9	1.83
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	14	1.79
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	20	1.77
(1,40)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	13	1.77
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	12	1.77
(1,36)	1:21:A:ASP:N	1:21:A:ASP:CA	1:21:A:ASP:C	1:22:A:ASP:N	13	1.74
(1,15)	1:9:A:VAL:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	20	1.74
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	5	1.67
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	11	1.67
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	12	1.66
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	5	1.66
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	14	1.66
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	2	1.63
(1,10)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:ILE:N	21	1.59
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	8	1.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1:8:A:ILE:N	16	1.55
(1,14)	1:9:A:VAL:N	1:9:A:VAL:CA	1:9:A:VAL:C	1:10:A:GLY:N	12	1.54
(1,8)	1:6:A:TYR:N	1:6:A:TYR:CA	1:6:A:TYR:C	1:7:A:ASP:N	12	1.53
(1,40)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	11	1.51
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	21	1.49
(1,17)	1:10:A:GLY:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	11	1.48
(1,60)	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	1:36:A:ALA:N	4	1.47
(1,94)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:ILE:N	12	1.46
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	10	1.46
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	14	1.45
(1,14)	1:9:A:VAL:N	1:9:A:VAL:CA	1:9:A:VAL:C	1:10:A:GLY:N	17	1.45
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	4	1.44
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	1	1.44
(1,8)	1:6:A:TYR:N	1:6:A:TYR:CA	1:6:A:TYR:C	1:7:A:ASP:N	11	1.44
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	1	1.43
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	9	1.43
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	6	1.42
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	10	1.39
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	8	1.38
(1,27)	1:15:A:TRP:C	1:16:A:GLY:N	1:16:A:GLY:CA	1:16:A:GLY:C	14	1.38
(1,48)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:LYS:N	2	1.37
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	6	1.36
(1,96)	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	1:54:A:THR:N	3	1.34
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	10	1.33
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	3	1.32
(1,96)	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	1:54:A:THR:N	11	1.31
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	21	1.3
(1,48)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:LYS:N	8	1.3
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	9	1.3
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	12	1.29
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	15	1.29
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	13	1.28
(1,40)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	6	1.28
(1,102)	1:56:A:PRO:N	1:56:A:PRO:CA	1:56:A:PRO:C	1:57:A:GLY:N	17	1.26
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	16	1.26
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	6	1.26
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	16	1.26
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	11	1.25
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	12	1.25
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	12	1.23
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	19	1.23
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	17	1.21
(1,23)	1:13:A:ASN:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	10	1.2
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	16	1.19
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	4	1.17
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	12	1.16
(1,46)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	5	1.15
(1,65)	1:37:A:ALA:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1	1.13
(1,26)	1:15:A:TRP:N	1:15:A:TRP:CA	1:15:A:TRP:C	1:16:A:GLY:N	13	1.1
(1,22)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:ARG:N	2	1.09
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	14	1.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:VAL:N	16	1.08
(1,38)	1:22:A:ASP:N	1:22:A:ASP:CA	1:22:A:ASP:C	1:23:A:PRO:N	8	1.07
(1,1)	1:2:A:GLY:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	3	1.07
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	4	1.05
(1,16)	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:SER:N	18	1.05
(1,102)	1:56:A:PRO:N	1:56:A:PRO:CA	1:56:A:PRO:C	1:57:A:GLY:N	12	1.04
(1,39)	1:23:A:PRO:C	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	13	1.03
(1,78)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:ILE:N	9	1.01
(1,66)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:ALA:N	2	1.01