



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:20 AM UTC

PDB ID : 8WLS / pdb_00008wls
BMRB ID : 36598
Title : Bcl-xL in complex with HBx BH3 delta C peptide
Authors : Kobayashi, N.; Nagata, T.; Kusunoki, H.
Deposited on : 2023-10-01

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

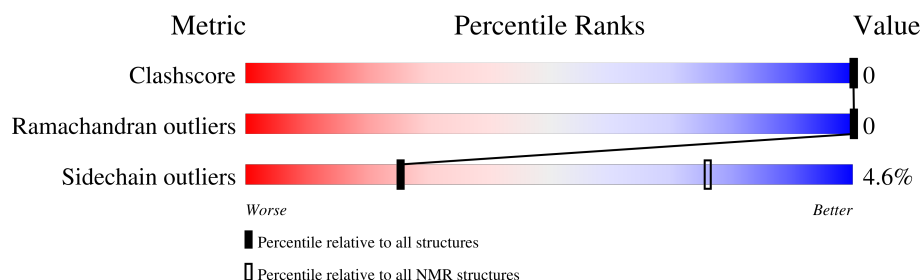
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	156	 87% 12%
2	B	25	 100%

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:27, A:43-A:155 (137)	0.54	10

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2815 atoms, of which 1357 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	156	Total	C	H	N	O	S	0
			2445	800	1182	211	248	4	

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP Q07817
A	?	-	GLU	deletion	UNP Q07817
A	?	-	THR	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ILE	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	TRP	deletion	UNP Q07817
A	?	-	HIS	deletion	UNP Q07817
A	?	-	LEU	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ASP	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	VAL	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	THR	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	HIS	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	LEU	deletion	UNP Q07817

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ARG	deletion	UNP Q07817
A	?	-	GLU	deletion	UNP Q07817
A	?	-	VAL	deletion	UNP Q07817
A	?	-	ILE	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	MET	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817

- Molecule 2 is a protein called Protein X.

Mol	Chain	Residues	Atoms						Trace
2	B	25	Total	C	H	N	O	S	0
			370	124	175	29	39	3	

There are 5 discrepancies between the modelled and reference sequences:

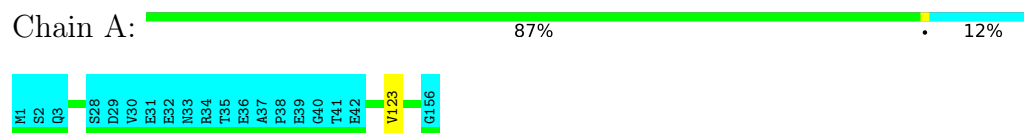
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	GLY	-	cloning artifact	UNP Q9YKJ6
B	302	SER	-	cloning artifact	UNP Q9YKJ6
B	303	HIS	-	cloning artifact	UNP Q9YKJ6
B	304	MET	-	cloning artifact	UNP Q9YKJ6
B	325	GLY	-	linker	UNP Q9YKJ6

4 Residue-property plots

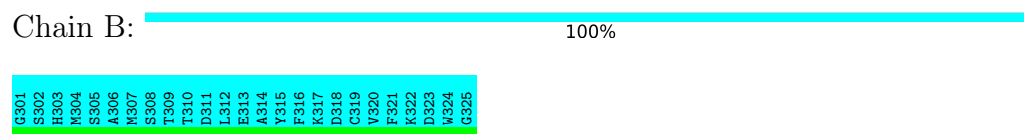
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Bcl-2-like protein 1



- Molecule 2: Protein X

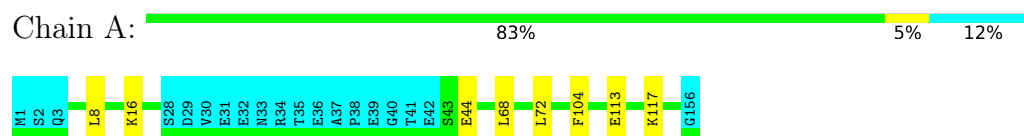


4.2 Scores per residue for each member of the ensemble

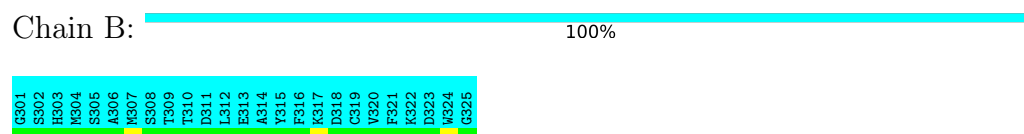
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Bcl-2-like protein 1

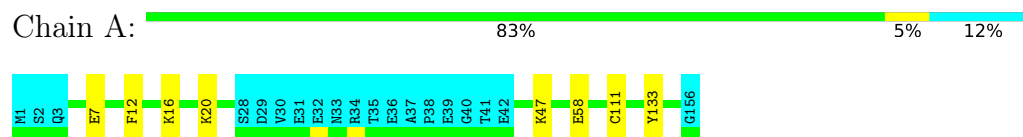


- Molecule 2: Protein X

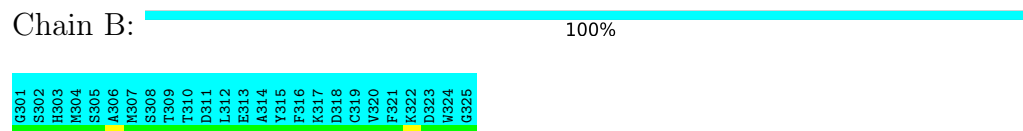


4.2.2 Score per residue for model 2

- Molecule 1: Bcl-2-like protein 1

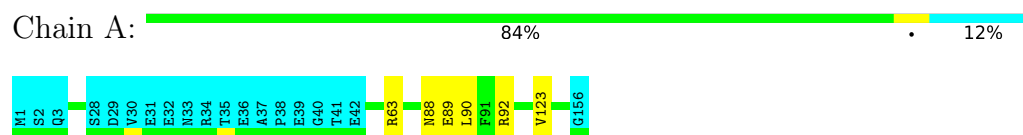


- Molecule 2: Protein X

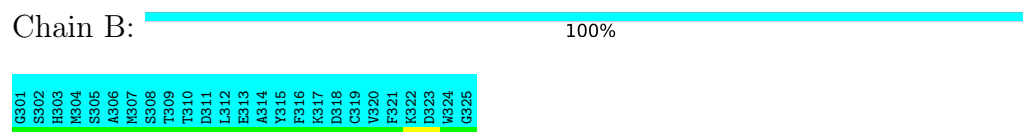


4.2.3 Score per residue for model 3

- Molecule 1: Bcl-2-like protein 1

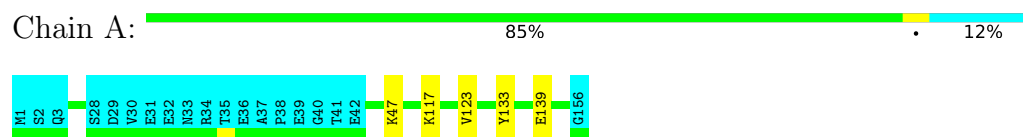


- Molecule 2: Protein X

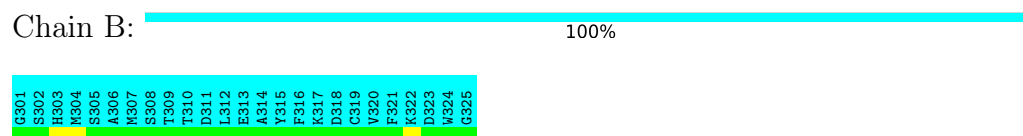


4.2.4 Score per residue for model 4

- Molecule 1: Bcl-2-like protein 1

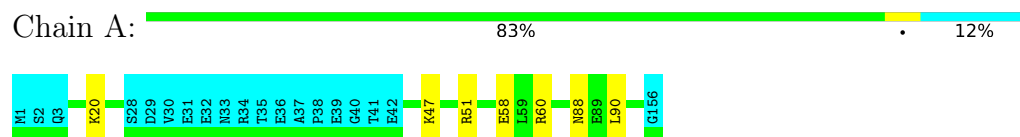


- Molecule 2: Protein X

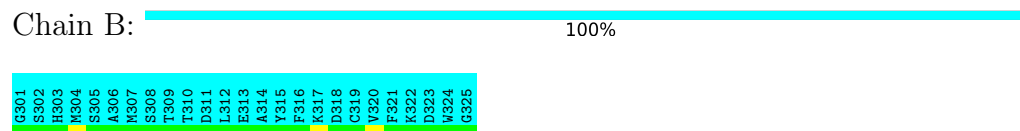


4.2.5 Score per residue for model 5

- Molecule 1: Bcl-2-like protein 1

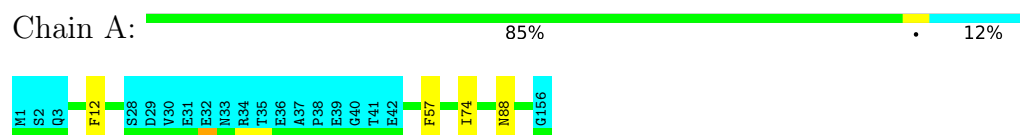


- Molecule 2: Protein X

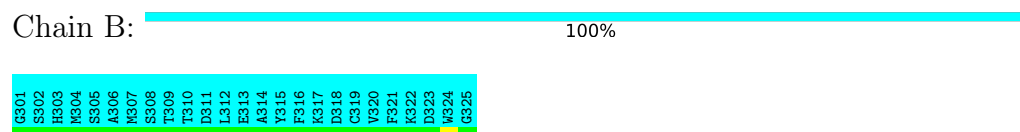


4.2.6 Score per residue for model 6

- Molecule 1: Bcl-2-like protein 1

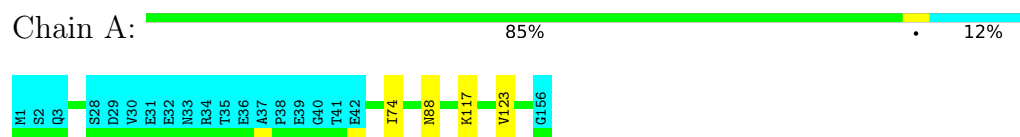


- Molecule 2: Protein X

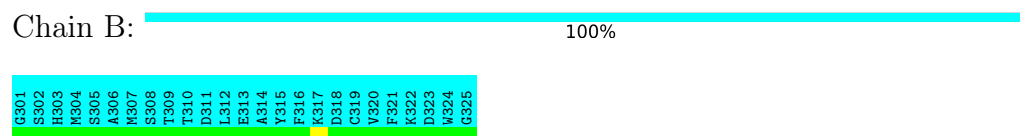


4.2.7 Score per residue for model 7

- Molecule 1: Bcl-2-like protein 1

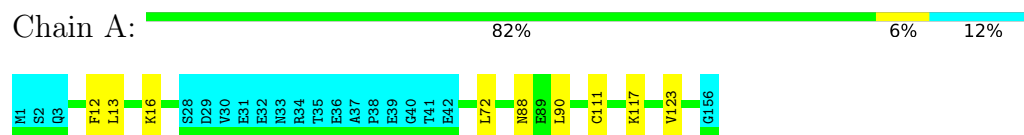


- Molecule 2: Protein X

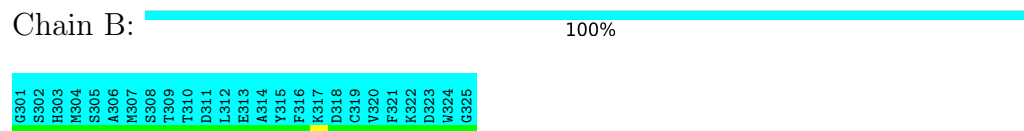


4.2.8 Score per residue for model 8

- Molecule 1: Bcl-2-like protein 1

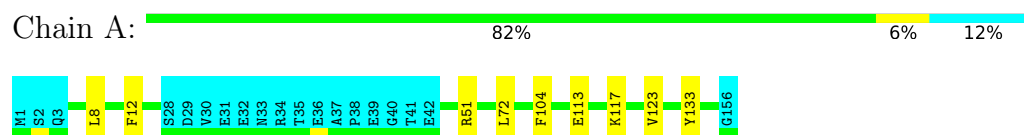


- Molecule 2: Protein X

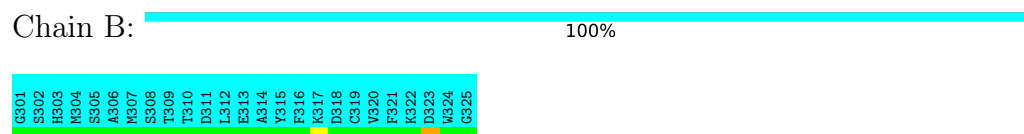


4.2.9 Score per residue for model 9

- Molecule 1: Bcl-2-like protein 1

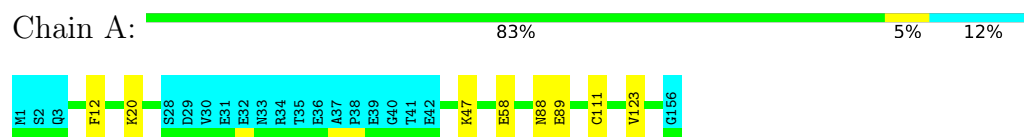


- Molecule 2: Protein X

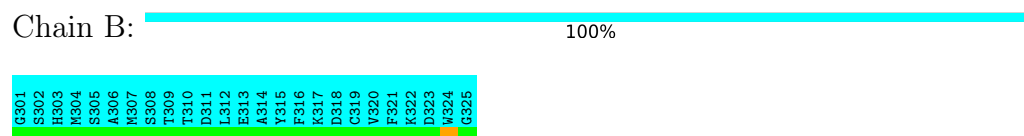


4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Bcl-2-like protein 1

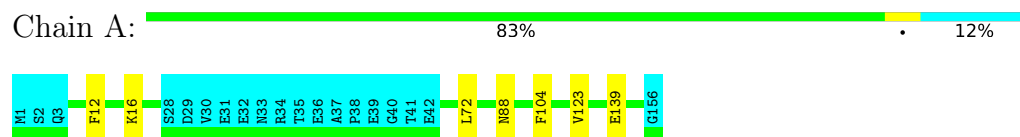


- Molecule 2: Protein X

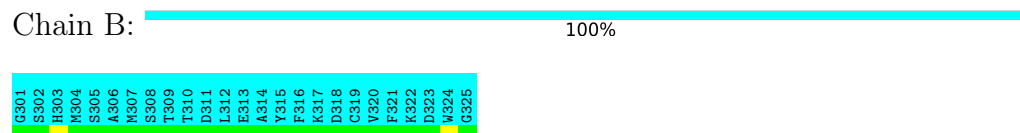


4.2.11 Score per residue for model 11

- Molecule 1: Bcl-2-like protein 1

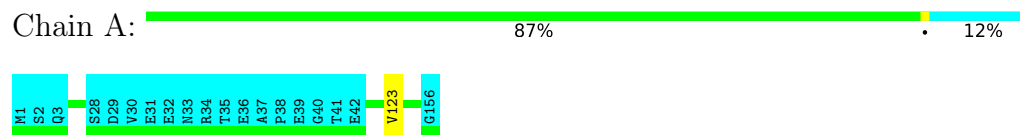


- Molecule 2: Protein X

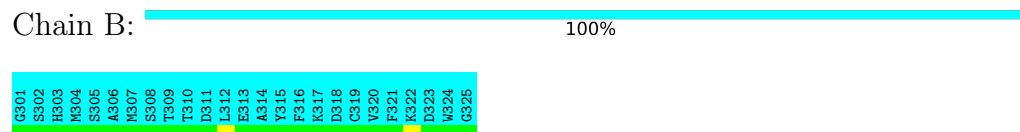


4.2.12 Score per residue for model 12

- Molecule 1: Bcl-2-like protein 1

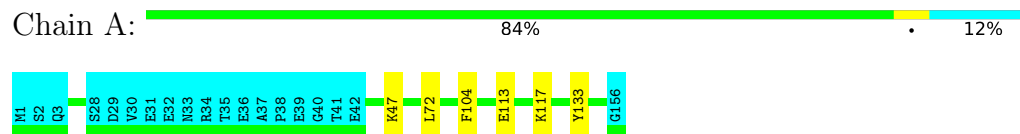


- Molecule 2: Protein X

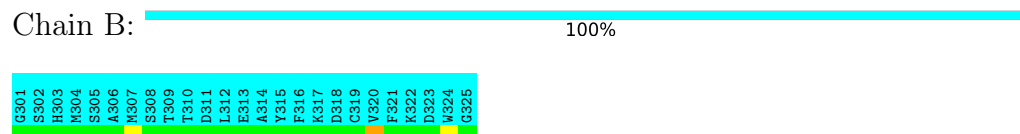


4.2.13 Score per residue for model 13

- Molecule 1: Bcl-2-like protein 1

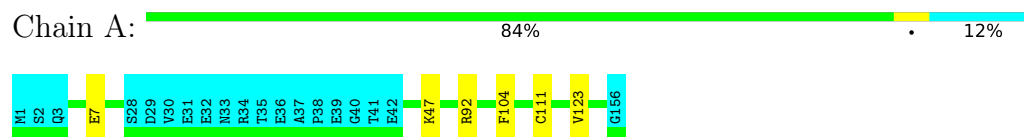


- Molecule 2: Protein X

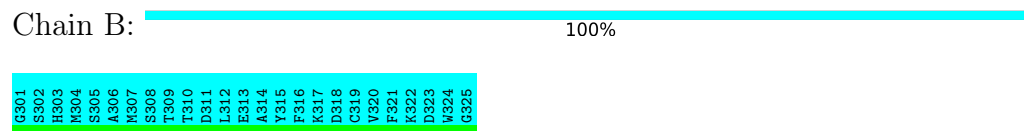


4.2.14 Score per residue for model 14

- Molecule 1: Bcl-2-like protein 1

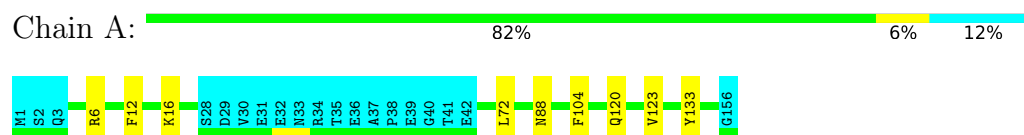


- Molecule 2: Protein X

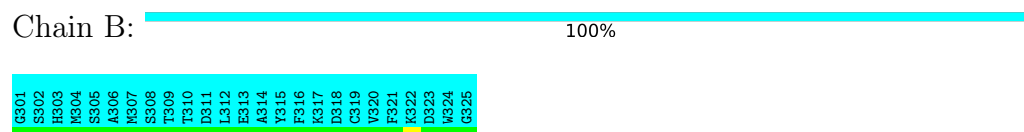


4.2.15 Score per residue for model 15

- Molecule 1: Bcl-2-like protein 1

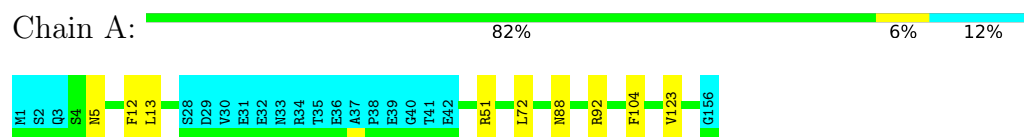


- Molecule 2: Protein X

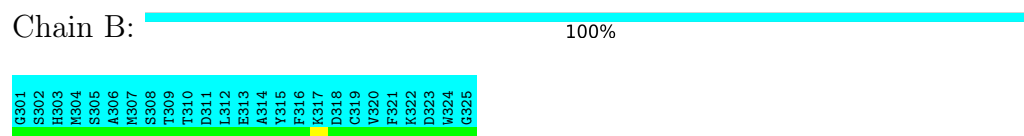


4.2.16 Score per residue for model 16

- Molecule 1: Bcl-2-like protein 1

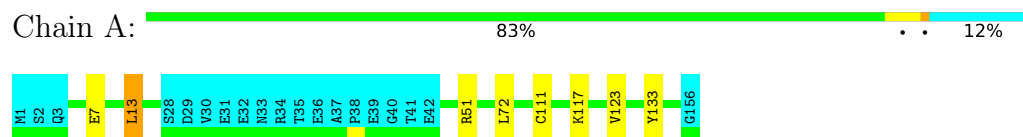


- Molecule 2: Protein X

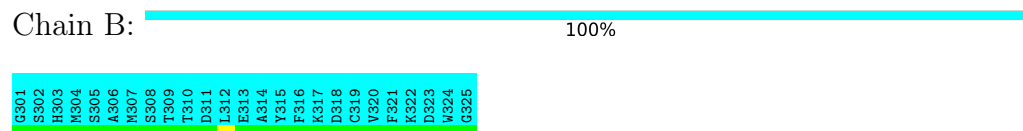


4.2.17 Score per residue for model 17

- Molecule 1: Bcl-2-like protein 1

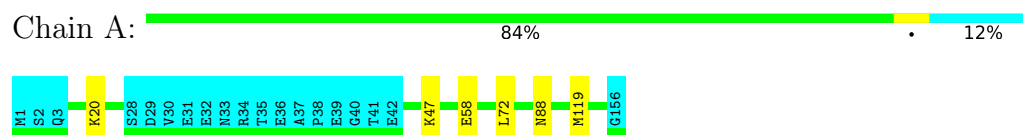


- Molecule 2: Protein X

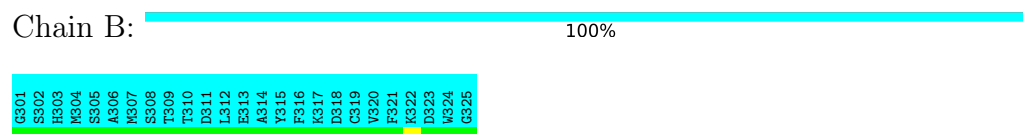


4.2.18 Score per residue for model 18

- Molecule 1: Bcl-2-like protein 1

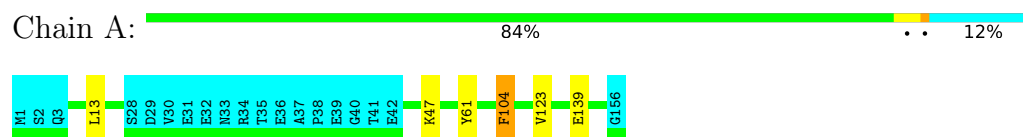


- Molecule 2: Protein X

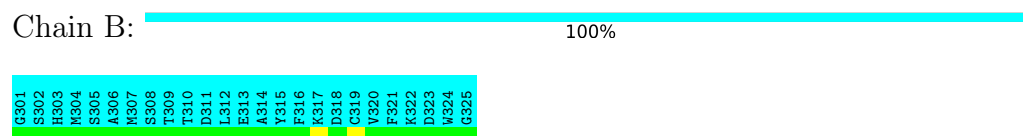


4.2.19 Score per residue for model 19

- Molecule 1: Bcl-2-like protein 1

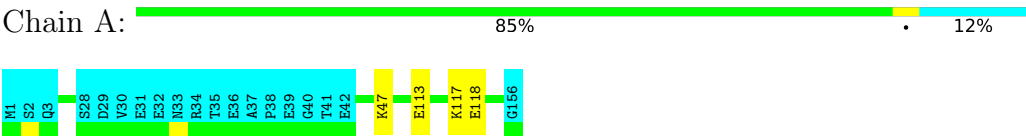


- Molecule 2: Protein X

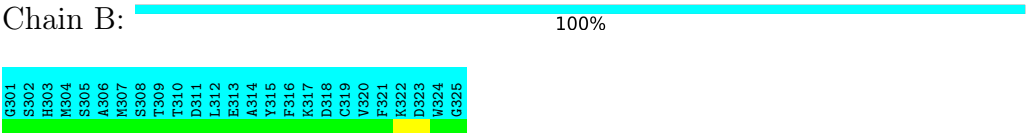


4.2.20 Score per residue for model 20

- Molecule 1: Bcl-2-like protein 1



- Molecule 2: Protein X



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CYANA	structure calculation	3.98
Amber	refinement	12

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	2129
Number of shifts mapped to atoms	2120
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.85±0.01	0±0/1151 (0.0± 0.0%)	1.36±0.02	1±1/1561 (0.0± 0.1%)
All	All	0.85	0/23020 (0.0%)	1.36	14/31220 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.4±0.5
All	All	0	8

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	PHE	CA-CB-CG	6.26	120.06	113.80	2	8
1	A	57	PHE	CA-CB-CG	5.84	119.64	113.80	6	1
1	A	74	ILE	CA-C-N	5.37	127.85	120.39	6	2
1	A	74	ILE	C-N-CA	5.37	127.85	120.39	6	2
1	A	104	PHE	CA-CB-CG	5.11	118.91	113.80	19	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	133	TYR	Sidechain	6
1	A	60	ARG	Sidechain	1
1	A	51	ARG	Sidechain	1

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	1121	1062	1062	0±0
2	B	0	0	0	0±0
All	All	22420	21240	21240	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:HD21	1:A:111:CYS:SG	0.40	2.56	17	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	137/156 (88%)	133±1 (97±1%)	4±1 (3±1%)	0±0 (0±0%)	100	100
2	B	0	-	-	-	-	-
All	All	2740/3620 (76%)	2665 (97%)	75 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	118/134 (88%)	113±2 (95±2%)	5±2 (5±2%)	25 76
2	B	0	-	-	-
All	All	2360/3100 (76%)	2251 (95%)	109 (5%)	25 76

All 27 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	123	VAL	13
1	A	88	ASN	10
1	A	72	LEU	9
1	A	47	LYS	9
1	A	104	PHE	8
1	A	117	LYS	8
1	A	16	LYS	5
1	A	113	GLU	4
1	A	20	LYS	4
1	A	58	GLU	4
1	A	111	CYS	4
1	A	13	LEU	4
1	A	7	GLU	3
1	A	90	LEU	3
1	A	92	ARG	3
1	A	139	GLU	3
1	A	51	ARG	3
1	A	8	LEU	2
1	A	89	GLU	2
1	A	44	GLU	1
1	A	68	LEU	1
1	A	63	ARG	1
1	A	6	ARG	1
1	A	120	GLN	1
1	A	5	ASN	1
1	A	119	MET	1
1	A	118	GLU	1

6.3.3 RNA ⓘ

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 89% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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

Total number of shifts	2129
Number of shifts mapped to atoms	2120
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	40

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

- No matching atom found in the structure. All 9 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	H	8.565	0.03	1
1	B	325	SER	H	8.263	0.03	1
1	B	325	SER	HA	4.481	0.03	1
1	B	325	SER	HB2	4.008	0.03	2
1	B	325	SER	HB3	4.008	0.03	2
1	B	325	SER	C	180.314	0.3	1
1	B	325	SER	CA	63.245	0.3	1
1	B	325	SER	CB	68.689	0.3	1
1	B	325	SER	N	115.712	0.3	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	174	-5.25 ± 0.14	Should be checked
$^{13}\text{C}_\beta$	163	-4.42 ± 0.05	Should be checked
$^{13}\text{C}'$	163	-4.89 ± 0.10	Should be applied
^{15}N	166	0.29 ± 0.17	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1690 atoms were assigned a chemical shift out of a possible 1898. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	660/690 (96%)	268/281 (95%)	262/274 (96%)	130/135 (96%)
Sidechain	849/980 (87%)	577/635 (91%)	255/304 (84%)	17/41 (41%)
Aromatic	181/228 (79%)	94/112 (84%)	82/109 (75%)	5/7 (71%)
Overall	1690/1898 (89%)	939/1028 (91%)	599/687 (87%)	152/183 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 2118 atoms were assigned a chemical shift out of a possible 2428. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	843/912 (92%)	343/372 (92%)	335/362 (93%)	165/178 (93%)
Sidechain	1059/1240 (85%)	718/801 (90%)	322/391 (82%)	19/48 (40%)
Aromatic	216/276 (78%)	112/136 (82%)	98/131 (75%)	6/9 (67%)
Overall	2118/2428 (87%)	1173/1309 (90%)	755/884 (85%)	190/235 (81%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	325	GLY	CA	54.88	38.93 – 51.79	7.4
1	A	141	TRP	HZ3	4.23	5.05 – 8.70	-7.3
1	A	47	LYS	CE	47.95	37.57 – 46.21	7.0
1	A	51	ARG	CD	48.87	38.57 – 47.75	6.2
1	A	125	ARG	CD	48.61	38.57 – 47.75	5.9
1	A	117	LYS	CE	47.00	37.57 – 46.21	5.9
1	A	145	ASN	HB2	1.00	1.27 – 4.34	-5.9

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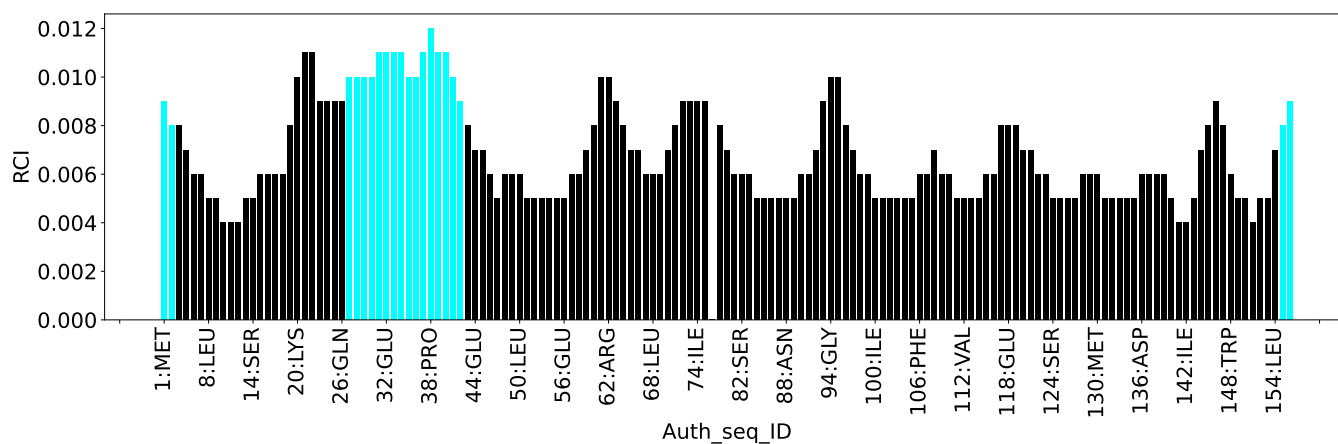
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	20	LYS	CE	46.91	37.57 – 46.21	5.8
1	B	317	LYS	CE	46.86	37.57 – 46.21	5.8
1	A	16	LYS	CE	46.83	37.57 – 46.21	5.7
1	A	83	PHE	CE2	137.49	124.80 – 136.72	5.7
1	A	107	GLY	CA	52.60	38.93 – 51.79	5.6
1	A	108	GLY	CA	52.54	38.93 – 51.79	5.6
1	B	322	LYS	CE	46.71	37.57 – 46.21	5.6
1	A	35	THR	C	184.01	166.08 – 183.07	5.6
1	A	134	LEU	CG	32.76	21.37 – 32.19	5.5
1	A	140	PRO	CG	33.24	21.69 – 32.72	5.5
1	A	95	VAL	HB	0.31	0.43 – 3.54	-5.4
1	A	98	GLY	CA	52.19	38.93 – 51.79	5.3
1	A	17	LEU	CG	32.48	21.37 – 32.19	5.3
1	A	60	ARG	CD	47.99	38.57 – 47.75	5.3
1	A	75	THR	CG2	27.31	16.06 – 27.03	5.3
1	A	62	ARG	CD	47.98	38.57 – 47.75	5.2
1	A	34	ARG	CD	47.96	38.57 – 47.75	5.2
1	A	92	ARG	CD	47.96	38.57 – 47.75	5.2
1	A	27	PHE	CE2	136.96	124.80 – 136.72	5.2
1	A	95	VAL	HG21	-0.63	-0.58 – 2.19	-5.2
1	A	95	VAL	HG22	-0.63	-0.58 – 2.19	-5.2
1	A	95	VAL	HG23	-0.63	-0.58 – 2.19	-5.2
1	A	76	PRO	CD	55.75	45.11 – 55.58	5.2
1	A	83	PHE	CE1	137.49	124.17 – 137.29	5.2
1	A	63	ARG	CD	47.87	38.57 – 47.75	5.1
1	A	6	ARG	CD	47.86	38.57 – 47.75	5.1
1	A	140	PRO	CA	71.03	55.85 – 70.84	5.1
1	A	81	GLN	CG	39.33	28.36 – 39.21	5.1
1	A	69	THR	CG2	27.12	16.06 – 27.03	5.1
1	A	54	GLY	CA	51.89	38.93 – 51.79	5.1
1	A	150	THR	CG2	27.12	16.06 – 27.03	5.1
1	A	152	VAL	CG2	28.96	13.71 – 28.88	5.0
1	A	18	SER	C	183.19	166.15 – 183.14	5.0

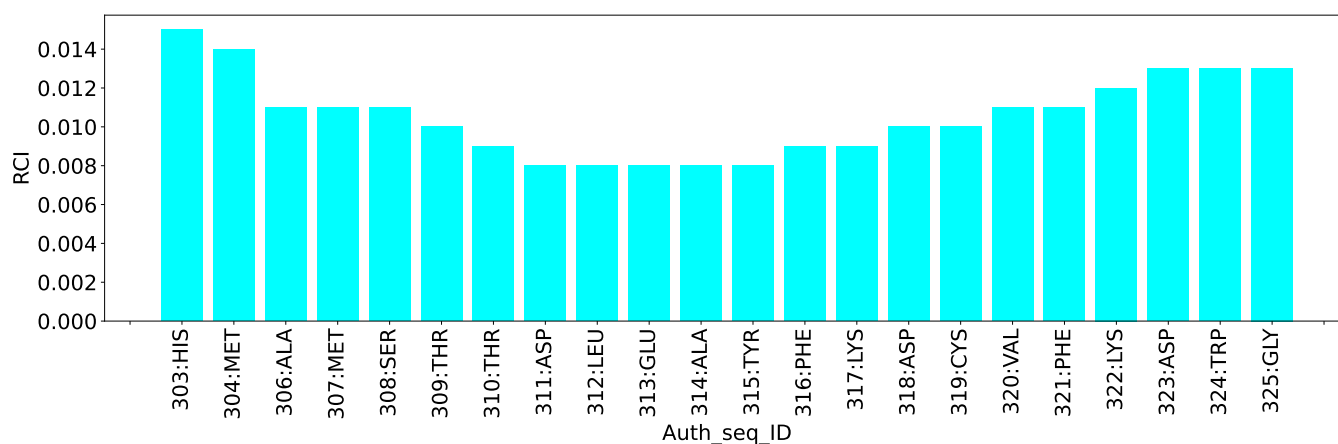
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3127
Intra-residue ($ i-j =0$)	763
Sequential ($ i-j =1$)	666
Medium range ($ i-j >1$ and $ i-j <5$)	1022
Long range ($ i-j \geq 5$)	512
Inter-chain	20
Hydrogen bond restraints	144
Disulfide bond restraints	0
Total dihedral-angle restraints	355
Number of unmapped restraints	0
Number of restraints per residue	19.2
Number of long range restraints per residue ¹	2.8

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)	12.9	0.2
0.2-0.5 (Medium)	11.8	0.5
>0.5 (Large)	14.7	2.6

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)	42.6	10.0
10.0-20.0 (Medium)	15.2	19.99
>20.0 (Large)	12.2	135.21

9 Distance violation analysis ⓘ

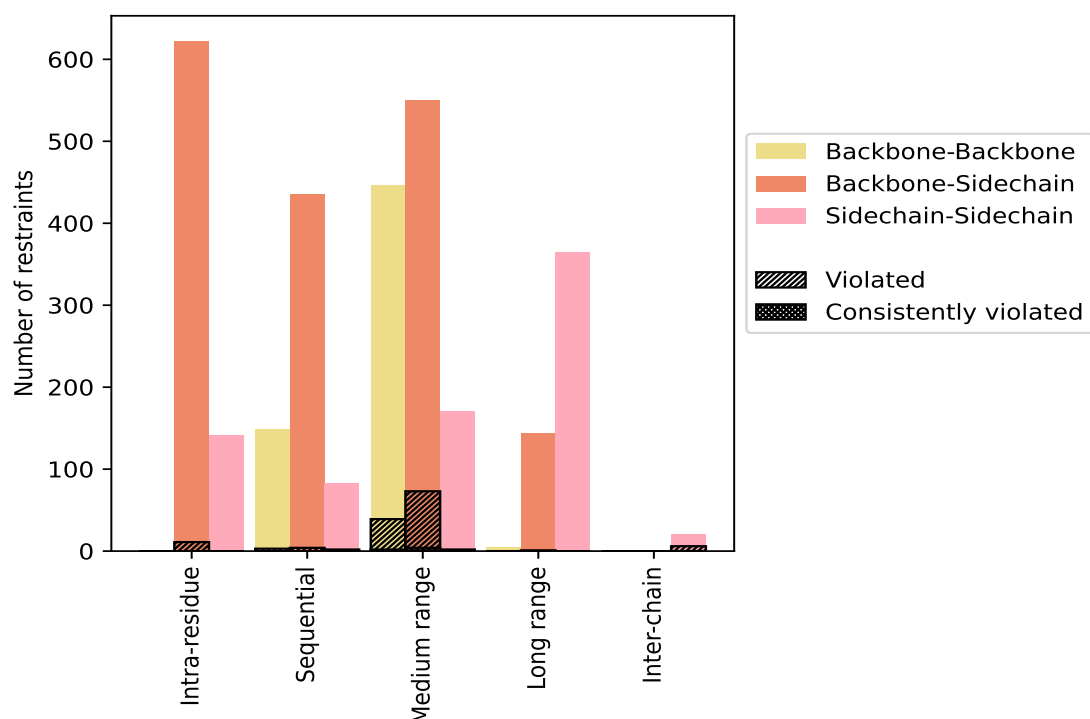
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	763	24.4	11	1.4	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	622	19.9	11	1.8	0.4	0	0.0	0.0
Sidechain-Sidechain	141	4.5	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	666	21.3	9	1.4	0.3	0	0.0	0.0
Backbone-Backbone	148	4.7	3	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	435	13.9	4	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	83	2.7	2	2.4	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	1022	32.7	46	4.5	1.5	2	0.2	0.1
Backbone-Backbone	446	14.3	39	8.7	1.2	2	0.4	0.1
Backbone-Sidechain	406	13.0	5	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	170	5.4	2	1.2	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	512	16.4	1	0.2	0.0	0	0.0	0.0
Backbone-Backbone	5	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	143	4.6	1	0.7	0.0	0	0.0	0.0
Sidechain-Sidechain	364	11.6	0	0.0	0.0	0	0.0	0.0
Inter-chain	20	0.6	6	30.0	0.2	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	20	0.6	6	30.0	0.2	0	0.0	0.0
Hydrogen bond	144	4.6	68	47.2	2.2	4	2.8	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3127	100.0	141	4.5	4.5	6	0.2	0.2
Backbone-Backbone	599	19.2	42	7.0	1.3	2	0.3	0.1
Backbone-Sidechain	1750	56.0	89	5.1	2.8	4	0.2	0.1
Sidechain-Sidechain	778	24.9	10	1.3	0.3	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	2	35	0	0	37	0.59	1.87	0.51	0.4
2	0	2	39	0	0	41	0.56	2.29	0.51	0.43
3	2	1	30	0	0	33	0.51	2.05	0.51	0.26
4	0	1	42	0	0	43	0.53	1.82	0.46	0.34
5	2	2	42	0	0	46	0.48	1.93	0.49	0.26
6	5	1	35	0	0	41	0.56	1.82	0.46	0.39
7	2	1	51	0	0	54	0.48	1.61	0.38	0.32
8	3	0	30	0	0	33	0.52	1.88	0.53	0.27
9	4	0	31	0	0	35	0.66	2.03	0.58	0.42
10	2	1	34	0	0	37	0.62	2.6	0.62	0.28

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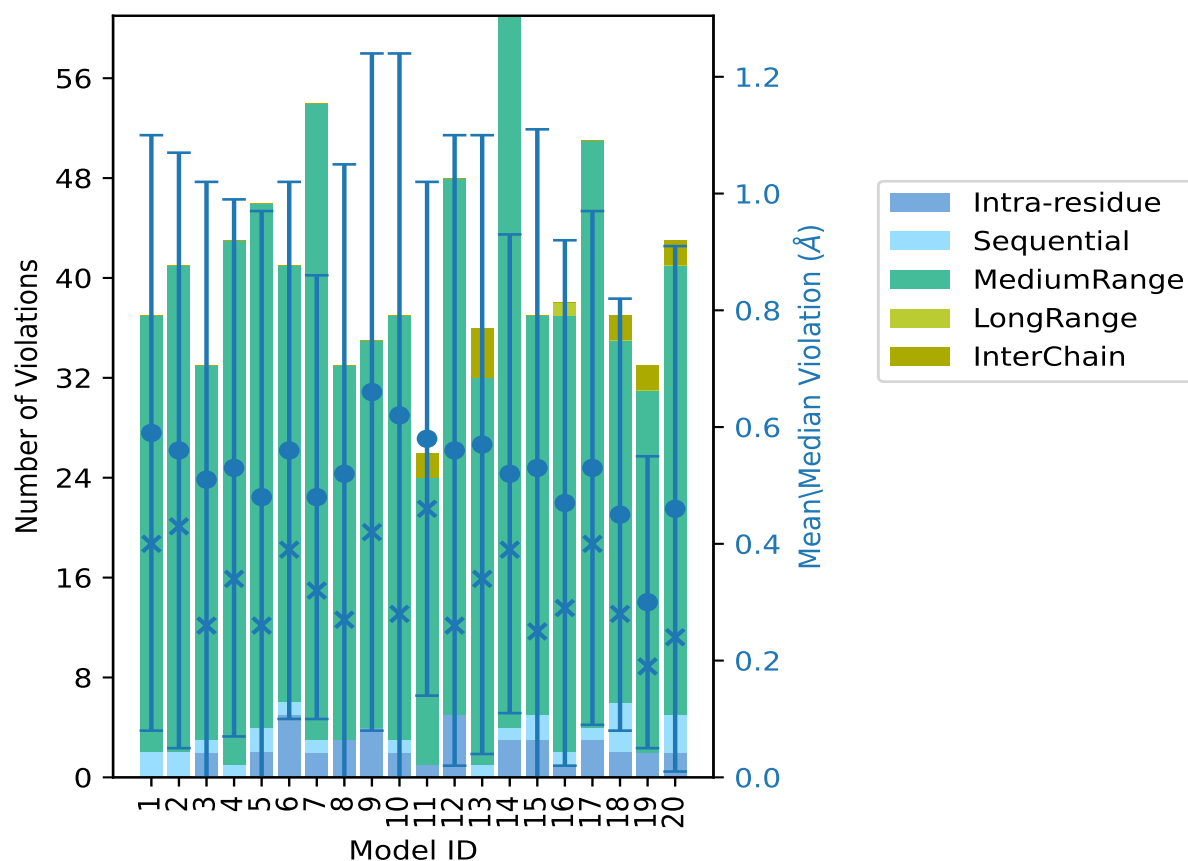
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	0	23	0	2	26	0.58	1.75	0.44	0.46
12	5	0	43	0	0	48	0.56	2.27	0.54	0.26
13	0	1	31	0	4	36	0.57	2.14	0.53	0.34
14	3	1	57	0	0	61	0.52	1.66	0.41	0.39
15	3	2	32	0	0	37	0.53	2.4	0.58	0.25
16	1	1	35	1	0	38	0.47	1.96	0.45	0.29
17	3	1	47	0	0	51	0.53	2.15	0.44	0.4
18	2	4	29	0	2	37	0.45	1.39	0.37	0.28
19	2	0	29	0	2	33	0.3	1.1	0.25	0.19
20	2	3	36	0	2	43	0.46	1.89	0.45	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

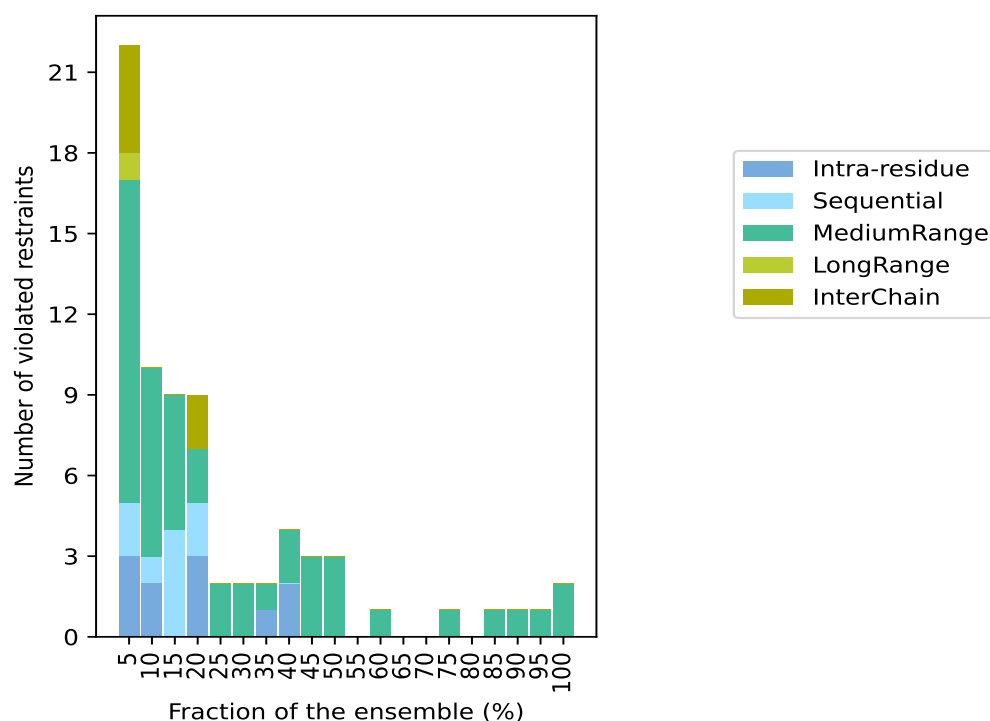
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2910(IR:752, SQ:657, MR:976, LR:511, IC:14) restraints are 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	%
3	2	12	1	4	22	1	5.0
2	1	7	0	0	10	2	10.0
0	4	5	0	0	9	3	15.0
3	2	2	0	2	9	4	20.0
0	0	2	0	0	2	5	25.0
0	0	2	0	0	2	6	30.0
1	0	1	0	0	2	7	35.0
2	0	2	0	0	4	8	40.0
0	0	3	0	0	3	9	45.0
0	0	3	0	0	3	10	50.0
0	0	0	0	0	0	11	55.0
0	0	1	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	1	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	1	0	0	1	17	85.0
0	0	1	0	0	1	18	90.0
0	0	1	0	0	1	19	95.0
0	0	2	0	0	2	20	100.0

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

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

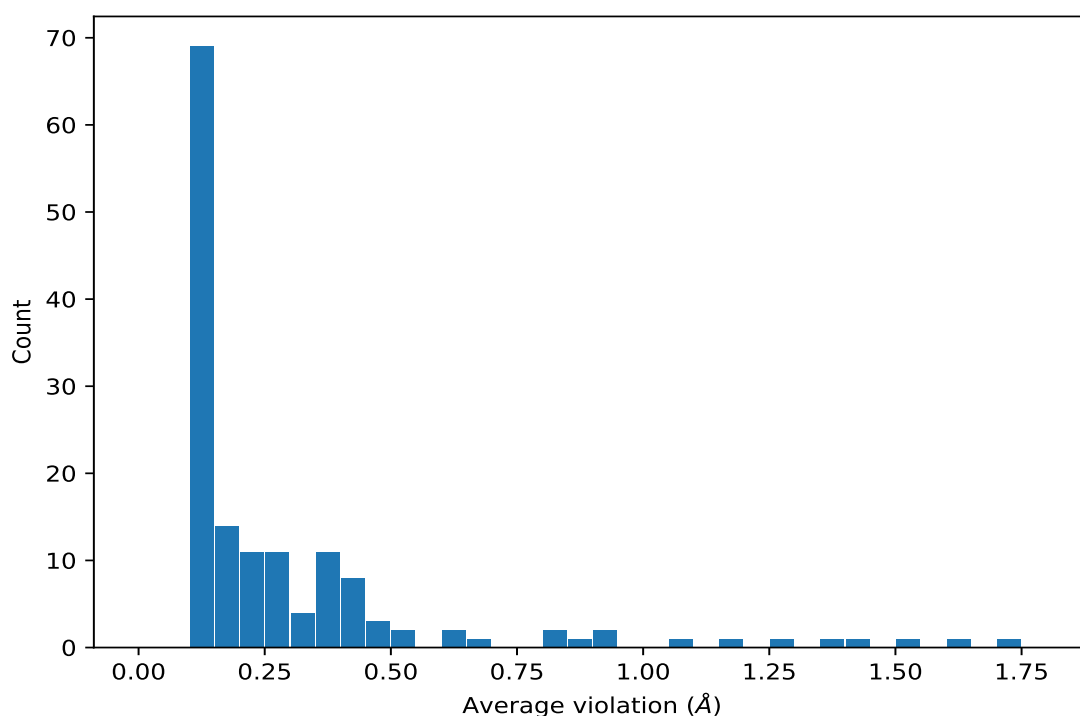
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	20	1.71	0.59	1.81
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	20	1.52	0.27	1.52
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	20	1.25	0.28	1.25
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	20	1.17	0.24	1.18
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	20	0.94	0.24	0.94
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	20	0.87	0.42	0.9
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	19	1.45	0.47	1.5
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	19	0.84	0.28	0.86
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	19	0.23	0.06	0.21
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	18	0.62	0.26	0.6
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	17	0.16	0.03	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	17	0.16	0.03	0.15
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	16	0.49	0.16	0.49
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	15	0.43	0.17	0.5
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	15	0.37	0.14	0.41
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	14	0.54	0.29	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	14	0.38	0.11	0.36
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	14	0.21	0.07	0.19
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	13	1.35	0.15	1.37
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	13	0.95	0.14	0.99
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	13	0.69	0.31	0.54
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	12	0.47	0.29	0.45
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	12	0.38	0.14	0.36
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	11	0.52	0.19	0.55
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	11	0.42	0.22	0.32
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	11	0.23	0.07	0.2
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	10	0.81	0.29	0.89
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	10	0.61	0.22	0.66
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	10	0.41	0.22	0.37
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	10	0.39	0.19	0.32
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	10	0.36	0.23	0.28
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	10	0.26	0.06	0.26
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	10	0.16	0.06	0.13
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	9	0.48	0.27	0.47
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	9	0.26	0.1	0.23
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	9	0.26	0.1	0.22
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	9	0.12	0.02	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	9	0.12	0.02	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	9	0.12	0.02	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	9	0.12	0.02	0.11
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	8	0.42	0.24	0.41
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	8	0.27	0.16	0.21
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	8	0.17	0.04	0.15
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	8	0.14	0.02	0.14
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	8	0.14	0.02	0.14
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	8	0.14	0.02	0.14
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	8	0.14	0.02	0.14
(3,6)	2:317:B:LYS:N	2:313:B:GLU:C	7	0.2	0.05	0.22
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG2	7	0.13	0.02	0.13
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG3	7	0.13	0.02	0.13
(3,2)	2:319:B:CYS:N	2:315:B:TYR:C	6	0.4	0.18	0.36
(3,10)	2:315:B:TYR:N	2:311:B:ASP:C	6	0.37	0.17	0.32
(9,51)	1:85:A:GLN:H	1:81:A:GLN:O	6	0.32	0.05	0.31
(9,21)	1:19:A:GLN:H	1:15:A:TYR:O	6	0.28	0.11	0.26
(9,79)	1:110:A:LEU:H	1:106:A:PHE:O	6	0.26	0.1	0.29
(9,52)	1:85:A:GLN:N	1:81:A:GLN:O	6	0.21	0.05	0.2
(9,10)	1:13:A:LEU:N	1:9:A:VAL:O	6	0.19	0.09	0.16
(9,84)	1:112:A:VAL:N	1:108:A:GLY:O	5	0.41	0.14	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(9,3)	1:9:A:VAL:H	1:5:A:ASN:O	5	0.39	0.19	0.41
(10,83)	1:112:A:VAL:H	1:108:A:GLY:C	5	0.34	0.12	0.42
(9,70)	1:105:A:SER:N	1:101:A:VAL:O	5	0.16	0.06	0.14
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB2	5	0.12	0.02	0.11
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB3	5	0.12	0.02	0.11
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB2	5	0.12	0.02	0.11
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB3	5	0.12	0.02	0.11
(2,3)	2:318:B:ASP:H	2:314:B:ALA:O	4	1.6	0.13	1.56
(2,4)	2:318:B:ASP:N	2:314:B:ALA:O	4	1.07	0.04	1.06
(10,84)	1:112:A:VAL:N	1:108:A:GLY:C	4	0.28	0.05	0.3
(10,9)	1:13:A:LEU:H	1:9:A:VAL:C	4	0.19	0.06	0.18
(9,15)	1:16:A:LYS:H	1:12:A:PHE:O	4	0.19	0.04	0.18
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	4	0.14	0.01	0.14
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	4	0.14	0.01	0.14
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB2	4	0.14	0.02	0.14
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB3	4	0.14	0.02	0.14
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB2	4	0.14	0.02	0.14
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB3	4	0.14	0.02	0.14
(7,17)	1:31:A:GLU:H	1:31:A:GLU:HB2	4	0.12	0.01	0.12
(7,1045)	1:133:A:TYR:HD1	1:134:A:LEU:HG	4	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(7,1045)	1:133:A:TYR:HD2	1:134:A:LEU:HG	4	0.11	0.0	0.11
(7,1766)	2:313:B:GLU:HG2	2:314:B:ALA:H	4	0.11	0.0	0.11
(7,1766)	2:313:B:GLU:HG3	2:314:B:ALA:H	4	0.11	0.0	0.11
(9,88)	1:114:A:SER:N	1:110:A:LEU:O	3	0.44	0.12	0.44
(9,85)	1:113:A:GLU:H	1:109:A:ALA:O	3	0.44	0.15	0.52
(9,29)	1:51:A:ARG:H	1:47:A:LYS:O	3	0.39	0.13	0.34
(10,87)	1:114:A:SER:H	1:110:A:LEU:C	3	0.37	0.14	0.4
(9,86)	1:113:A:GLU:N	1:109:A:ALA:O	3	0.28	0.13	0.35
(7,1526)	1:87:A:VAL:HA	1:90:A:LEU:HG	3	0.21	0.04	0.19
(9,128)	1:153:A:GLU:N	1:149:A:ASP:O	3	0.21	0.06	0.22
(9,30)	1:51:A:ARG:N	1:47:A:LYS:O	3	0.19	0.09	0.14
(9,63)	1:100:A:ILE:H	1:96:A:ASN:O	3	0.14	0.02	0.15
(10,79)	1:110:A:LEU:H	1:106:A:PHE:C	3	0.14	0.02	0.13
(5,18)	2:323:B:ASP:HA	2:324:B:TRP:H	3	0.13	0.01	0.12
(7,2433)	2:323:B:ASP:HA	2:324:B:TRP:H	3	0.13	0.01	0.12
(10,60)	1:92:A:ARG:N	1:88:A:ASN:C	3	0.13	0.01	0.13
(7,1881)	1:13:A:LEU:HD11	1:14:A:SER:HA	3	0.11	0.01	0.11
(7,1881)	1:13:A:LEU:HD12	1:14:A:SER:HA	3	0.11	0.01	0.11
(7,1881)	1:13:A:LEU:HD13	1:14:A:SER:HA	3	0.11	0.01	0.11
(7,1881)	1:13:A:LEU:HD21	1:14:A:SER:HA	3	0.11	0.01	0.11
(7,1881)	1:13:A:LEU:HD22	1:14:A:SER:HA	3	0.11	0.01	0.11
(7,1881)	1:13:A:LEU:HD23	1:14:A:SER:HA	3	0.11	0.01	0.11
(9,80)	1:110:A:LEU:N	1:106:A:PHE:O	3	0.11	0.0	0.11
(7,2292)	1:120:A:GLN:HG2	1:121:A:VAL:H	3	0.11	0.0	0.11
(7,2292)	1:120:A:GLN:HG3	1:121:A:VAL:H	3	0.11	0.0	0.11
(7,283)	1:115:A:VAL:HB	1:119:A:MET:H	3	0.1	0.0	0.1
(9,77)	1:109:A:ALA:H	1:105:A:SER:O	2	0.38	0.19	0.38
(9,47)	1:82:A:SER:H	1:78:A:THR:O	2	0.36	0.06	0.36
(10,85)	1:113:A:GLU:H	1:109:A:ALA:C	2	0.34	0.02	0.34
(9,1)	1:8:A:LEU:H	1:4:A:SER:O	2	0.31	0.0	0.31
(9,57)	1:90:A:LEU:H	1:86:A:VAL:O	2	0.3	0.19	0.3
(10,88)	1:114:A:SER:N	1:110:A:LEU:C	2	0.3	0.06	0.3
(9,4)	1:9:A:VAL:N	1:5:A:ASN:O	2	0.25	0.03	0.25
(9,89)	1:115:A:VAL:H	1:111:A:CYS:O	2	0.24	0.12	0.24
(9,48)	1:82:A:SER:N	1:78:A:THR:O	2	0.22	0.06	0.22
(9,124)	1:151:A:PHE:N	1:147:A:GLY:O	2	0.21	0.01	0.21
(10,86)	1:113:A:GLU:N	1:109:A:ALA:C	2	0.2	0.02	0.2
(9,2)	1:8:A:LEU:N	1:4:A:SER:O	2	0.19	0.01	0.19
(9,8)	1:11:A:ASP:N	1:7:A:GLU:O	2	0.18	0.02	0.18
(10,1)	1:8:A:LEU:H	1:4:A:SER:C	2	0.16	0.04	0.16
(9,22)	1:19:A:GLN:N	1:15:A:TYR:O	2	0.16	0.05	0.16
(10,10)	1:13:A:LEU:N	1:9:A:VAL:C	2	0.16	0.04	0.16

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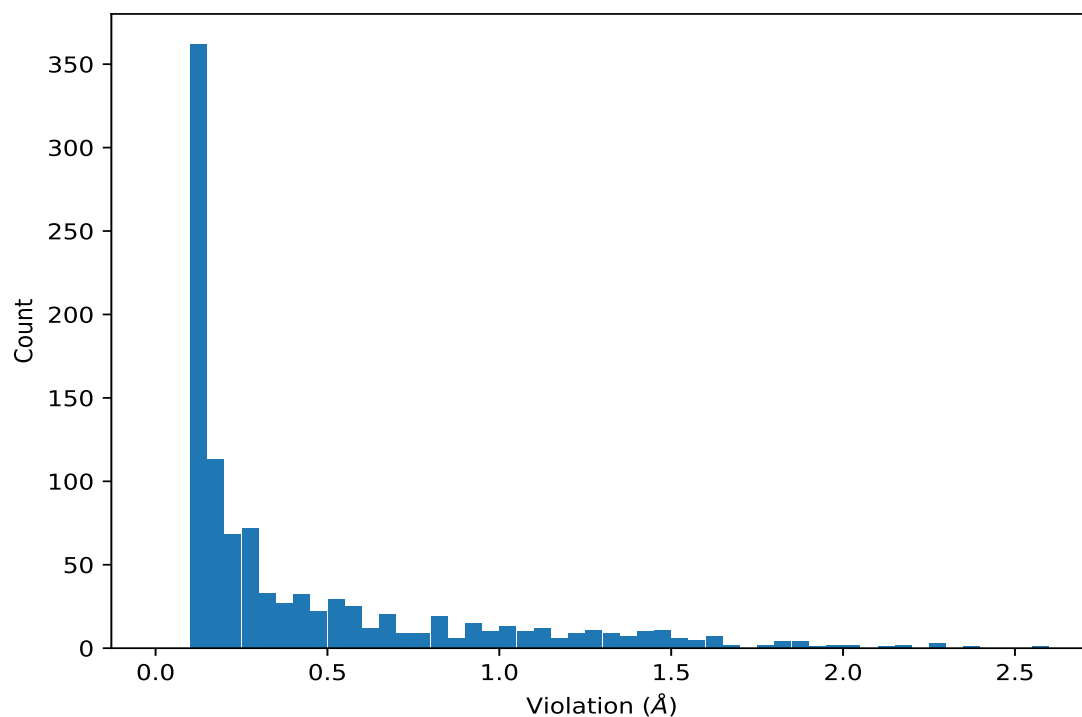
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(7,111)	1:31:A:GLU:HA	1:32:A:GLU:H	2	0.15	0.04	0.15
(5,30)	2:324:B:TRP:HA	2:324:B:TRP:HE3	2	0.14	0.01	0.14
(7,2446)	2:324:B:TRP:HA	2:324:B:TRP:HE3	2	0.14	0.01	0.14
(10,51)	1:85:A:GLN:H	1:81:A:GLN:C	2	0.12	0.02	0.12
(9,25)	1:49:A:ALA:H	1:45:A:ALA:O	2	0.12	0.0	0.12
(10,123)	1:151:A:PHE:H	1:147:A:GLY:C	2	0.12	0.01	0.12
(9,43)	1:59:A:LEU:H	1:55:A:ASP:O	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	10	2.6
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	15	2.4
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	2	2.29
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	12	2.27
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	10	2.25
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	12	2.15
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	17	2.15
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	13	2.14
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	3	2.05
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	9	2.03
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	13	1.99
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	16	1.96
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	5	1.93
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	15	1.9
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	20	1.89
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	8	1.88
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	1	1.87
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	2	1.84
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	4	1.82
(2,3)	2:318:B:ASP:H	2:314:B:ALA:O	6	1.82
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	9	1.8
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	17	1.76
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	11	1.75
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	5	1.7
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	14	1.66
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	9	1.65
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	9	1.63
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	1	1.63
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	6	1.62
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	4	1.61
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	7	1.61
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	15	1.6
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	8	1.57
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	20	1.57
(2,3)	2:318:B:ASP:H	2:314:B:ALA:O	12	1.56
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	2	1.55
(2,3)	2:318:B:ASP:H	2:314:B:ALA:O	9	1.55
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	5	1.54
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	8	1.54
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	16	1.53
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	8	1.52
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	3	1.51
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	9	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	10	1.49
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	7	1.49
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	5	1.49
(2,3)	2:318:B:ASP:H	2:314:B:ALA:O	7	1.49
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	17	1.48
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	5	1.47
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	20	1.47
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	14	1.47
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	1	1.46
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	3	1.46
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	1	1.46
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	6	1.45
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	13	1.45
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	12	1.44
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	4	1.43
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	13	1.43
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	4	1.43
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	10	1.43
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	9	1.42
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	9	1.41
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	12	1.41
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	14	1.4
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	8	1.4
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	18	1.39
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	11	1.38
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	3	1.37
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	11	1.37
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	4	1.36
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	10	1.34
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	15	1.34
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	5	1.33
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	17	1.33
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	2	1.32
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	1	1.32
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	18	1.3
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	10	1.3
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	14	1.3
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	15	1.29
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	1	1.29
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	6	1.29
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	1	1.29
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	14	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	14	1.28
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	7	1.28
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	14	1.27
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	16	1.27
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	6	1.26
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	4	1.25
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	12	1.24
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	15	1.24
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	20	1.24
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	8	1.21
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	20	1.21
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	6	1.21
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	2	1.21
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	15	1.21
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	12	1.21
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	8	1.2
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	16	1.2
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	13	1.19
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	17	1.18
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	2	1.18
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	10	1.16
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	3	1.15
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	11	1.14
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	1	1.13
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	5	1.13
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	6	1.12
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	4	1.12
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	20	1.12
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	18	1.12
(2,4)	2:318:B:ASP:N	2:314:B:ALA:O	12	1.12
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	12	1.1
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	13	1.1
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	19	1.1
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	10	1.09
(2,4)	2:318:B:ASP:N	2:314:B:ALA:O	9	1.09
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	16	1.07
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	3	1.07
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	2	1.06
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	13	1.06
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	7	1.06
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	1	1.06
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	17	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	10	1.05
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	12	1.04
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	6	1.04
(2,5)	2:317:B:LYS:H	2:313:B:GLU:O	2	1.04
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	2	1.03
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	10	1.03
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	5	1.03
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	18	1.03
(2,4)	2:318:B:ASP:N	2:314:B:ALA:O	6	1.03
(2,4)	2:318:B:ASP:N	2:314:B:ALA:O	7	1.03
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	17	1.01
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	16	1.0
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	20	1.0
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	10	1.0
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	15	0.99
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	7	0.99
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	18	0.99
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	14	0.99
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	3	0.99
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	4	0.99
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	11	0.98
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	15	0.97
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	14	0.96
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	18	0.96
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	12	0.95
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	12	0.95
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	13	0.95
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	10	0.95
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	9	0.95
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	7	0.94
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	17	0.94
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	19	0.94
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	3	0.94
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	4	0.94
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	14	0.93
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	17	0.93
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	14	0.92
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	6	0.9
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	14	0.9
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	12	0.89
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	1	0.88
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	1	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	14	0.87
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	13	0.86
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	7	0.86
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	4	0.85
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	14	0.85
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	16	0.85
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	3	0.84
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	11	0.84
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	5	0.84
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	2	0.83
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	15	0.83
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	16	0.83
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	14	0.83
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	13	0.83
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	18	0.83
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	16	0.82
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	17	0.82
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	11	0.82
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	12	0.82
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	8	0.81
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	16	0.8
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	20	0.8
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	6	0.77
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	7	0.77
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	14	0.77
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	17	0.77
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	11	0.77
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	20	0.76
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	10	0.75
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	7	0.75
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	7	0.75
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	14	0.74
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	2	0.73
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	17	0.72
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	14	0.72
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	9	0.72
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	18	0.71
(9,3)	1:9:A:VAL:H	1:5:A:ASN:O	5	0.71
(3,2)	2:319:B:CYS:N	2:315:B:TYR:C	10	0.71
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	13	0.71
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	7	0.7
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	19	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	12	0.7
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	11	0.7
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	6	0.7
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	14	0.69
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	17	0.69
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	8	0.69
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	7	0.68
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	7	0.68
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	19	0.68
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	6	0.67
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	18	0.66
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	9	0.66
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	18	0.66
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	18	0.66
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	13	0.65
(3,10)	2:315:B:TYR:N	2:311:B:ASP:C	14	0.65
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	13	0.65
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	1	0.65
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	6	0.64
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	20	0.64
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	2	0.64
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	1	0.63
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	6	0.63
(2,6)	2:317:B:LYS:N	2:313:B:GLU:O	19	0.63
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	2	0.62
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	9	0.62
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	9	0.62
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	17	0.62
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	9	0.61
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	17	0.61
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	14	0.6
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	14	0.6
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	11	0.59
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	6	0.59
(9,88)	1:114:A:SER:N	1:110:A:LEU:O	17	0.59
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	5	0.59
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	15	0.59
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	7	0.59
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	15	0.59
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	11	0.59
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	12	0.58
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	12	0.57
(9,85)	1:113:A:GLU:H	1:109:A:ALA:O	17	0.57
(9,29)	1:51:A:ARG:H	1:47:A:LYS:O	4	0.57
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	5	0.57
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	2	0.56
(9,77)	1:109:A:ALA:H	1:105:A:SER:O	14	0.56
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	3	0.56
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	4	0.55
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	1	0.55
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	8	0.55
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	9	0.55
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	4	0.55
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	18	0.55
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	6	0.54
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	16	0.54
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	4	0.54
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	16	0.54
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	20	0.54
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	20	0.54
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	7	0.54
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	17	0.54
(10,87)	1:114:A:SER:H	1:110:A:LEU:C	17	0.53
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	14	0.53
(9,84)	1:112:A:VAL:N	1:108:A:GLY:O	17	0.53
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	14	0.53
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	3	0.53
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	12	0.53
(3,2)	2:319:B:CYS:N	2:315:B:TYR:C	14	0.53
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	12	0.53
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	4	0.52
(9,85)	1:113:A:GLU:H	1:109:A:ALA:O	7	0.52
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	16	0.52
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	13	0.52
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	2	0.52
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	6	0.52
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	4	0.51
(9,84)	1:112:A:VAL:N	1:108:A:GLY:O	6	0.51
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	17	0.51
(3,10)	2:315:B:TYR:N	2:311:B:ASP:C	13	0.51
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	1	0.51
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	17	0.5
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	18	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	13	0.49
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	7	0.49
(9,57)	1:90:A:LEU:H	1:86:A:VAL:O	10	0.49
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	5	0.49
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	20	0.49
(9,21)	1:19:A:GLN:H	1:15:A:TYR:O	2	0.49
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	11	0.49
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	19	0.48
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	1	0.48
(9,84)	1:112:A:VAL:N	1:108:A:GLY:O	7	0.48
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	18	0.48
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	8	0.48
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	10	0.48
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	4	0.47
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	11	0.47
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	12	0.47
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	20	0.47
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	2	0.46
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	8	0.46
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	11	0.46
(10,83)	1:112:A:VAL:H	1:108:A:GLY:C	17	0.45
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	2	0.45
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	1	0.44
(9,88)	1:114:A:SER:N	1:110:A:LEU:O	7	0.44
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	2	0.44
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	9	0.44
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	19	0.44
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	11	0.44
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	1	0.44
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	18	0.44
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	17	0.44
(10,83)	1:112:A:VAL:H	1:108:A:GLY:C	7	0.43
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	13	0.43
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	14	0.43
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	15	0.43
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	4	0.43
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	20	0.43
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	18	0.43
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	2	0.43
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	2	0.43
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	8	0.43
(10,83)	1:112:A:VAL:H	1:108:A:GLY:C	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,51)	1:85:A:GLN:H	1:81:A:GLN:O	16	0.42
(9,47)	1:82:A:SER:H	1:78:A:THR:O	14	0.42
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	14	0.42
(9,3)	1:9:A:VAL:H	1:5:A:ASN:O	9	0.42
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	14	0.41
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	11	0.41
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	17	0.41
(9,3)	1:9:A:VAL:H	1:5:A:ASN:O	4	0.41
(10,87)	1:114:A:SER:H	1:110:A:LEU:C	7	0.4
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	17	0.4
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	1	0.4
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	3	0.4
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	20	0.39
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	3	0.39
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	12	0.39
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	14	0.39
(9,78)	1:109:A:ALA:N	1:105:A:SER:O	14	0.39
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	5	0.39
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	9	0.39
(3,3)	2:318:B:ASP:H	2:314:B:ALA:C	6	0.39
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	17	0.38
(9,86)	1:113:A:GLU:N	1:109:A:ALA:O	17	0.38
(9,84)	1:112:A:VAL:N	1:108:A:GLY:O	14	0.38
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	4	0.38
(3,2)	2:319:B:CYS:N	2:315:B:TYR:C	18	0.38
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	7	0.37
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	6	0.37
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	19	0.37
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	13	0.37
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	15	0.37
(10,88)	1:114:A:SER:N	1:110:A:LEU:C	17	0.36
(10,85)	1:113:A:GLU:H	1:109:A:ALA:C	17	0.36
(9,89)	1:115:A:VAL:H	1:111:A:CYS:O	7	0.36
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	6	0.36
(9,79)	1:110:A:LEU:H	1:106:A:PHE:O	2	0.36
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	20	0.36
(3,10)	2:315:B:TYR:N	2:311:B:ASP:C	20	0.36
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	4	0.36
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	15	0.36
(9,86)	1:113:A:GLU:N	1:109:A:ALA:O	7	0.35
(9,51)	1:85:A:GLN:H	1:81:A:GLN:O	2	0.35
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	1	0.35
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	2	0.34
(9,79)	1:110:A:LEU:H	1:106:A:PHE:O	4	0.34
(9,79)	1:110:A:LEU:H	1:106:A:PHE:O	14	0.34
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	18	0.34
(9,51)	1:85:A:GLN:H	1:81:A:GLN:O	4	0.34
(9,29)	1:51:A:ARG:H	1:47:A:LYS:O	20	0.34
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	12	0.33
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	5	0.33
(3,2)	2:319:B:CYS:N	2:315:B:TYR:C	1	0.33
(10,85)	1:113:A:GLU:H	1:109:A:ALA:C	7	0.32
(10,84)	1:112:A:VAL:N	1:108:A:GLY:C	17	0.32
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	16	0.32
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	4	0.32
(9,21)	1:19:A:GLN:H	1:15:A:TYR:O	14	0.32
(9,10)	1:13:A:LEU:N	1:9:A:VAL:O	14	0.32
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	19	0.32
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	1	0.32
(10,84)	1:112:A:VAL:N	1:108:A:GLY:C	6	0.31
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	4	0.31
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	3	0.31
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	7	0.31
(9,52)	1:85:A:GLN:N	1:81:A:GLN:O	16	0.31
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	3	0.31
(9,30)	1:51:A:ARG:N	1:47:A:LYS:O	4	0.31
(9,1)	1:8:A:LEU:H	1:4:A:SER:O	5	0.31
(9,1)	1:8:A:LEU:H	1:4:A:SER:O	10	0.31
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	19	0.31
(3,2)	2:319:B:CYS:N	2:315:B:TYR:C	11	0.31
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	7	0.31
(10,83)	1:112:A:VAL:H	1:108:A:GLY:C	14	0.3
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	16	0.3
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	13	0.3
(9,88)	1:114:A:SER:N	1:110:A:LEU:O	4	0.3
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	9	0.3
(7,2481)	2:315:B:TYR:HE2	1:64:A:ALA:HA	13	0.3
(6,8)	2:315:B:TYR:HE2	1:64:A:ALA:HA	13	0.3
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	8	0.3
(2,9)	2:315:B:TYR:H	2:311:B:ASP:O	10	0.3
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	16	0.29
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	16	0.29
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	7	0.29
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	8	0.29
(9,47)	1:82:A:SER:H	1:78:A:THR:O	7	0.29
(9,21)	1:19:A:GLN:H	1:15:A:TYR:O	16	0.29
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	6	0.29
(2,1)	2:319:B:CYS:H	2:315:B:TYR:O	9	0.29
(10,84)	1:112:A:VAL:N	1:108:A:GLY:C	7	0.28
(10,57)	1:90:A:LEU:H	1:86:A:VAL:C	10	0.28
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	9	0.28
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	18	0.28
(10,9)	1:13:A:LEU:H	1:9:A:VAL:C	14	0.28
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	11	0.28
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	5	0.28
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	19	0.28
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	10	0.28
(9,70)	1:105:A:SER:N	1:101:A:VAL:O	5	0.28
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	20	0.28
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	10	0.28
(9,58)	1:90:A:LEU:N	1:86:A:VAL:O	10	0.28
(9,51)	1:85:A:GLN:H	1:81:A:GLN:O	5	0.28
(9,51)	1:85:A:GLN:H	1:81:A:GLN:O	12	0.28
(9,48)	1:82:A:SER:N	1:78:A:THR:O	14	0.28
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	1	0.28
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	8	0.28
(9,10)	1:13:A:LEU:N	1:9:A:VAL:O	17	0.28
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	20	0.28
(9,4)	1:9:A:VAL:N	1:5:A:ASN:O	5	0.28
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	17	0.28
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	7	0.27
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	15	0.27
(9,128)	1:153:A:GLU:N	1:149:A:ASP:O	1	0.27
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	16	0.27
(9,51)	1:85:A:GLN:H	1:81:A:GLN:O	19	0.27
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	8	0.27
(3,10)	2:315:B:TYR:N	2:311:B:ASP:C	2	0.27
(3,10)	2:315:B:TYR:N	2:311:B:ASP:C	12	0.27
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	7	0.26
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	5	0.26
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	14	0.26
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	6	0.26
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	3	0.26
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	3	0.26
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	7	0.26
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	17	0.26
(9,3)	1:9:A:VAL:H	1:5:A:ASN:O	1	0.26
(7,1526)	1:87:A:VAL:HA	1:90:A:LEU:HG	13	0.26
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	15	0.26
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	7	0.26
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	5	0.25
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	9	0.25
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	15	0.25
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	19	0.25
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	12	0.25
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	19	0.25
(9,29)	1:51:A:ARG:H	1:47:A:LYS:O	15	0.25
(9,15)	1:16:A:LYS:H	1:12:A:PHE:O	7	0.25
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	12	0.25
(3,6)	2:317:B:LYS:N	2:313:B:GLU:C	5	0.25
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	12	0.25
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	8	0.24
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	20	0.24
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	20	0.24
(9,52)	1:85:A:GLN:N	1:81:A:GLN:O	2	0.24
(9,45)	1:61:A:TYR:H	1:57:A:PHE:O	18	0.24
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	11	0.24
(9,21)	1:19:A:GLN:H	1:15:A:TYR:O	17	0.24
(3,6)	2:317:B:LYS:N	2:313:B:GLU:C	11	0.24
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	3	0.24
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	12	0.24
(10,88)	1:114:A:SER:N	1:110:A:LEU:C	7	0.23
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	17	0.23
(9,79)	1:110:A:LEU:H	1:106:A:PHE:O	6	0.23
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	6	0.23
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	7	0.23
(10,86)	1:113:A:GLU:N	1:109:A:ALA:C	17	0.22
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	17	0.22
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	15	0.22
(10,9)	1:13:A:LEU:H	1:9:A:VAL:C	17	0.22
(9,128)	1:153:A:GLU:N	1:149:A:ASP:O	3	0.22
(9,124)	1:151:A:PHE:N	1:147:A:GLY:O	14	0.22
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	20	0.22
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	5	0.22
(9,90)	1:115:A:VAL:N	1:111:A:CYS:O	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,85)	1:113:A:GLU:H	1:109:A:ALA:O	4	0.22
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	19	0.22
(9,65)	1:101:A:VAL:H	1:97:A:TRP:O	13	0.22
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	20	0.22
(9,4)	1:9:A:VAL:N	1:5:A:ASN:O	9	0.22
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	5	0.22
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	5	0.22
(3,6)	2:317:B:LYS:N	2:313:B:GLU:C	17	0.22
(3,6)	2:317:B:LYS:N	2:313:B:GLU:C	18	0.22
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	19	0.21
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	12	0.21
(10,1)	1:8:A:LEU:H	1:4:A:SER:C	5	0.21
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	2	0.21
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	8	0.21
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	4	0.21
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	12	0.21
(9,52)	1:85:A:GLN:N	1:81:A:GLN:O	4	0.21
(9,40)	1:57:A:PHE:N	1:53:A:ALA:O	3	0.21
(9,21)	1:19:A:GLN:H	1:15:A:TYR:O	7	0.21
(9,8)	1:11:A:ASP:N	1:7:A:GLU:O	3	0.21
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	5	0.21
(7,2197)	1:99:A:ARG:H	1:99:A:ARG:HG2	6	0.21
(7,2197)	1:99:A:ARG:H	1:99:A:ARG:HG3	6	0.21
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	4	0.21
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	15	0.21
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	2	0.2
(10,3)	1:9:A:VAL:H	1:5:A:ASN:C	5	0.2
(9,124)	1:151:A:PHE:N	1:147:A:GLY:O	12	0.2
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	1	0.2
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	11	0.2
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	13	0.2
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	18	0.2
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	12	0.2
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	3	0.2
(9,22)	1:19:A:GLN:N	1:15:A:TYR:O	2	0.2
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	5	0.2
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	12	0.2
(9,2)	1:8:A:LEU:N	1:4:A:SER:O	5	0.2
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	6	0.2
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	6	0.2
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	17	0.2
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	2:317:B:LYS:N	2:313:B:GLU:C	10	0.2
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	9	0.2
(10,86)	1:113:A:GLU:N	1:109:A:ALA:C	7	0.19
(10,84)	1:112:A:VAL:N	1:108:A:GLY:C	14	0.19
(10,81)	1:111:A:CYS:H	1:107:A:GLY:C	9	0.19
(10,10)	1:13:A:LEU:N	1:9:A:VAL:C	14	0.19
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	2	0.19
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	3	0.19
(9,77)	1:109:A:ALA:H	1:105:A:SER:O	17	0.19
(9,10)	1:13:A:LEU:N	1:9:A:VAL:O	19	0.19
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	7	0.19
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	7	0.19
(7,1526)	1:87:A:VAL:HA	1:90:A:LEU:HG	14	0.19
(7,111)	1:31:A:GLU:HA	1:32:A:GLU:H	20	0.19
(3,9)	2:315:B:TYR:H	2:311:B:ASP:C	10	0.19
(3,1)	2:319:B:CYS:H	2:315:B:TYR:C	20	0.19
(10,89)	1:115:A:VAL:H	1:111:A:CYS:C	7	0.18
(10,87)	1:114:A:SER:H	1:110:A:LEU:C	4	0.18
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	5	0.18
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	8	0.18
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	13	0.18
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	7	0.18
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	9	0.18
(9,82)	1:111:A:CYS:N	1:107:A:GLY:O	5	0.18
(9,52)	1:85:A:GLN:N	1:81:A:GLN:O	5	0.18
(9,52)	1:85:A:GLN:N	1:81:A:GLN:O	12	0.18
(9,15)	1:16:A:LYS:H	1:12:A:PHE:O	10	0.18
(9,15)	1:16:A:LYS:H	1:12:A:PHE:O	15	0.18
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	18	0.18
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	15	0.18
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	16	0.18
(9,2)	1:8:A:LEU:N	1:4:A:SER:O	10	0.18
(7,1526)	1:87:A:VAL:HA	1:90:A:LEU:HG	6	0.18
(10,79)	1:110:A:LEU:H	1:106:A:PHE:C	14	0.17
(10,77)	1:109:A:ALA:H	1:105:A:SER:C	14	0.17
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	4	0.17
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	4	0.17
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	18	0.17
(9,63)	1:100:A:ILE:H	1:96:A:ASN:O	13	0.17
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	3	0.17
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	14	0.17
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	20	0.17
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	20	0.17
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	20	0.17
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	4	0.17
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	4	0.17
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	14	0.17
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	14	0.17
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	18	0.17
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	18	0.17
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	20	0.17
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	20	0.17
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	20	0.17
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	20	0.17
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	9	0.16
(10,39)	1:57:A:PHE:H	1:53:A:ALA:C	8	0.16
(10,21)	1:19:A:GLN:H	1:15:A:TYR:C	2	0.16
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	10	0.16
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	16	0.16
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	17	0.16
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	20	0.16
(9,84)	1:112:A:VAL:N	1:108:A:GLY:O	4	0.16
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	8	0.16
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	15	0.16
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	16	0.16
(9,48)	1:82:A:SER:N	1:78:A:THR:O	7	0.16
(9,39)	1:57:A:PHE:H	1:53:A:ALA:O	10	0.16
(9,8)	1:11:A:ASP:N	1:7:A:GLU:O	1	0.16
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	13	0.16
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	18	0.16
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	18	0.16
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	18	0.16
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	18	0.16
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	18	0.16
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	18	0.16
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	18	0.16
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	18	0.16
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	18	0.16
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	18	0.16
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	18	0.16
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	18	0.16
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	13	0.16
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB2	17	0.16
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB3	17	0.16
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	6	0.16
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	6	0.16
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	13	0.16
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	13	0.16
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG2	11	0.16
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG3	11	0.16
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	18	0.16
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	18	0.16
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	18	0.16
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	18	0.16
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	18	0.16
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	18	0.16
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	18	0.16
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	18	0.16
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	18	0.16
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	18	0.16
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	18	0.16
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	18	0.16
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	13	0.16
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	13	0.16
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB2	17	0.16
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB3	17	0.16
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	6	0.16
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	6	0.16
(3,5)	2:317:B:LYS:H	2:313:B:GLU:C	16	0.16
(3,2)	2:319:B:CYS:N	2:315:B:TYR:C	17	0.16
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	19	0.16
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	15	0.16
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	2	0.16
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	16	0.15
(10,69)	1:105:A:SER:H	1:101:A:VAL:C	5	0.15
(10,59)	1:92:A:ARG:H	1:88:A:ASN:C	3	0.15
(10,47)	1:82:A:SER:H	1:78:A:THR:C	14	0.15
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	15	0.15
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	18	0.15
(9,127)	1:153:A:GLU:H	1:149:A:ASP:O	19	0.15
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	6	0.15
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	10	0.15
(9,63)	1:100:A:ILE:H	1:96:A:ASN:O	12	0.15
(9,52)	1:85:A:GLN:N	1:81:A:GLN:O	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,21)	1:19:A:GLN:H	1:15:A:TYR:O	6	0.15
(9,7)	1:11:A:ASP:H	1:7:A:GLU:O	10	0.15
(7,2433)	2:323:B:ASP:HA	2:324:B:TRP:H	18	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	3	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	3	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	10	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	10	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	15	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	15	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	19	0.15
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	19	0.15
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB2	8	0.15
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB3	8	0.15
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB2	8	0.15
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB3	8	0.15
(5,18)	2:323:B:ASP:HA	2:324:B:TRP:H	18	0.15
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	8	0.15
(10,60)	1:92:A:ARG:N	1:88:A:ASN:C	6	0.14
(10,51)	1:85:A:GLN:H	1:81:A:GLN:C	16	0.14
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	5	0.14
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	14	0.14
(10,40)	1:57:A:PHE:N	1:53:A:ALA:C	20	0.14
(10,9)	1:13:A:LEU:H	1:9:A:VAL:C	19	0.14
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	1	0.14
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	19	0.14
(9,79)	1:110:A:LEU:H	1:106:A:PHE:O	16	0.14
(9,71)	1:106:A:PHE:H	1:102:A:ALA:O	5	0.14
(9,70)	1:105:A:SER:N	1:101:A:VAL:O	9	0.14
(9,70)	1:105:A:SER:N	1:101:A:VAL:O	19	0.14
(9,30)	1:51:A:ARG:N	1:47:A:LYS:O	20	0.14
(9,15)	1:16:A:LYS:H	1:12:A:PHE:O	6	0.14
(9,10)	1:13:A:LEU:N	1:9:A:VAL:O	12	0.14
(9,3)	1:9:A:VAL:H	1:5:A:ASN:O	16	0.14
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	19	0.14
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	19	0.14
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	19	0.14
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	19	0.14
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	19	0.14
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	19	0.14
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	19	0.14
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	19	0.14
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	19	0.14
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	19	0.14
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	19	0.14
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	20	0.14
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	20	0.14
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	20	0.14
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	20	0.14
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	20	0.14
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	20	0.14
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	20	0.14
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	20	0.14
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	20	0.14
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	20	0.14
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	20	0.14
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	20	0.14
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB2	12	0.14
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB3	12	0.14
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	7	0.14
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	7	0.14
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	8	0.14
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	8	0.14
(7,2446)	2:324:B:TRP:HA	2:324:B:TRP:HE3	18	0.14
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	1	0.14
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	1	0.14
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	8	0.14
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	8	0.14
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	16	0.14
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	16	0.14
(7,303)	1:30:A:VAL:H	1:30:A:VAL:HB	3	0.14
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG2	8	0.14
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG3	8	0.14
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	19	0.14
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	19	0.14
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	19	0.14
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	19	0.14
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	19	0.14
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	19	0.14
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	19	0.14
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	19	0.14
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	19	0.14
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	19	0.14
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	19	0.14
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	20	0.14
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	20	0.14
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	20	0.14
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	20	0.14
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	20	0.14
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	20	0.14
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	20	0.14
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	20	0.14
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	20	0.14
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	20	0.14
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	20	0.14
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	20	0.14
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB2	12	0.14
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB3	12	0.14
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	7	0.14
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	7	0.14
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	8	0.14
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	8	0.14
(5,30)	2:324:B:TRP:HA	2:324:B:TRP:HE3	18	0.14
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	6	0.14
(3,10)	2:315:B:TYR:N	2:311:B:ASP:C	7	0.14
(10,123)	1:151:A:PHE:H	1:147:A:GLY:C	14	0.13
(10,79)	1:110:A:LEU:H	1:106:A:PHE:C	2	0.13
(10,60)	1:92:A:ARG:N	1:88:A:ASN:C	12	0.13
(9,129)	1:154:A:LEU:H	1:150:A:THR:O	3	0.13
(9,128)	1:153:A:GLU:N	1:149:A:ASP:O	13	0.13
(9,105)	1:133:A:TYR:H	1:129:A:TRP:O	12	0.13
(9,95)	1:128:A:ALA:H	1:124:A:SER:O	1	0.13
(9,83)	1:112:A:VAL:H	1:108:A:GLY:O	16	0.13
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	13	0.13
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	20	0.13
(9,60)	1:92:A:ARG:N	1:88:A:ASN:O	3	0.13
(9,9)	1:13:A:LEU:H	1:9:A:VAL:O	1	0.13
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	16	0.13
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	16	0.13
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB2	15	0.13
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB3	15	0.13
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	12	0.13
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	12	0.13
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	19	0.13
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,2446)	2:324:B:TRP:HA	2:324:B:TRP:HE3	5	0.13
(7,1881)	1:13:A:LEU:HD11	1:14:A:SER:HA	2	0.13
(7,1881)	1:13:A:LEU:HD12	1:14:A:SER:HA	2	0.13
(7,1881)	1:13:A:LEU:HD13	1:14:A:SER:HA	2	0.13
(7,1881)	1:13:A:LEU:HD21	1:14:A:SER:HA	2	0.13
(7,1881)	1:13:A:LEU:HD22	1:14:A:SER:HA	2	0.13
(7,1881)	1:13:A:LEU:HD23	1:14:A:SER:HA	2	0.13
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG2	3	0.13
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG3	3	0.13
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG2	15	0.13
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG3	15	0.13
(7,17)	1:31:A:GLU:H	1:31:A:GLU:HB2	10	0.13
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	16	0.13
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	16	0.13
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB2	15	0.13
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB3	15	0.13
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	12	0.13
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	12	0.13
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	19	0.13
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	19	0.13
(5,30)	2:324:B:TRP:HA	2:324:B:TRP:HE3	5	0.13
(3,6)	2:317:B:LYS:N	2:313:B:GLU:C	4	0.13
(2,10)	2:315:B:TYR:N	2:311:B:ASP:O	10	0.13
(2,2)	2:319:B:CYS:N	2:315:B:TYR:O	15	0.13
(10,83)	1:112:A:VAL:H	1:108:A:GLY:C	4	0.12
(10,79)	1:110:A:LEU:H	1:106:A:PHE:C	4	0.12
(10,58)	1:90:A:LEU:N	1:86:A:VAL:C	10	0.12
(10,10)	1:13:A:LEU:N	1:9:A:VAL:C	17	0.12
(10,9)	1:13:A:LEU:H	1:9:A:VAL:C	12	0.12
(10,1)	1:8:A:LEU:H	1:4:A:SER:C	10	0.12
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	7	0.12
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	11	0.12
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	12	0.12
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	16	0.12
(9,89)	1:115:A:VAL:H	1:111:A:CYS:O	12	0.12
(9,81)	1:111:A:CYS:H	1:107:A:GLY:O	12	0.12
(9,80)	1:110:A:LEU:N	1:106:A:PHE:O	4	0.12
(9,79)	1:110:A:LEU:H	1:106:A:PHE:O	5	0.12
(9,70)	1:105:A:SER:N	1:101:A:VAL:O	3	0.12
(9,70)	1:105:A:SER:N	1:101:A:VAL:O	7	0.12
(9,69)	1:105:A:SER:H	1:101:A:VAL:O	1	0.12
(9,25)	1:49:A:ALA:H	1:45:A:ALA:O	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,25)	1:49:A:ALA:H	1:45:A:ALA:O	17	0.12
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	11	0.12
(7,2476)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	11	0.12
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	11	0.12
(7,2476)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	11	0.12
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	11	0.12
(7,2476)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	11	0.12
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	11	0.12
(7,2476)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	11	0.12
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	11	0.12
(7,2476)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	11	0.12
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	11	0.12
(7,2476)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	11	0.12
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	2	0.12
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	2	0.12
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	9	0.12
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	9	0.12
(7,2433)	2:323:B:ASP:HA	2:324:B:TRP:H	5	0.12
(7,2433)	2:323:B:ASP:HA	2:324:B:TRP:H	20	0.12
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	11	0.12
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	11	0.12
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB2	16	0.12
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB3	16	0.12
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB2	16	0.12
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB3	16	0.12
(7,17)	1:31:A:GLU:H	1:31:A:GLU:HB2	16	0.12
(7,17)	1:31:A:GLU:H	1:31:A:GLU:HB2	17	0.12
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE1	11	0.12
(6,3)	2:320:B:VAL:HG11	1:61:A:TYR:HE2	11	0.12
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE1	11	0.12
(6,3)	2:320:B:VAL:HG12	1:61:A:TYR:HE2	11	0.12
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE1	11	0.12
(6,3)	2:320:B:VAL:HG13	1:61:A:TYR:HE2	11	0.12
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE1	11	0.12
(6,3)	2:320:B:VAL:HG21	1:61:A:TYR:HE2	11	0.12
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE1	11	0.12
(6,3)	2:320:B:VAL:HG22	1:61:A:TYR:HE2	11	0.12
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE1	11	0.12
(6,3)	2:320:B:VAL:HG23	1:61:A:TYR:HE2	11	0.12
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	2	0.12
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	2	0.12
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	9	0.12
(5,18)	2:323:B:ASP:HA	2:324:B:TRP:H	5	0.12
(5,18)	2:323:B:ASP:HA	2:324:B:TRP:H	20	0.12
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	18	0.12
(3,6)	2:317:B:LYS:N	2:313:B:GLU:C	8	0.12
(10,123)	1:151:A:PHE:H	1:147:A:GLY:C	12	0.11
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	7	0.11
(10,82)	1:111:A:CYS:N	1:107:A:GLY:C	8	0.11
(10,60)	1:92:A:ARG:N	1:88:A:ASN:C	14	0.11
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	17	0.11
(9,93)	1:127:A:ALA:H	1:123:A:VAL:O	2	0.11
(9,87)	1:114:A:SER:H	1:110:A:LEU:O	18	0.11
(9,80)	1:110:A:LEU:N	1:106:A:PHE:O	2	0.11
(9,80)	1:110:A:LEU:N	1:106:A:PHE:O	14	0.11
(9,63)	1:100:A:ILE:H	1:96:A:ASN:O	5	0.11
(9,43)	1:59:A:LEU:H	1:55:A:ASP:O	18	0.11
(9,31)	1:53:A:ALA:H	1:49:A:ALA:O	7	0.11
(9,30)	1:51:A:ARG:N	1:47:A:LYS:O	15	0.11
(9,22)	1:19:A:GLN:N	1:15:A:TYR:O	14	0.11
(7,2474)	2:324:B:TRP:HH2	1:90:A:LEU:HD11	13	0.11
(7,2474)	2:324:B:TRP:HH2	1:90:A:LEU:HD12	13	0.11
(7,2474)	2:324:B:TRP:HH2	1:90:A:LEU:HD13	13	0.11
(7,2474)	2:324:B:TRP:HH2	1:90:A:LEU:HD21	13	0.11
(7,2474)	2:324:B:TRP:HH2	1:90:A:LEU:HD22	13	0.11
(7,2474)	2:324:B:TRP:HH2	1:90:A:LEU:HD23	13	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	1	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	1	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	8	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	8	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	14	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	14	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	19	0.11
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	19	0.11
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB2	9	0.11
(7,2471)	2:324:B:TRP:H	2:324:B:TRP:HB3	9	0.11
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG2	14	0.11
(7,2462)	2:313:B:GLU:H	2:313:B:GLU:HG3	14	0.11
(7,2432)	2:322:B:LYS:HA	2:324:B:TRP:H	19	0.11
(7,2292)	1:120:A:GLN:HG2	1:121:A:VAL:H	14	0.11
(7,2292)	1:120:A:GLN:HG3	1:121:A:VAL:H	14	0.11
(7,2292)	1:120:A:GLN:HG2	1:121:A:VAL:H	17	0.11
(7,2292)	1:120:A:GLN:HG3	1:121:A:VAL:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,1881)	1:13:A:LEU:HD11	1:14:A:SER:HA	18	0.11
(7,1881)	1:13:A:LEU:HD12	1:14:A:SER:HA	18	0.11
(7,1881)	1:13:A:LEU:HD13	1:14:A:SER:HA	18	0.11
(7,1881)	1:13:A:LEU:HD21	1:14:A:SER:HA	18	0.11
(7,1881)	1:13:A:LEU:HD22	1:14:A:SER:HA	18	0.11
(7,1881)	1:13:A:LEU:HD23	1:14:A:SER:HA	18	0.11
(7,1766)	2:313:B:GLU:HG2	2:314:B:ALA:H	1	0.11
(7,1766)	2:313:B:GLU:HG3	2:314:B:ALA:H	1	0.11
(7,1766)	2:313:B:GLU:HG2	2:314:B:ALA:H	15	0.11
(7,1766)	2:313:B:GLU:HG3	2:314:B:ALA:H	15	0.11
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD1	20	0.11
(7,1690)	2:312:B:LEU:HG	2:316:B:PHE:HD2	20	0.11
(7,1379)	1:52:A:GLU:HB2	1:53:A:ALA:HB1	15	0.11
(7,1379)	1:52:A:GLU:HB2	1:53:A:ALA:HB2	15	0.11
(7,1379)	1:52:A:GLU:HB2	1:53:A:ALA:HB3	15	0.11
(7,1379)	1:52:A:GLU:HB3	1:53:A:ALA:HB1	15	0.11
(7,1379)	1:52:A:GLU:HB3	1:53:A:ALA:HB2	15	0.11
(7,1379)	1:52:A:GLU:HB3	1:53:A:ALA:HB3	15	0.11
(7,1097)	1:38:A:PRO:HA	1:47:A:LYS:HD2	16	0.11
(7,1097)	1:38:A:PRO:HA	1:47:A:LYS:HD3	16	0.11
(7,1045)	1:133:A:TYR:HD1	1:134:A:LEU:HG	1	0.11
(7,1045)	1:133:A:TYR:HD2	1:134:A:LEU:HG	1	0.11
(7,1045)	1:133:A:TYR:HD1	1:134:A:LEU:HG	18	0.11
(7,1045)	1:133:A:TYR:HD2	1:134:A:LEU:HG	18	0.11
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB2	19	0.11
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB3	19	0.11
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB2	19	0.11
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB3	19	0.11
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB2	20	0.11
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB3	20	0.11
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB2	20	0.11
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB3	20	0.11
(7,283)	1:115:A:VAL:HB	1:119:A:MET:H	13	0.11
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG2	6	0.11
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG3	6	0.11
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG2	12	0.11
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG3	12	0.11
(7,17)	1:31:A:GLU:H	1:31:A:GLU:HB2	6	0.11
(6,1)	2:324:B:TRP:HH2	1:90:A:LEU:HD11	13	0.11
(6,1)	2:324:B:TRP:HH2	1:90:A:LEU:HD12	13	0.11
(6,1)	2:324:B:TRP:HH2	1:90:A:LEU:HD13	13	0.11
(6,1)	2:324:B:TRP:HH2	1:90:A:LEU:HD21	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,1)	2:324:B:TRP:HH2	1:90:A:LEU:HD22	13	0.11
(6,1)	2:324:B:TRP:HH2	1:90:A:LEU:HD23	13	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	1	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	1	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	8	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	8	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	14	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	14	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	19	0.11
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	19	0.11
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB2	9	0.11
(5,54)	2:324:B:TRP:H	2:324:B:TRP:HB3	9	0.11
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG2	14	0.11
(5,45)	2:313:B:GLU:H	2:313:B:GLU:HG3	14	0.11
(5,17)	2:322:B:LYS:HA	2:324:B:TRP:H	19	0.11
(10,51)	1:85:A:GLN:H	1:81:A:GLN:C	2	0.1
(9,115)	1:138:A:LEU:H	1:134:A:LEU:O	8	0.1
(9,94)	1:127:A:ALA:N	1:123:A:VAL:O	5	0.1
(9,86)	1:113:A:GLU:N	1:109:A:ALA:O	4	0.1
(9,57)	1:90:A:LEU:H	1:86:A:VAL:O	20	0.1
(9,43)	1:59:A:LEU:H	1:55:A:ASP:O	1	0.1
(9,10)	1:13:A:LEU:N	1:9:A:VAL:O	5	0.1
(9,10)	1:13:A:LEU:N	1:9:A:VAL:O	20	0.1
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB2	15	0.1
(7,2473)	2:315:B:TYR:H	2:318:B:ASP:HB3	15	0.1
(7,2316)	1:125:A:ARG:H	1:125:A:ARG:HG2	10	0.1
(7,2316)	1:125:A:ARG:H	1:125:A:ARG:HG3	10	0.1
(7,2292)	1:120:A:GLN:HG2	1:121:A:VAL:H	10	0.1
(7,2292)	1:120:A:GLN:HG3	1:121:A:VAL:H	10	0.1
(7,1881)	1:13:A:LEU:HD11	1:14:A:SER:HA	6	0.1
(7,1881)	1:13:A:LEU:HD12	1:14:A:SER:HA	6	0.1
(7,1881)	1:13:A:LEU:HD13	1:14:A:SER:HA	6	0.1
(7,1881)	1:13:A:LEU:HD21	1:14:A:SER:HA	6	0.1
(7,1881)	1:13:A:LEU:HD22	1:14:A:SER:HA	6	0.1
(7,1881)	1:13:A:LEU:HD23	1:14:A:SER:HA	6	0.1
(7,1767)	2:314:B:ALA:HA	2:317:B:LYS:HG2	9	0.1
(7,1767)	2:314:B:ALA:HA	2:317:B:LYS:HG3	9	0.1
(7,1766)	2:313:B:GLU:HG2	2:314:B:ALA:H	2	0.1
(7,1766)	2:313:B:GLU:HG3	2:314:B:ALA:H	2	0.1
(7,1766)	2:313:B:GLU:HG2	2:314:B:ALA:H	3	0.1
(7,1766)	2:313:B:GLU:HG3	2:314:B:ALA:H	3	0.1
(7,1141)	1:90:A:LEU:HG	1:91:A:PHE:HA	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,1045)	1:133:A:TYR:HD1	1:134:A:LEU:HG	4	0.1
(7,1045)	1:133:A:TYR:HD2	1:134:A:LEU:HG	4	0.1
(7,1045)	1:133:A:TYR:HD1	1:134:A:LEU:HG	16	0.1
(7,1045)	1:133:A:TYR:HD2	1:134:A:LEU:HG	16	0.1
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB2	3	0.1
(7,980)	2:313:B:GLU:HB2	2:317:B:LYS:HB3	3	0.1
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB2	3	0.1
(7,980)	2:313:B:GLU:HB3	2:317:B:LYS:HB3	3	0.1
(7,283)	1:115:A:VAL:HB	1:119:A:MET:H	2	0.1
(7,283)	1:115:A:VAL:HB	1:119:A:MET:H	15	0.1
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG2	14	0.1
(7,272)	1:113:A:GLU:H	1:113:A:GLU:HG3	14	0.1
(7,111)	1:31:A:GLU:HA	1:32:A:GLU:H	7	0.1
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB2	15	0.1
(5,56)	2:315:B:TYR:H	2:318:B:ASP:HB3	15	0.1

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

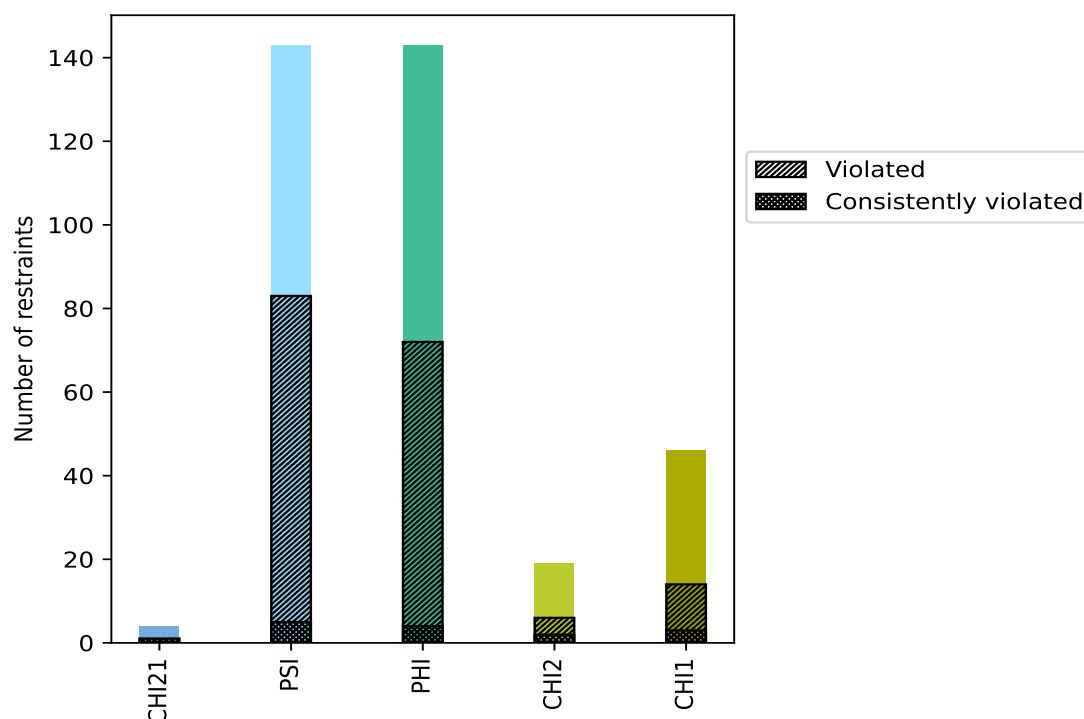
10.1 Summary of dihedral-angle violations [i](#)

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
CHI21	4	1.1	1	25.0	0.3	1	25.0	0.3
PSI	143	40.3	83	58.0	23.4	5	3.5	1.4
PHI	143	40.3	72	50.3	20.3	4	2.8	1.1
CHI2	19	5.4	6	31.6	1.7	2	10.5	0.6
CHI1	46	13.0	14	30.4	3.9	3	6.5	0.8
Total	355	100.0	176	49.6	49.6	15	4.2	4.2

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](#)



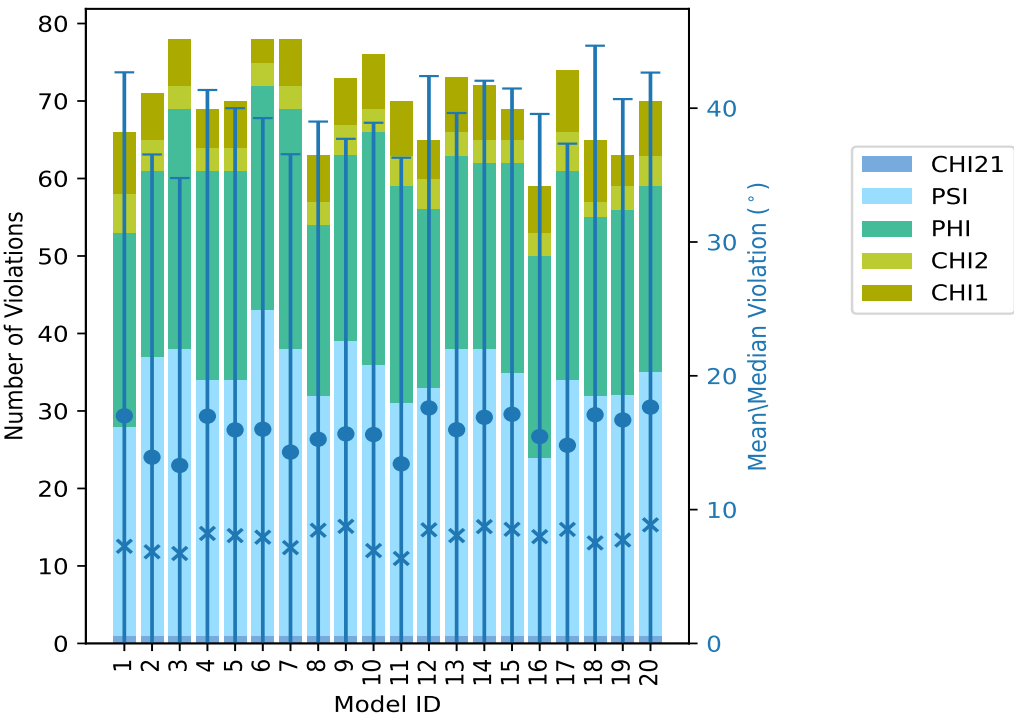
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	CHI21	PSI	PHI	CHI2	CHI1	Total				
1	1	27	25	5	8	66	17.01	130.26	25.67	7.26
2	1	36	24	4	6	71	13.92	128.17	22.62	6.85
3	1	37	31	3	6	78	13.3	133.61	21.48	6.72
4	1	33	27	3	5	69	16.98	132.83	24.38	8.22
5	1	33	27	3	6	70	15.96	129.29	24.04	8.06
6	1	42	29	3	3	78	16.01	131.63	23.25	7.94
7	1	37	31	3	6	78	14.3	131.61	22.26	7.16
8	1	31	22	3	6	63	15.26	132.37	23.74	8.46
9	1	38	24	4	6	73	15.66	130.82	22.05	8.75
10	1	35	30	3	7	76	15.61	135.02	23.3	6.94
11	1	30	28	4	7	70	13.42	131.51	22.88	6.35
12	1	32	23	4	5	65	17.6	135.21	24.8	8.49
13	1	37	25	3	7	73	15.97	129.58	23.67	8.06
14	1	37	24	3	7	72	16.9	133.52	25.15	8.73
15	1	34	27	3	4	69	17.13	131.47	24.34	8.53
16	1	23	26	3	6	59	15.46	129.75	24.11	7.98
17	1	33	27	5	8	74	14.81	131.06	22.54	8.52
18	1	31	23	2	8	65	17.09	129.51	27.58	7.51
19	1	31	24	3	4	63	16.7	131.13	23.98	7.73
20	1	34	24	4	7	70	17.66	127.23	25.0	8.86

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	
CHI21	PSI	PHI	CHI2	CHI1	Total	Count ¹	%
0	11	13	1	2	27	1	5.0
0	10	12	0	3	25	2	10.0
0	7	2	1	1	11	3	15.0
0	9	7	0	1	17	4	20.0
0	8	1	0	1	10	5	25.0
0	2	4	0	0	6	6	30.0
0	0	6	1	0	7	7	35.0
0	2	2	0	0	4	8	40.0
0	2	2	0	0	4	9	45.0
0	3	1	0	0	4	10	50.0
0	1	2	0	0	3	11	55.0

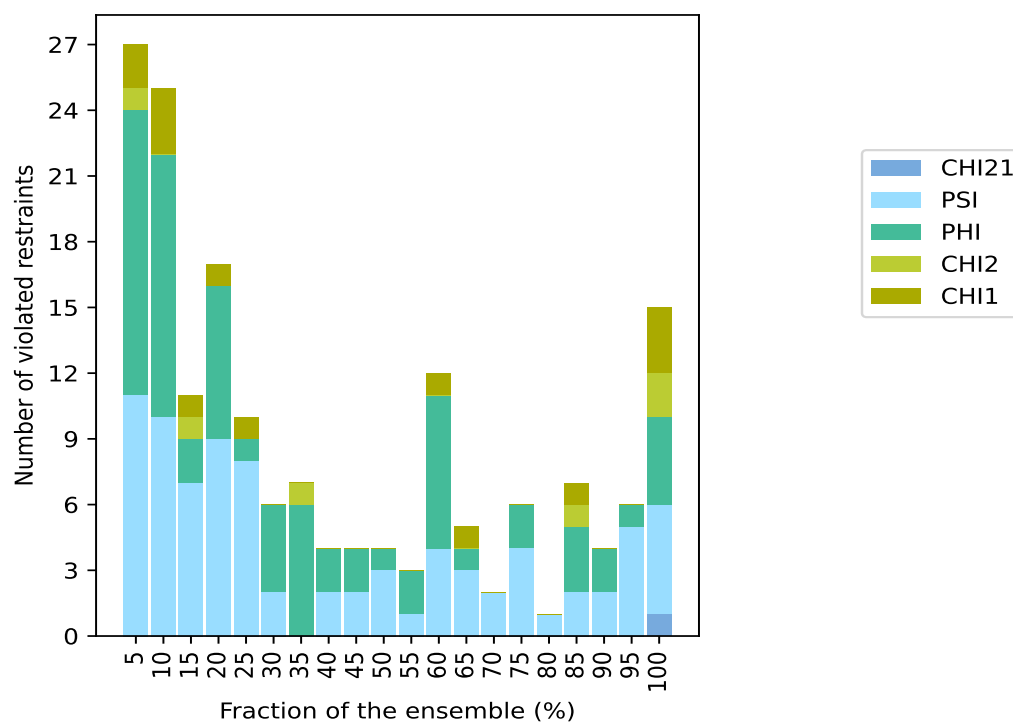
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Number of violated restraints						Fraction of the ensemble	
CHI21	PSI	PHI	CHI2	CHI1	Total	Count ¹	%
0	4	7	0	1	12	12	60.0
0	3	1	0	1	5	13	65.0
0	2	0	0	0	2	14	70.0
0	4	2	0	0	6	15	75.0
0	1	0	0	0	1	16	80.0
0	2	3	1	1	7	17	85.0
0	2	2	0	0	4	18	90.0
0	5	1	0	0	6	19	95.0
1	5	4	2	3	15	20	100.0

¹ Number of models with violations

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

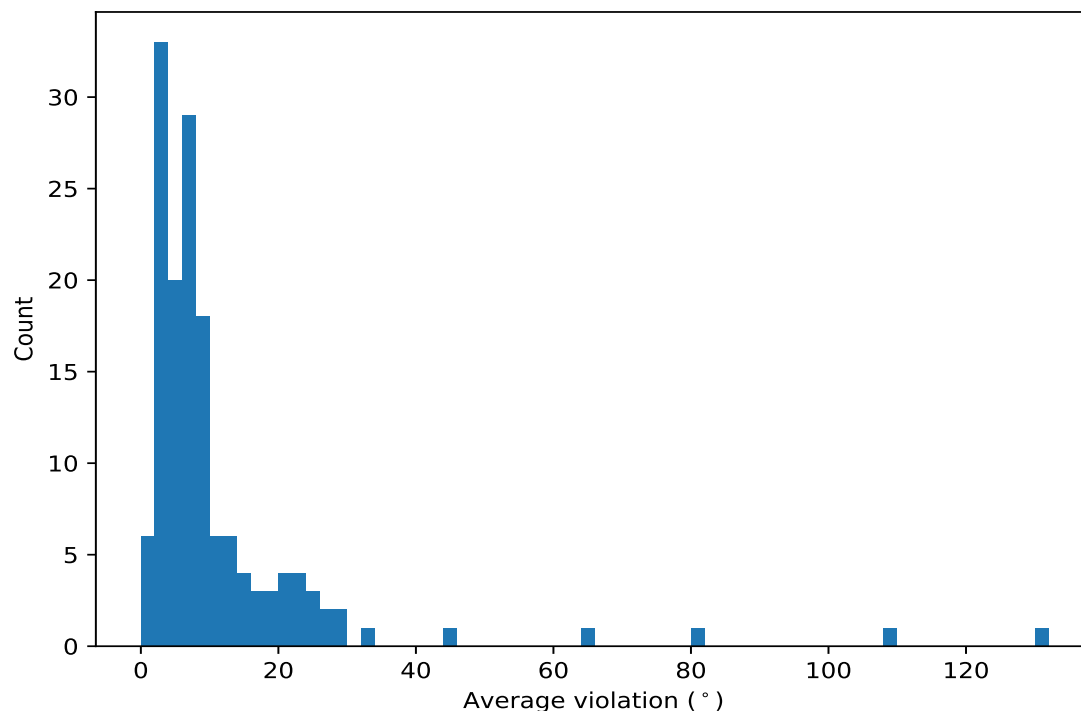


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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 ⓘ

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	Med
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	20	131.28	2.04	131.28
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	20	108.9	5.65	108.9
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	20	64.1	4.32	65.1
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	20	45.39	3.36	44.9
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	20	33.1	36.67	10.6
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	20	22.44	9.77	20.1
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	20	18.76	23.74	8.9
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	20	14.94	5.24	15.3
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	20	14.25	2.15	14.3
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	20	12.22	3.53	13.4
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	20	12.0	6.57	10.2
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	20	11.72	2.99	11.4
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	20	9.4	3.86	8.1
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	20	8.67	2.42	9.5
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	20	5.7	1.56	5.9
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	19	28.87	31.15	9.3
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	19	20.66	9.12	19.6
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	19	12.8	1.06	12.7
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	19	8.86	2.31	8.9
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	19	7.93	2.87	7.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Med
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	19	3.54	1.21	3.3
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	18	24.84	8.79	23.
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	18	22.81	15.22	22.6
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	18	9.05	2.96	8.6
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	18	4.41	1.12	4.4
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	17	80.41	4.71	81.0
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	17	24.81	9.49	29.6
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	17	17.84	10.32	17.5
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	17	17.02	11.37	16.
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	17	16.83	9.8	18.
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	17	7.31	2.76	8.0
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	17	6.05	4.82	5.1
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	16	8.73	6.9	7.5
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	15	13.76	14.61	5.9
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	15	10.55	4.36	9.9
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	15	9.21	5.26	10.3
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	15	8.08	3.94	8.0
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	15	7.83	4.93	6.5
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	15	5.96	1.21	5.8
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	14	11.79	9.01	9.7
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	14	6.57	3.79	6.0
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	13	8.27	5.28	7.7
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	13	7.89	3.42	7.7
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	13	7.53	4.32	6.4
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	13	6.01	4.59	5.0
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	13	5.16	3.39	3.5
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	12	18.68	13.58	15.0
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	12	10.32	6.59	8.6
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	12	9.84	6.68	7.8
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	12	9.49	3.91	8.8
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	12	8.75	6.09	6.0
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	12	7.54	3.58	8.2
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	12	7.54	4.31	7.2
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	12	7.32	4.64	6.2
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	12	6.37	3.18	7.2
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	12	5.44	1.88	5.9
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	12	4.72	2.95	3.8
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	12	3.73	1.31	3.7
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	11	6.92	5.85	4.3
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	11	6.22	4.17	6.0
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	11	2.71	1.18	2.7
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	10	20.94	16.55	16.9
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	10	6.17	1.87	6.0
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	10	5.66	4.34	4.5
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	10	3.25	1.13	3.2
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	9	10.15	6.33	9.6
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	9	8.63	6.1	5.9
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	9	5.84	3.88	4.1
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	9	3.45	1.89	3.0
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	8	23.66	15.25	24.4
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	8	7.62	4.84	7.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Med
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	8	5.26	2.3	5.4
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	8	2.8	1.31	2.3
(2,65)	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2:312:B:LEU:CD1	7	21.33	17.81	13.1
(1,51)	1:41:A:THR:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	7	18.05	22.15	5.9
(1,281)	2:317:B:LYS:C	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	7	6.09	7.13	4.1
(1,257)	1:153:A:GLU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	7	5.71	4.14	4.9
(1,57)	1:44:A:GLU:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	7	4.7	2.64	3.8
(1,143)	1:90:A:LEU:C	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:C	7	3.67	0.98	3.5
(1,11)	1:7:A:GLU:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	7	3.59	1.77	3.3
(1,97)	1:65:A:PHE:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	6	25.58	26.21	13.0
(1,117)	1:77:A:GLY:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	6	22.88	18.92	12.6
(1,284)	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	2:320:B:VAL:N	6	14.13	13.47	5.6
(1,1)	1:2:A:SER:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	6	10.2	7.91	7.6
(1,53)	1:42:A:GLU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	6	8.15	3.94	7.9
(1,118)	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1:79:A:ALA:N	6	4.7	2.77	4.1
(2,68)	2:324:B:TRP:N	2:324:B:TRP:CA	2:324:B:TRP:CB	2:324:B:TRP:CG	5	29.12	28.43	26.1
(1,98)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	1:67:A:ASP:N	5	15.07	11.74	12.3
(1,282)	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	2:319:B:CYS:N	5	7.29	2.92	5.5
(1,6)	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	1:6:A:ARG:N	5	6.32	2.93	7.5
(1,88)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:TYR:N	5	4.83	3.99	4.3
(1,256)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:LEU:N	5	3.95	0.77	4.2
(1,258)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:TYR:N	5	3.54	2.51	2.0
(1,116)	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1:76:A:PRO:N	5	3.25	1.95	2.5
(1,64)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	5	2.25	0.54	2.1
(1,217)	1:129:A:TRP:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	5	1.85	0.83	1.4
(1,123)	1:80:A:TYR:C	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	4	12.74	11.01	7.3
(1,196)	1:118:A:GLU:N	1:118:A:GLU:CA	1:118:A:GLU:C	1:119:A:MET:N	4	8.97	2.58	7.6
(1,5)	1:4:A:SER:C	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	4	8.47	2.31	7.4
(1,278)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:C	2:317:B:LYS:N	4	7.38	4.4	7.0
(1,122)	1:80:A:TYR:N	1:80:A:TYR:CA	1:80:A:TYR:C	1:81:A:GLN:N	4	7.04	8.2	2.9
(1,7)	1:5:A:ASN:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	4	6.36	3.92	6.1
(1,156)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	4	5.91	4.57	5.0
(1,101)	1:67:A:ASP:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	4	5.7	3.98	4.7
(1,136)	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	1:88:A:ASN:N	4	4.75	1.96	4.8
(2,42)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	4	4.24	2.09	4.3
(1,124)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:SER:N	4	3.36	1.32	3.2
(1,263)	2:308:B:SER:C	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	4	3.1	2.07	2.3
(1,181)	1:110:A:LEU:C	1:111:A:CYS:N	1:111:A:CYS:CA	1:111:A:CYS:C	4	2.68	0.39	2.5
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:LEU:N	4	2.64	1.06	2.6
(1,194)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:GLU:N	4	2.56	1.44	1.9
(1,37)	1:20:A:LYS:C	1:21:A:GLY:N	1:21:A:GLY:CA	1:21:A:GLY:C	4	2.44	0.99	2.3
(1,216)	1:129:A:TRP:N	1:129:A:TRP:CA	1:129:A:TRP:C	1:130:A:MET:N	4	1.9	0.57	1.8
(1,96)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:SER:N	3	27.08	21.68	20.1
(2,43)	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	1:65:A:PHE:CD1	3	21.03	9.61	21.6
(1,109)	1:71:A:GLN:C	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	3	8.31	4.78	10.4
(1,110)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:HIS:N	3	7.2	5.69	4.9
(1,48)	1:26:A:GLN:N	1:26:A:GLN:CA	1:26:A:GLN:C	1:27:A:PHE:N	3	6.51	2.96	7.1
(1,259)	1:154:A:LEU:C	1:155:A:TYR:N	1:155:A:TYR:CA	1:155:A:TYR:C	3	6.47	3.57	6.9
(1,142)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:PHE:N	3	6.42	2.76	8.2
(1,102)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:THR:N	3	5.23	3.11	4.4
(1,44)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:SER:N	3	2.56	1.63	1.4

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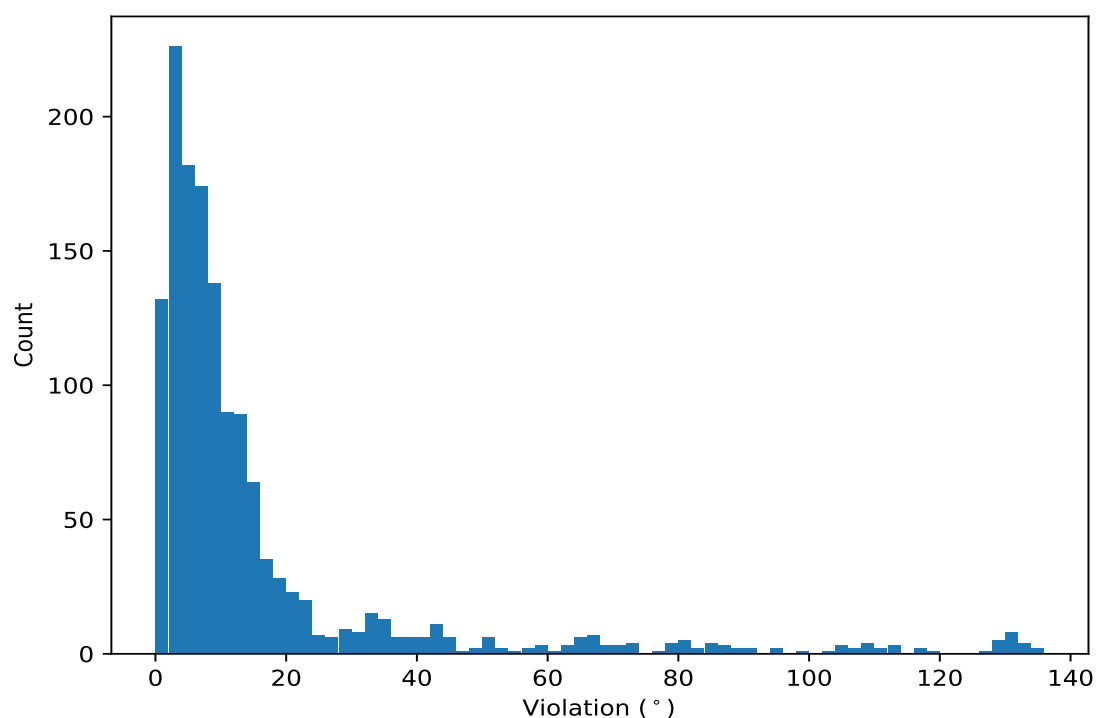
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Med
(2,46)	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:CB	1:91:A:PHE:CG	3	2.45	1.02	2.8
(1,226)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:ASN:N	3	2.11	0.5	1.8
(2,1)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:CB	1:68:A:LEU:CG	2	26.5	24.49	26.
(1,157)	1:98:A:GLY:C	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	2	12.73	2.74	12.7
(2,64)	2:312:B:LEU:N	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2	9.96	5.02	9.9
(1,283)	2:318:B:ASP:C	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	2	8.07	1.16	8.0
(1,52)	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	1:43:A:SER:N	2	7.5	2.44	7.5
(1,187)	1:113:A:GLU:C	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	2	7.39	5.64	7.3
(1,86)	1:59:A:LEU:N	1:59:A:LEU:CA	1:59:A:LEU:C	1:60:A:ARG:N	2	7.36	3.06	7.3
(1,269)	2:311:B:ASP:C	2:312:B:LEU:N	2:312:B:LEU:CA	2:312:B:LEU:C	2	4.85	1.01	4.8
(1,8)	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	1:7:A:GLU:N	2	4.34	0.49	4.3
(1,158)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:ILE:N	2	3.83	1.19	3.8
(1,188)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:VAL:N	2	3.73	0.02	3.7
(1,141)	1:89:A:GLU:C	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	2	3.65	1.55	3.6
(1,82)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:GLU:N	2	3.3	1.53	3.3
(1,107)	1:70:A:SER:C	1:71:A:GLN:N	1:71:A:GLN:CA	1:71:A:GLN:C	2	2.86	1.25	2.8
(1,4)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:ASN:N	2	2.8	0.52	2.8
(1,91)	1:62:A:ARG:C	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	2	2.62	0.14	2.6
(1,175)	1:107:A:GLY:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	2	2.52	0.5	2.5
(1,254)	1:152:A:VAL:N	1:152:A:VAL:CA	1:152:A:VAL:C	1:153:A:GLU:N	2	2.33	0.86	2.3
(1,61)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	2	2.26	1.11	2.2
(1,174)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:GLY:N	2	2.22	0.62	2.2
(1,145)	1:91:A:PHE:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	2	2.2	0.57	2.2
(1,176)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ALA:N	2	1.97	0.56	1.9
(1,131)	1:84:A:GLU:C	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	2	1.82	0.36	1.8
(1,85)	1:58:A:GLU:C	1:59:A:LEU:N	1:59:A:LEU:CA	1:59:A:LEU:C	2	1.78	0.19	1.7
(2,63)	1:155:A:TYR:N	1:155:A:TYR:CA	1:155:A:TYR:CB	1:155:A:TYR:CG	2	1.5	0.15	1.5

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 (°)
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	12	135.21
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	10	135.02
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	3	133.61
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	14	133.52
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	4	132.83
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	8	132.37
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	6	131.63
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	7	131.61
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	11	131.51
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	15	131.47
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	19	131.13
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	17	131.06
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	9	130.82
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	1	130.26
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	16	129.75
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	13	129.58
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	18	129.51
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	5	129.29
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	2	128.17
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	20	127.23
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1	118.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	20	116.55
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	8	116.33
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	14	113.74
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	18	112.57
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	2	112.16
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	16	111.98
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	15	110.8
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	12	109.66
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	7	108.91
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	17	108.89
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	4	108.88
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	6	107.96
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	11	107.44
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	19	105.88
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	5	105.56
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	13	105.41
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	3	103.98
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	10	98.58
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	18	95.88
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	9	94.4
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	20	91.93
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	18	90.95
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	5	89.73
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	13	88.27
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	6	87.31
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	10	86.48
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	18	86.05
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	1	85.61
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	2	85.23
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	12	84.71
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	19	84.66
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	15	83.18
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	17	83.02
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	11	81.66
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	7	81.07
(2,68)	2:324:B:TRP:N	2:324:B:TRP:CA	2:324:B:TRP:CB	2:324:B:TRP:CG	14	80.84
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1	80.65
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	16	80.6
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	6	78.71
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	4	78.42
(1,97)	1:65:A:PHE:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	14	78.37
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	9	78.29
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	20	76.11
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	14	73.95
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	3	73.67
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	5	72.91
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	13	72.53
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	15	70.85
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	9	70.74
(2,7)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	8	70.25
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	4	69.33

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	11	68.64
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	5	68.4
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	8	67.74
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	12	67.29
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	15	67.17
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	20	66.91
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	14	66.79
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	18	66.58
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	17	66.05
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	2	65.25
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	10	65.05
(1,51)	1:41:A:THR:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	15	64.88
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	19	64.26
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	7	64.11
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	4	64.09
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	16	63.47
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	13	63.38
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	6	62.36
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	1	61.4
(1,117)	1:77:A:GLY:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	10	59.56
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	4	59.46
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	3	58.9
(2,65)	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2:312:B:LEU:CD1	20	57.1
(1,96)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:SER:N	14	56.25
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	5	55.81
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	10	53.28
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	13	52.84
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	7	51.73
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	11	51.65
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	12	51.64
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	9	51.54
(2,1)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:CB	1:68:A:LEU:CG	1	51.0
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	19	50.4
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	18	49.33
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	10	48.7
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	3	47.62
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	1	45.96
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	12	45.92
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	1	45.34
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	13	45.3
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	17	45.11
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	2	44.72
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	20	43.91
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	17	43.82
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	9	43.81
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	8	43.47
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	20	43.44
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	9	43.23
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	19	43.14
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	15	43.03
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	3	42.91

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	14	42.55
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	4	42.15
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	7	41.9
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	5	41.46
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	7	41.39
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	16	40.88
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	6	40.77
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	12	40.11
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	10	39.54
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	9	39.19
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	17	39.05
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	7	38.74
(1,97)	1:65:A:PHE:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	4	38.53
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	6	38.3
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	12	37.69
(1,98)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	1:67:A:ASP:N	4	37.29
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	9	36.95
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	3	36.55
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	6	36.48
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	19	36.05
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	12	35.98
(1,117)	1:77:A:GLY:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	19	35.78
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	4	35.48
(1,51)	1:41:A:THR:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	20	35.24
(2,65)	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2:312:B:LEU:CD1	12	35.22
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	12	35.21
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	12	35.15
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	4	34.94
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	10	34.87
(1,284)	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	2:320:B:VAL:N	13	34.37
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	20	34.26
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	10	34.25
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	14	34.12
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	6	33.87
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	13	33.76
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	7	33.4
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	11	33.31
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	15	33.15
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	5	33.14
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	13	33.02
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	18	32.97
(2,43)	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	1:65:A:PHE:CD1	1	32.5
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	18	32.46
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	18	32.45
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	8	32.4
(2,68)	2:324:B:TRP:N	2:324:B:TRP:CA	2:324:B:TRP:CB	2:324:B:TRP:CG	10	32.35
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	12	32.32
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	17	32.18
(1,284)	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	2:320:B:VAL:N	6	31.86
(1,123)	1:80:A:TYR:C	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	20	31.58
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	2	31.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	6	31.35
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	3	31.15
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	17	30.7
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	10	30.35
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	11	30.07
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	16	29.93
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	19	29.66
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	15	29.57
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	6	29.2
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	8	29.19
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	9	29.0
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	13	28.25
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	7	28.19
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	5	28.07
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	16	27.71
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	3	27.4
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	19	26.65
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	3	26.59
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	6	26.08
(2,68)	2:324:B:TRP:N	2:324:B:TRP:CA	2:324:B:TRP:CB	2:324:B:TRP:CG	13	26.0
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	5	25.96
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	2	25.88
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	17	25.41
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	7	25.18
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	10	25.09
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	15	24.85
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	6	24.73
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	19	23.94
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	8	23.67
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	15	23.64
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	1	23.56
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	15	23.48
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	6	23.46
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	20	23.34
(1,281)	2:317:B:LYS:C	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	6	23.27
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	14	23.14
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	15	23.02
(2,65)	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2:312:B:LEU:CD1	2	22.98
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	12	22.9
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	16	22.89
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	4	22.67
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	2	22.63
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1	22.58
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	2	22.55
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	20	22.2
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	6	22.09
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2	22.05
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	16	21.95
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	1	21.85
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	19	21.67
(2,43)	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	1:65:A:PHE:CD1	20	21.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1)	1:2:A:SER:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	10	21.58
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	14	21.54
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	16	21.33
(1,122)	1:80:A:TYR:N	1:80:A:TYR:CA	1:80:A:TYR:C	1:81:A:GLN:N	20	21.17
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1	21.13
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	10	21.12
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	17	21.03
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	13	21.01
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	17	20.89
(1,96)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:SER:N	4	20.7
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	8	20.65
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	10	20.5
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	19	20.44
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	9	20.39
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	1	20.31
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	1	20.3
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	20	20.3
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	14	20.05
(1,1)	1:2:A:SER:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	15	20.01
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	14	19.99
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	6	19.97
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	14	19.95
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	14	19.93
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	1	19.78
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	3	19.77
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	18	19.67
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	4	19.66
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	18	19.56
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	8	19.33
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	16	19.25
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	19	19.22
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	4	19.14
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	7	19.13
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	19	19.04
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	9	18.98
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	11	18.95
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	18	18.94
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	19	18.74
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	5	18.7
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	12	18.62
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	11	18.58
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	13	18.54
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	8	18.49
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1	18.49
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	17	18.2
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	4	18.11
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	5	18.03
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	15	17.99
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	20	17.89
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	4	17.83
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	15	17.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	14	17.66
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	16	17.51
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	12	17.48
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	9	17.36
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	10	17.33
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	18	17.26
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	2	17.22
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	6	17.21
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	6	17.19
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	13	17.19
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	5	17.15
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	5	17.15
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	16	17.13
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	3	17.03
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	9	16.96
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	4	16.96
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	16	16.89
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	7	16.86
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	18	16.8
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	5	16.77
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	8	16.75
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	11	16.72
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	5	16.72
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	15	16.68
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	7	16.59
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	19	16.58
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	19	16.49
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	16	16.47
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	8	16.46
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	17	16.22
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	6	16.21
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	9	15.99
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	16	15.96
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	12	15.84
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	15	15.74
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	8	15.65
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	17	15.65
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	3	15.64
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	13	15.56
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	15	15.55
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	20	15.52
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	14	15.49
(1,157)	1:98:A:GLY:C	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	20	15.47
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	12	15.45
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	9	15.37
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	14	15.35
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	11	15.27
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	1	15.26
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	13	15.23
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	20	15.22
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	9	15.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	8	15.14
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	9	15.11
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	20	15.06
(1,110)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:HIS:N	5	15.03
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	20	15.02
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	8	14.99
(2,64)	2:312:B:LEU:N	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	13	14.98
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	20	14.96
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	20	14.92
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	10	14.91
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	2	14.88
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	10	14.87
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	11	14.85
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	18	14.8
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	4	14.79
(1,51)	1:41:A:THR:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	9	14.79
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	3	14.78
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	11	14.74
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	3	14.71
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	3	14.7
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	11	14.65
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	2	14.63
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	13	14.6
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	1	14.58
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	9	14.53
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	17	14.52
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	5	14.51
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	12	14.49
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	17	14.45
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	14	14.4
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	8	14.35
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	1	14.27
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	9	14.27
(1,257)	1:153:A:GLU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	13	14.24
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	19	14.19
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	2	14.19
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	19	14.17
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	15	14.12
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	15	14.11
(1,53)	1:42:A:GLU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	17	14.11
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	9	14.1
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	7	14.08
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	1	14.04
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	9	14.02
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	9	13.98
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	8	13.95
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	7	13.91
(1,278)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:C	2:317:B:LYS:N	20	13.9
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	17	13.9
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	17	13.84
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	7	13.84

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	14	13.84
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	4	13.69
(1,117)	1:77:A:GLY:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	9	13.67
(1,97)	1:65:A:PHE:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	6	13.67
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	4	13.64
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	19	13.63
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	8	13.62
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	13	13.61
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	7	13.6
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	15	13.58
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	15	13.56
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	20	13.47
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	10	13.45
(1,98)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	1:67:A:ASP:N	2	13.45
(1,196)	1:118:A:GLU:N	1:118:A:GLU:CA	1:118:A:GLU:C	1:119:A:MET:N	20	13.43
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	5	13.42
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	4	13.35
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	9	13.33
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	3	13.32
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	17	13.31
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	4	13.27
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	13	13.27
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	9	13.22
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	12	13.22
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1	13.22
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	17	13.21
(2,65)	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2:312:B:LEU:CD1	9	13.19
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	13	13.08
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	11	13.08
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	11	13.08
(1,187)	1:113:A:GLU:C	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	6	13.03
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	5	13.02
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	6	13.02
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	14	13.01
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	10	12.99
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	1	12.9
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	12	12.85
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	6	12.85
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	18	12.84
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	5	12.82
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	4	12.82
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	2	12.78
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	2	12.77
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	9	12.77
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	2	12.76
(1,109)	1:71:A:GLN:C	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	5	12.76
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	13	12.71
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	20	12.66
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	4	12.64
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	3	12.64
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	8	12.62

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	19	12.58
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	7	12.55
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	8	12.52
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	8	12.51
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	2	12.51
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	14	12.51
(1,97)	1:65:A:PHE:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	2	12.48
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	18	12.42
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	14	12.41
(1,5)	1:4:A:SER:C	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	17	12.4
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	8	12.39
(1,98)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	1:67:A:ASP:N	7	12.32
(2,65)	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2:312:B:LEU:CD1	17	12.3
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	14	12.3
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	2	12.28
(1,282)	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	2:319:B:CYS:N	14	12.27
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	1	12.25
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	2	12.24
(1,88)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:TYR:N	16	12.23
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	17	12.22
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	7	12.21
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	4	12.19
(1,156)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	20	12.18
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	10	12.16
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	14	12.15
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	10	12.15
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	13	12.14
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	20	12.14
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	19	12.12
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	3	12.04
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	10	12.04
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	10	11.97
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	3	11.96
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	15	11.94
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	7	11.93
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	19	11.92
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	11	11.91
(1,101)	1:67:A:ASP:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	8	11.88
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	7	11.88
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	8	11.8
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	19	11.79
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	8	11.79
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	12	11.78
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	12	11.77
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	7	11.73
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	5	11.7
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	10	11.69
(1,117)	1:77:A:GLY:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	17	11.69
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	15	11.63
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	8	11.62
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	2	11.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	6	11.6
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	11	11.43
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	14	11.39
(1,7)	1:5:A:ASN:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	9	11.38
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	4	11.37
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	12	11.36
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	13	11.34
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	16	11.33
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	5	11.26
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	2	11.25
(1,53)	1:42:A:GLU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	5	11.25
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	16	11.24
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	18	11.22
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	12	11.21
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	18	11.19
(1,242)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:GLY:N	11	11.18
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	6	11.1
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	3	11.09
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	10	11.09
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	1	11.08
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	14	11.05
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	11	11.04
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	18	11.0
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	14	10.99
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	11	10.91
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	7	10.88
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	20	10.88
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	17	10.85
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	13	10.83
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	20	10.81
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	1	10.75
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	6	10.75
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	17	10.73
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	4	10.7
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	18	10.63
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	16	10.58
(1,259)	1:154:A:LEU:C	1:155:A:TYR:N	1:155:A:TYR:CA	1:155:A:TYR:C	7	10.57
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	4	10.54
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	2	10.54
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	10	10.54
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	6	10.5
(1,109)	1:71:A:GLN:C	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	12	10.49
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	14	10.48
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	6	10.45
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	20	10.43
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	15	10.42
(1,86)	1:59:A:LEU:N	1:59:A:LEU:CA	1:59:A:LEU:C	1:60:A:ARG:N	7	10.42
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	3	10.37
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	14	10.36
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	13	10.34
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	19	10.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	10	10.33
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	9	10.31
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	3	10.3
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	3	10.3
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	3	10.24
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	4	10.22
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	6	10.19
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	18	10.19
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	5	10.17
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	10	10.16
(1,53)	1:42:A:GLU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	10	10.15
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	10	10.11
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	17	10.11
(1,41)	1:22:A:TYR:C	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	11	10.08
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	15	10.08
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	5	10.07
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	2	10.07
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	11	10.02
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	7	10.0
(1,157)	1:98:A:GLY:C	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	3	9.98
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	3	9.96
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	6	9.95
(1,52)	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	1:43:A:SER:N	2	9.94
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	10	9.92
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	4	9.91
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	4	9.9
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	5	9.89
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	11	9.88
(1,6)	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	1:6:A:ARG:N	20	9.88
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	7	9.87
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	6	9.84
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	2	9.84
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	5	9.83
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	6	9.81
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	7	9.8
(1,48)	1:26:A:GLN:N	1:26:A:GLN:CA	1:26:A:GLN:C	1:27:A:PHE:N	14	9.8
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	8	9.79
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	8	9.78
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	7	9.72
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	10	9.72
(1,118)	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1:79:A:ALA:N	13	9.68
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	8	9.67
(1,98)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	1:67:A:ASP:N	11	9.67
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	18	9.66
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	12	9.66
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	16	9.66
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	18	9.65
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	3	9.65
(1,140)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LEU:N	14	9.64
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	9	9.62
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	9	9.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	3	9.59
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	6	9.56
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	13	9.56
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	6	9.53
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	17	9.51
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	14	9.49
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	11	9.47
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	5	9.46
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	2	9.42
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	6	9.41
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	12	9.4
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	1	9.39
(1,102)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:THR:N	15	9.39
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	19	9.37
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	16	9.31
(1,1)	1:2:A:SER:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	17	9.3
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1	9.29
(1,123)	1:80:A:TYR:C	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	9	9.28
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	16	9.27
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	18	9.25
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	15	9.24
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	17	9.23
(1,283)	2:318:B:ASP:C	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	3	9.23
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	5	9.22
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	14	9.19
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	11	9.16
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	13	9.13
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	15	9.12
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	7	9.07
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	12	9.06
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1	9.04
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	12	9.02
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	4	9.01
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	14	9.0
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	17	8.98
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	20	8.98
(2,43)	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	1:65:A:PHE:CD1	17	8.97
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	12	8.96
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	3	8.94
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	17	8.93
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	18	8.9
(1,7)	1:5:A:ASN:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	5	8.9
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	16	8.89
(1,282)	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	2:319:B:CYS:N	9	8.85
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	18	8.84
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	9	8.83
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	5	8.83
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	5	8.81
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	16	8.8
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	15	8.79
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	15	8.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	12	8.76
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	9	8.75
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	20	8.74
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	20	8.7
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	13	8.64
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	17	8.63
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	15	8.63
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	16	8.62
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	17	8.62
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	15	8.57
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	5	8.56
(1,117)	1:77:A:GLY:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	15	8.53
(1,97)	1:65:A:PHE:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	16	8.53
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	4	8.52
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	19	8.51
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	8	8.49
(1,57)	1:44:A:GLU:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	12	8.49
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	8	8.46
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	19	8.46
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	19	8.46
(1,142)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:PHE:N	14	8.46
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	17	8.42
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	17	8.41
(1,57)	1:44:A:GLU:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	6	8.41
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	7	8.4
(1,156)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	3	8.37
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	7	8.36
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	15	8.36
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	18	8.36
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	12	8.36
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	7	8.33
(1,258)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:TYR:N	18	8.31
(1,142)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:PHE:N	13	8.29
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	15	8.27
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	15	8.27
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	15	8.26
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	13	8.26
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	13	8.23
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	4	8.22
(1,6)	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	1:6:A:ARG:N	15	8.13
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	3	8.12
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	13	8.09
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	1	8.09
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	9	8.08
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	13	8.06
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	16	8.05
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	8	8.05
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	16	8.04
(1,117)	1:77:A:GLY:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	2	8.03
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	9	8.02
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	10	8.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	8	8.01
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	7	8.01
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	15	8.0
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	9	8.0
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	6	7.99
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	16	7.98
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	11	7.96
(1,65)	1:48:A:GLN:C	1:49:A:ALA:N	1:49:A:ALA:CA	1:49:A:ALA:C	14	7.95
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	8	7.94
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	11	7.94
(1,62)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:GLN:N	4	7.92
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	3	7.9
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	6	7.9
(1,241)	1:144:A:GLU:C	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	16	7.88
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	15	7.88
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	1	7.86
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	13	7.86
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	15	7.86
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	14	7.85
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	4	7.84
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	14	7.83
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	1	7.79
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	19	7.77
(1,5)	1:4:A:SER:C	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	15	7.77
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	15	7.76
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	14	7.76
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	12	7.76
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	19	7.73
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	12	7.73
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	19	7.69
(1,196)	1:118:A:GLU:N	1:118:A:GLU:CA	1:118:A:GLU:C	1:119:A:MET:N	9	7.66
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	4	7.65
(1,196)	1:118:A:GLU:N	1:118:A:GLU:CA	1:118:A:GLU:C	1:119:A:MET:N	18	7.65
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	7	7.62
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	18	7.58
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	1	7.57
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	17	7.57
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	9	7.57
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	5	7.55
(1,257)	1:153:A:GLU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	3	7.54
(1,93)	1:63:A:ARG:C	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	19	7.53
(1,6)	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	1:6:A:ARG:N	17	7.52
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	2	7.51
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	16	7.51
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	18	7.51
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	12	7.46
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	12	7.42
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	8	7.4
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	14	7.4
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	20	7.39
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	9	7.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	18	7.35
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	13	7.35
(1,278)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:C	2:317:B:LYS:N	17	7.31
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	12	7.29
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	10	7.29
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	19	7.28
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	4	7.28
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	3	7.27
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	17	7.26
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	9	7.25
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2	7.23
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	7	7.23
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	13	7.21
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	10	7.2
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	2	7.18
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	7	7.17
(1,196)	1:118:A:GLU:N	1:118:A:GLU:CA	1:118:A:GLU:C	1:119:A:MET:N	2	7.15
(1,5)	1:4:A:SER:C	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	7	7.15
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	8	7.14
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	19	7.14
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	15	7.13
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	14	7.12
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	8	7.12
(1,48)	1:26:A:GLN:N	1:26:A:GLN:CA	1:26:A:GLN:C	1:27:A:PHE:N	8	7.11
(2,42)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	18	7.09
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	4	7.03
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	13	7.02
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	5	7.0
(1,257)	1:153:A:GLU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	11	6.98
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	3	6.98
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	13	6.97
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	6	6.97
(1,259)	1:154:A:LEU:C	1:155:A:TYR:N	1:155:A:TYR:CA	1:155:A:TYR:C	13	6.96
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	5	6.96
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	10	6.95
(2,65)	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2:312:B:LEU:CD1	1	6.94
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	14	6.94
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	10	6.93
(1,283)	2:318:B:ASP:C	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	16	6.92
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	10	6.92
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	11	6.92
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	3	6.89
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	16	6.86
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	3	6.86
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	2	6.85
(1,278)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:C	2:317:B:LYS:N	8	6.85
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	17	6.85
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	5	6.85
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	11	6.84
(1,136)	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	1:88:A:ASN:N	14	6.78
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	6	6.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	7	6.76
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	9	6.74
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	15	6.69
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	7	6.69
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	7	6.68
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	9	6.67
(1,136)	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	1:88:A:ASN:N	6	6.63
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	1	6.62
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	6	6.62
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	12	6.61
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	3	6.59
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	20	6.59
(1,11)	1:7:A:GLU:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	10	6.59
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	17	6.58
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	3	6.57
(1,5)	1:4:A:SER:C	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	20	6.57
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	20	6.56
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	6	6.56
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	11	6.56
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	7	6.55
(1,263)	2:308:B:SER:C	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	7	6.55
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	11	6.55
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	2	6.54
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	5	6.54
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	3	6.51
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	3	6.48
(1,113)	1:73:A:HIS:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	11	6.46
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	19	6.45
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	18	6.42
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	5	6.4
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	17	6.4
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	2	6.4
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	10	6.4
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	6	6.39
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	2	6.38
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	19	6.38
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	19	6.37
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	10	6.35
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	4	6.35
(1,101)	1:67:A:ASP:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	4	6.35
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	7	6.35
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	12	6.32
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	9	6.31
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	10	6.3
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	10	6.3
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	2	6.26
(1,111)	1:72:A:LEU:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	16	6.25
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	6	6.24
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	13	6.24
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	11	6.24
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	18	6.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	11	6.21
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	15	6.2
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	16	6.2
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	7	6.19
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	5	6.18
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	6	6.17
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	4	6.16
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	6	6.14
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	2	6.13
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	11	6.13
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	16	6.13
(1,118)	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1:79:A:ALA:N	6	6.12
(1,116)	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1:76:A:PRO:N	3	6.12
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	2	6.11
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	16	6.11
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	6	6.09
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	11	6.09
(2,48)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:CB	1:103:A:PHE:CG	12	6.07
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	1	6.07
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	10	6.07
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	4	6.05
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	18	6.05
(1,1)	1:2:A:SER:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	20	6.01
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	8	6.0
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	3	6.0
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	15	5.99
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	1	5.97
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	2	5.96
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1	5.95
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	1	5.95
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	20	5.95
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	10	5.93
(1,51)	1:41:A:THR:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	13	5.92
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	19	5.91
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	18	5.91
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	16	5.91
(1,284)	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	2:320:B:VAL:N	12	5.89
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	2	5.89
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	3	5.87
(1,269)	2:311:B:ASP:C	2:312:B:LEU:N	2:312:B:LEU:CA	2:312:B:LEU:C	11	5.86
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	5	5.82
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	5	5.82
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	9	5.82
(1,232)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	5	5.79
(1,53)	1:42:A:GLU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	11	5.79
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	16	5.71
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	4	5.71
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	19	5.7
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	3	5.7
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	15	5.69
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	1	5.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	2	5.66
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	3	5.62
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	15	5.59
(1,118)	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1:79:A:ALA:N	7	5.57
(1,282)	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	2:319:B:CYS:N	12	5.56
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	15	5.56
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	14	5.54
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	9	5.52
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	17	5.51
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	11	5.5
(1,282)	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	2:319:B:CYS:N	10	5.49
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	14	5.47
(1,284)	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	2:320:B:VAL:N	7	5.41
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	13	5.39
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	20	5.39
(1,123)	1:80:A:TYR:C	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	15	5.38
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	4	5.32
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	12	5.31
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	19	5.31
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	5	5.31
(1,57)	1:44:A:GLU:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	20	5.28
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	14	5.27
(1,11)	1:7:A:GLU:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	3	5.26
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	13	5.25
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	18	5.23
(1,124)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:SER:N	18	5.23
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	14	5.21
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	6	5.21
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	4	5.2
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	12	5.2
(1,267)	2:310:B:THR:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	20	5.2
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	20	5.2
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	1	5.2
(1,141)	1:89:A:GLU:C	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	6	5.19
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	9	5.18
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	12	5.18
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	10	5.17
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	13	5.17
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	8	5.16
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	19	5.15
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	15	5.14
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	19	5.11
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	14	5.11
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	19	5.1
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	19	5.1
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	1	5.08
(1,285)	2:319:B:CYS:C	2:320:B:VAL:N	2:320:B:VAL:CA	2:320:B:VAL:C	9	5.08
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	11	5.07
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	7	5.06
(1,52)	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	1:43:A:SER:N	19	5.06
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	1	5.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	15	5.04
(1,158)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:ILE:N	13	5.02
(1,194)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:GLU:N	20	5.01
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	18	5.0
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	17	4.98
(1,88)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:TYR:N	13	4.95
(2,64)	2:312:B:LEU:N	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	14	4.94
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	12	4.94
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	17	4.93
(1,281)	2:317:B:LYS:C	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	19	4.92
(1,257)	1:153:A:GLU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	4	4.92
(1,256)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:LEU:N	1	4.91
(1,116)	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1:76:A:PRO:N	9	4.91
(1,110)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:HIS:N	19	4.91
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	5	4.89
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	2	4.89
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	6	4.89
(1,44)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:SER:N	8	4.87
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	16	4.86
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	19	4.85
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	12	4.85
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	2	4.84
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	9	4.83
(1,143)	1:90:A:LEU:C	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:C	20	4.83
(1,82)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:GLU:N	15	4.83
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	7	4.82
(1,8)	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	1:7:A:GLU:N	9	4.82
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	14	4.78
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	5	4.76
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	4	4.76
(1,123)	1:80:A:TYR:C	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1	4.74
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	6	4.72
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	13	4.71
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	3	4.71
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	18	4.68
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	5	4.64
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	14	4.63
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	4	4.62
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	16	4.62
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2	4.6
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1	4.6
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	20	4.6
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	15	4.6
(1,143)	1:90:A:LEU:C	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:C	11	4.59
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	2	4.57
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	13	4.57
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	11	4.54
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	19	4.54
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	9	4.54
(1,256)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:LEU:N	3	4.51
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	11	4.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1	4.44
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	12	4.44
(1,143)	1:90:A:LEU:C	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:C	17	4.43
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	1	4.41
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	19	4.41
(1,102)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:THR:N	12	4.41
(1,6)	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	1:6:A:ARG:N	7	4.41
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	5	4.4
(1,2)	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	1:4:A:SER:N	17	4.4
(2,42)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	20	4.39
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	20	4.39
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	12	4.39
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	4	4.38
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	11	4.37
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	12	4.36
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	1	4.36
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	14	4.35
(1,11)	1:7:A:GLU:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	17	4.34
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	20	4.32
(1,88)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:TYR:N	11	4.32
(1,53)	1:42:A:GLU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	6	4.32
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1	4.31
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	7	4.3
(1,96)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:SER:N	6	4.3
(1,86)	1:59:A:LEU:N	1:59:A:LEU:CA	1:59:A:LEU:C	1:60:A:ARG:N	3	4.3
(2,42)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	1	4.29
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	7	4.28
(1,282)	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	2:319:B:CYS:N	7	4.28
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	7	4.28
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	16	4.26
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	16	4.25
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	13	4.25
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	11	4.25
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	15	4.24
(1,256)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:LEU:N	13	4.22
(1,199)	1:120:A:GLN:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	20	4.22
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	5	4.2
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	3	4.18
(1,281)	2:317:B:LYS:C	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	5	4.14
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	17	4.14
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	11	4.13
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	5	4.12
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	9	4.12
(1,281)	2:317:B:LYS:C	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	16	4.11
(1,107)	1:70:A:SER:C	1:71:A:GLN:N	1:71:A:GLN:CA	1:71:A:GLN:C	14	4.11
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	13	4.11
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	10	4.1
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	10	4.09
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	3	4.08
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	18	4.07
(2,68)	2:324:B:TRP:N	2:324:B:TRP:CA	2:324:B:TRP:CB	2:324:B:TRP:CG	16	4.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	20	4.06
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	7	4.06
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:LEU:N	7	4.02
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	2	3.99
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	7	3.98
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	9	3.93
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	2	3.91
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	6	3.89
(1,57)	1:44:A:GLU:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	5	3.89
(1,124)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:SER:N	9	3.88
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	6	3.85
(1,8)	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	1:7:A:GLU:N	5	3.85
(1,269)	2:311:B:ASP:C	2:312:B:LEU:N	2:312:B:LEU:CA	2:312:B:LEU:C	5	3.84
(1,258)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:TYR:N	5	3.82
(1,240)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:ASN:N	1	3.81
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	20	3.8
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	3	3.8
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	7	3.79
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	13	3.78
(1,55)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	11	3.78
(1,273)	2:313:B:GLU:C	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	17	3.75
(1,188)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:VAL:N	9	3.75
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	16	3.75
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	20	3.75
(1,37)	1:20:A:LYS:C	1:21:A:GLY:N	1:21:A:GLY:CA	1:21:A:GLY:C	5	3.75
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	13	3.74
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	17	3.74
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	10	3.74
(1,188)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:VAL:N	2	3.71
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	16	3.7
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	17	3.67
(1,284)	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	2:320:B:VAL:N	8	3.64
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	6	3.64
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	17	3.64
(1,284)	2:319:B:CYS:N	2:319:B:CYS:CA	2:319:B:CYS:C	2:320:B:VAL:N	4	3.63
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	11	3.63
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	3	3.61
(1,16)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:ASP:N	14	3.61
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	13	3.6
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	9	3.59
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	15	3.58
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	7	3.57
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	16	3.56
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	20	3.55
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	5	3.55
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	10	3.54
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	5	3.51
(1,143)	1:90:A:LEU:C	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:C	10	3.5
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	13	3.5
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	16	3.49
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	2	3.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	17	3.46
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	18	3.46
(1,94)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:PHE:N	18	3.46
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	4	3.44
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	17	3.43
(2,46)	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:CB	1:91:A:PHE:CG	20	3.42
(1,281)	2:317:B:LYS:C	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	8	3.39
(1,61)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1	3.37
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	2	3.36
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	14	3.35
(1,217)	1:129:A:TRP:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	9	3.34
(1,186)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:SER:N	9	3.34
(1,143)	1:90:A:LEU:C	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:C	15	3.33
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	8	3.32
(1,4)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:ASN:N	18	3.32
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	2	3.31
(1,11)	1:7:A:GLU:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	15	3.31
(1,7)	1:5:A:ASN:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	4	3.31
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	14	3.3
(1,99)	1:66:A:SER:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	10	3.3
(1,181)	1:110:A:LEU:C	1:111:A:CYS:N	1:111:A:CYS:CA	1:111:A:CYS:C	14	3.29
(1,53)	1:42:A:GLU:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	20	3.29
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:LEU:N	14	3.29
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	12	3.26
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	8	3.26
(1,143)	1:90:A:LEU:C	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:C	18	3.24
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	7	3.24
(1,90)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ARG:N	20	3.23
(1,256)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:LEU:N	11	3.19
(1,108)	1:71:A:GLN:N	1:71:A:GLN:CA	1:71:A:GLN:C	1:72:A:LEU:N	12	3.19
(1,254)	1:152:A:VAL:N	1:152:A:VAL:CA	1:152:A:VAL:C	1:153:A:GLU:N	6	3.18
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	3	3.18
(1,57)	1:44:A:GLU:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	2	3.18
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	8	3.17
(1,101)	1:67:A:ASP:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	3	3.16
(1,231)	1:136:A:ASP:C	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	11	3.15
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	11	3.14
(1,17)	1:10:A:VAL:C	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	14	3.14
(1,257)	1:153:A:GLU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	2	3.11
(1,130)	1:84:A:GLU:N	1:84:A:GLU:CA	1:84:A:GLU:C	1:85:A:GLN:N	1	3.09
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	5	3.08
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	7	3.07
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	5	3.05
(1,37)	1:20:A:LYS:C	1:21:A:GLY:N	1:21:A:GLY:CA	1:21:A:GLY:C	10	3.05
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	10	3.04
(1,122)	1:80:A:TYR:N	1:80:A:TYR:CA	1:80:A:TYR:C	1:81:A:GLN:N	7	3.04
(1,1)	1:2:A:SER:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	7	3.03
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	14	3.02
(1,175)	1:107:A:GLY:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	3	3.02
(1,136)	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	1:88:A:ASN:N	10	3.02
(1,178)	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	1:110:A:LEU:N	6	3.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	12	3.01
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	13	3.0
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	14	2.99
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	11	2.99
(1,50)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:SER:N	3	2.99
(1,106)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:GLN:N	7	2.96
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	13	2.96
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	12	2.93
(1,122)	1:80:A:TYR:N	1:80:A:TYR:CA	1:80:A:TYR:C	1:81:A:GLN:N	9	2.93
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	16	2.93
(1,256)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:LEU:N	4	2.92
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	20	2.92
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	1	2.92
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	10	2.91
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	10	2.9
(2,46)	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:CB	1:91:A:PHE:CG	3	2.89
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	6	2.89
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	7	2.87
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	6	2.85
(1,64)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	20	2.85
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	2	2.84
(1,174)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:GLY:N	8	2.84
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	12	2.83
(2,51)	1:106:A:PHE:CA	1:106:A:PHE:CB	1:106:A:PHE:CG	1:106:A:PHE:CD1	16	2.82
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	3	2.81
(1,226)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:ASN:N	19	2.81
(1,118)	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1:79:A:ALA:N	3	2.81
(1,263)	2:308:B:SER:C	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	9	2.79
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	8	2.79
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	19	2.79
(1,64)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	15	2.79
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	13	2.78
(1,216)	1:129:A:TRP:N	1:129:A:TRP:CA	1:129:A:TRP:C	1:130:A:MET:N	5	2.78
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	4	2.78
(1,63)	1:47:A:LYS:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	4	2.78
(1,145)	1:91:A:PHE:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	3	2.77
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	4	2.76
(1,91)	1:62:A:ARG:C	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	16	2.76
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	17	2.73
(1,181)	1:110:A:LEU:C	1:111:A:CYS:N	1:111:A:CYS:CA	1:111:A:CYS:C	4	2.73
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	11	2.72
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	7	2.71
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	11	2.7
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	18	2.69
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	3	2.68
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	19	2.66
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	9	2.64
(1,158)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:ILE:N	18	2.64
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	17	2.64
(1,48)	1:26:A:GLN:N	1:26:A:GLN:CA	1:26:A:GLN:C	1:27:A:PHE:N	12	2.63
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	5	2.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,60)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:CB	1:61:A:TYR:CG	17	2.6
(1,98)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	1:67:A:ASP:N	15	2.6
(1,116)	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1:76:A:PRO:N	5	2.58
(1,124)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:SER:N	15	2.57
(1,136)	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	1:88:A:ASN:N	13	2.56
(1,280)	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	2:318:B:ASP:N	1	2.53
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	16	2.53
(1,176)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ALA:N	3	2.53
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	10	2.53
(1,142)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:PHE:N	6	2.52
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	18	2.52
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	18	2.5
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	10	2.49
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	17	2.49
(1,11)	1:7:A:GLU:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	7	2.49
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	14	2.48
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	11	2.48
(1,91)	1:62:A:ARG:C	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	8	2.48
(1,57)	1:44:A:GLU:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	13	2.48
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	18	2.47
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	4	2.47
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	8	2.47
(1,181)	1:110:A:LEU:C	1:111:A:CYS:N	1:111:A:CYS:CA	1:111:A:CYS:C	3	2.44
(1,118)	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1:79:A:ALA:N	11	2.44
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	14	2.43
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	6	2.43
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	7	2.41
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	2	2.4
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	10	2.39
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	19	2.37
(1,87)	1:59:A:LEU:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	18	2.37
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	8	2.36
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	5	2.36
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	2	2.36
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	18	2.35
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	3	2.35
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	19	2.35
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	6	2.34
(2,68)	2:324:B:TRP:N	2:324:B:TRP:CA	2:324:B:TRP:CB	2:324:B:TRP:CG	11	2.33
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	15	2.33
(1,92)	1:63:A:ARG:N	1:63:A:ARG:CA	1:63:A:ARG:C	1:64:A:ALA:N	20	2.33
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	8	2.31
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	13	2.29
(1,4)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:ASN:N	5	2.28
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	17	2.27
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	8	2.27
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	10	2.27
(1,181)	1:110:A:LEU:C	1:111:A:CYS:N	1:111:A:CYS:CA	1:111:A:CYS:C	19	2.26
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	18	2.24
(1,51)	1:41:A:THR:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	16	2.24
(1,229)	1:135:A:ASN:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	13	2.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,131)	1:84:A:GLU:C	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	4	2.19
(1,3)	1:3:A:GLN:C	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	9	2.18
(1,275)	2:314:B:ALA:C	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	4	2.17
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	11	2.17
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	16	2.16
(1,217)	1:129:A:TRP:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	5	2.15
(1,64)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	4	2.15
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	8	2.13
(1,257)	1:153:A:GLU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1	2.12
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	6	2.12
(1,141)	1:89:A:GLU:C	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	13	2.1
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	7	2.09
(1,45)	1:24:A:TRP:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	4	2.08
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	17	2.07
(1,84)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:LEU:N	10	2.07
(1,258)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:TYR:N	6	2.06
(1,64)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	8	2.05
(1,76)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:ASP:N	8	2.04
(1,194)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:GLU:N	10	2.02
(1,175)	1:107:A:GLY:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	6	2.02
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	12	2.02
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	5	2.02
(2,61)	1:80:A:TYR:N	1:80:A:TYR:CA	1:80:A:TYR:CB	1:80:A:TYR:CG	1	2.01
(2,1)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:CB	1:68:A:LEU:CG	5	2.01
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	14	2.0
(1,85)	1:58:A:GLU:C	1:59:A:LEU:N	1:59:A:LEU:CA	1:59:A:LEU:C	2	1.98
(2,26)	1:126:A:ILE:CA	1:126:A:ILE:CB	1:126:A:ILE:CG1	1:126:A:ILE:CD1	6	1.96
(1,138)	1:88:A:ASN:N	1:88:A:ASN:CA	1:88:A:ASN:C	1:89:A:GLU:N	6	1.96
(1,112)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ILE:N	10	1.96
(1,216)	1:129:A:TRP:N	1:129:A:TRP:CA	1:129:A:TRP:C	1:130:A:MET:N	6	1.93
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	11	1.91
(1,279)	2:316:B:PHE:C	2:317:B:LYS:N	2:317:B:LYS:CA	2:317:B:LYS:C	9	1.9
(1,194)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:GLU:N	14	1.9
(1,102)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:THR:N	11	1.9
(1,43)	1:23:A:SER:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	4	1.9
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:LEU:N	10	1.9
(1,263)	2:308:B:SER:C	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	10	1.88
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	12	1.87
(1,259)	1:154:A:LEU:C	1:155:A:TYR:N	1:155:A:TYR:CA	1:155:A:TYR:C	3	1.87
(1,226)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:ASN:N	8	1.87
(1,97)	1:65:A:PHE:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	10	1.87
(2,66)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:CB	2:316:B:PHE:CG	7	1.86
(1,18)	1:11:A:ASP:N	1:11:A:ASP:CA	1:11:A:ASP:C	1:12:A:PHE:N	18	1.84
(1,7)	1:5:A:ASN:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	1	1.84
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	3	1.83
(1,258)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:TYR:N	20	1.79
(1,156)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	13	1.79
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	14	1.78
(1,51)	1:41:A:THR:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	7	1.78
(1,276)	2:315:B:TYR:N	2:315:B:TYR:CA	2:315:B:TYR:C	2:316:B:PHE:N	6	1.77
(1,143)	1:90:A:LEU:C	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:C	7	1.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,124)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:SER:N	19	1.77
(1,82)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:GLU:N	2	1.77
(1,281)	2:317:B:LYS:C	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	3	1.76
(1,187)	1:113:A:GLU:C	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	17	1.75
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	14	1.74
(1,11)	1:7:A:GLU:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1	1.74
(1,146)	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	1:93:A:ASP:N	15	1.72
(1,258)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:TYR:N	9	1.7
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1	1.7
(1,216)	1:129:A:TRP:N	1:129:A:TRP:CA	1:129:A:TRP:C	1:130:A:MET:N	2	1.69
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	18	1.69
(1,125)	1:81:A:GLN:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	17	1.68
(1,109)	1:71:A:GLN:C	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	2	1.67
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	3	1.66
(1,262)	2:308:B:SER:N	2:308:B:SER:CA	2:308:B:SER:C	2:309:B:THR:N	18	1.66
(1,110)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:HIS:N	17	1.66
(2,63)	1:155:A:TYR:N	1:155:A:TYR:CA	1:155:A:TYR:CB	1:155:A:TYR:CG	18	1.65
(1,226)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:ASN:N	11	1.65
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	8	1.65
(1,6)	1:5:A:ASN:N	1:5:A:ASN:CA	1:5:A:ASN:C	1:6:A:ARG:N	2	1.65
(1,54)	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	1:44:A:GLU:N	17	1.64
(1,145)	1:91:A:PHE:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	12	1.63
(1,107)	1:70:A:SER:C	1:71:A:GLN:N	1:71:A:GLN:CA	1:71:A:GLN:C	7	1.62
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	2	1.61
(1,193)	1:116:A:ASP:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	9	1.6
(1,12)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:VAL:N	10	1.6
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	1	1.59
(1,174)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:GLY:N	10	1.59
(1,85)	1:58:A:GLU:C	1:59:A:LEU:N	1:59:A:LEU:CA	1:59:A:LEU:C	3	1.59
(1,118)	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1:79:A:ALA:N	16	1.58
(1,116)	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1:76:A:PRO:N	4	1.58
(1,37)	1:20:A:LYS:C	1:21:A:GLY:N	1:21:A:GLY:CA	1:21:A:GLY:C	17	1.58
(2,65)	2:312:B:LEU:CA	2:312:B:LEU:CB	2:312:B:LEU:CG	2:312:B:LEU:CD1	11	1.57
(1,148)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:GLY:N	13	1.57
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	13	1.56
(1,147)	1:92:A:ARG:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	18	1.56
(1,115)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1	1.55
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	16	1.53
(1,243)	1:145:A:ASN:C	1:146:A:GLY:N	1:146:A:GLY:CA	1:146:A:GLY:C	12	1.52
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	3	1.51
(1,89)	1:60:A:ARG:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	16	1.5
(1,51)	1:41:A:THR:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	11	1.5
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	6	1.49
(1,278)	2:316:B:PHE:N	2:316:B:PHE:CA	2:316:B:PHE:C	2:317:B:LYS:N	19	1.48
(1,49)	1:26:A:GLN:C	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	19	1.48
(1,254)	1:152:A:VAL:N	1:152:A:VAL:CA	1:152:A:VAL:C	1:153:A:GLU:N	15	1.47
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	4	1.46
(1,131)	1:84:A:GLU:C	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	11	1.46
(1,88)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:TYR:N	6	1.43
(1,217)	1:129:A:TRP:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	3	1.42
(1,101)	1:67:A:ASP:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	19	1.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,44)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:SER:N	14	1.42
(1,176)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ALA:N	2	1.41
(1,103)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	18	1.39
(1,64)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:ALA:N	2	1.39
(1,44)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:SER:N	3	1.39
(1,37)	1:20:A:LYS:C	1:21:A:GLY:N	1:21:A:GLY:CA	1:21:A:GLY:C	18	1.39
(1,272)	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	2:314:B:ALA:N	9	1.38
(1,26)	1:15:A:TYR:N	1:15:A:TYR:CA	1:15:A:TYR:C	1:16:A:LYS:N	10	1.38
(1,11)	1:7:A:GLU:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	12	1.38
(1,104)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:SER:N	2	1.36
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:LEU:N	3	1.36
(2,63)	1:155:A:TYR:N	1:155:A:TYR:CA	1:155:A:TYR:CB	1:155:A:TYR:CG	9	1.35
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	20	1.35
(1,42)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:TRP:N	9	1.35
(1,194)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:GLU:N	17	1.32
(1,139)	1:88:A:ASN:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	10	1.32
(1,81)	1:56:A:GLU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	20	1.32
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	9	1.32
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	17	1.31
(1,156)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	2	1.3
(1,114)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	20	1.3
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:SER:N	8	1.3
(1,205)	1:123:A:VAL:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	19	1.29
(1,100)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:LEU:N	15	1.28
(1,1)	1:2:A:SER:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	14	1.28
(1,217)	1:129:A:TRP:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	15	1.25
(1,228)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ASP:N	8	1.24
(1,88)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:TYR:N	12	1.23
(1,216)	1:129:A:TRP:N	1:129:A:TRP:CA	1:129:A:TRP:C	1:130:A:MET:N	3	1.22
(2,21)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:CB	1:74:A:ILE:CG1	10	1.2
(1,236)	1:142:A:ILE:N	1:142:A:ILE:CA	1:142:A:ILE:C	1:143:A:GLN:N	1	1.2
(2,42)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:CB	1:65:A:PHE:CG	8	1.18
(1,263)	2:308:B:SER:C	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	13	1.18
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	11	1.18
(1,268)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:LEU:N	18	1.16
(1,61)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	7	1.16
(1,57)	1:44:A:GLU:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	4	1.15
(1,271)	2:312:B:LEU:C	2:313:B:GLU:N	2:313:B:GLU:CA	2:313:B:GLU:C	20	1.14
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	2	1.14
(1,246)	1:148:A:TRP:N	1:148:A:TRP:CA	1:148:A:TRP:C	1:149:A:ASP:N	6	1.13
(1,13)	1:8:A:LEU:C	1:9:A:VAL:N	1:9:A:VAL:CA	1:9:A:VAL:C	14	1.12
(1,40)	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	1:23:A:SER:N	10	1.09
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:GLY:N	7	1.09
(1,217)	1:129:A:TRP:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	13	1.08
(1,133)	1:85:A:GLN:C	1:86:A:VAL:N	1:86:A:VAL:CA	1:86:A:VAL:C	18	1.07
(1,265)	2:309:B:THR:C	2:310:B:THR:N	2:310:B:THR:CA	2:310:B:THR:C	1	1.06
(1,257)	1:153:A:GLU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	7	1.05
(1,116)	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1:76:A:PRO:N	11	1.05
(1,10)	1:7:A:GLU:N	1:7:A:GLU:CA	1:7:A:GLU:C	1:8:A:LEU:N	6	1.05
(2,4)	1:110:A:LEU:CA	1:110:A:LEU:CB	1:110:A:LEU:CG	1:110:A:LEU:CD1	4	1.04
(1,155)	1:97:A:TRP:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	13	1.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,46)	1:91:A:PHE:N	1:91:A:PHE:CA	1:91:A:PHE:CB	1:91:A:PHE:CG	17	1.03
(1,281)	2:317:B:LYS:C	2:318:B:ASP:N	2:318:B:ASP:CA	2:318:B:ASP:C	20	1.03
(1,264)	2:309:B:THR:N	2:309:B:THR:CA	2:309:B:THR:C	2:310:B:THR:N	17	1.02
(1,122)	1:80:A:TYR:N	1:80:A:TYR:CA	1:80:A:TYR:C	1:81:A:GLN:N	1	1.0