



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:13 AM UTC

PDB ID : 7AFR / pdb_00007afr
BMRB ID : 34562
Title : Ribosome maturation factor RimP (apo)
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Deposited on : 2020-09-19

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<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

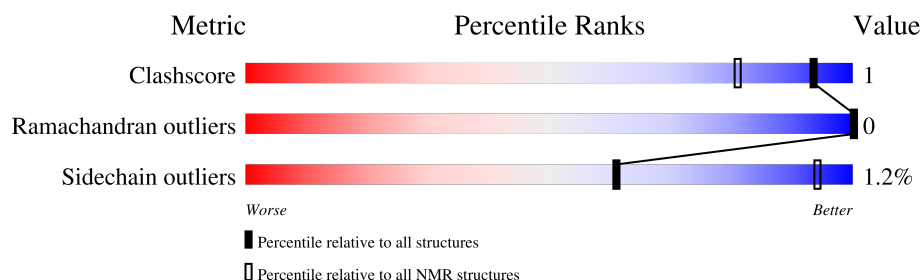
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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	X	151	

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 1 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	X:4-X:78 (75)	0.71	10
2	X:84-X:148 (65)	0.65	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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2349 atoms, of which 1174 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome maturation factor RimP.

Mol	Chain	Residues	Atoms						Trace
1	X	151	Total	C	H	N	O	S	0
			2349	742	1174	197	231	5	

There is a discrepancy between the modelled and reference sequences:

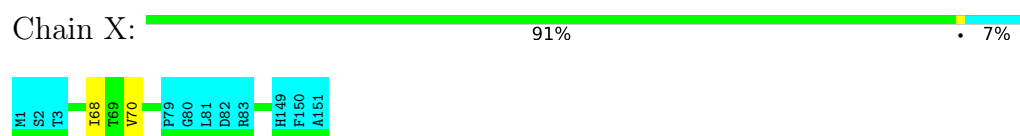
Chain	Residue	Modelled	Actual	Comment	Reference
X	151	ALA	-	expression tag	UNP A0A0J3VRH1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ribosome maturation factor RimP

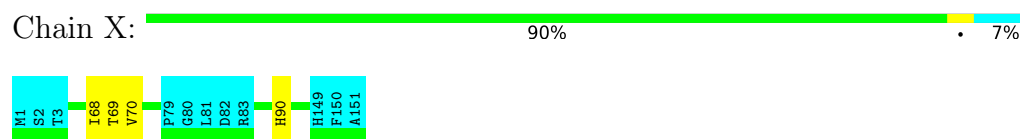


4.2 Scores per residue for each member of the ensemble

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

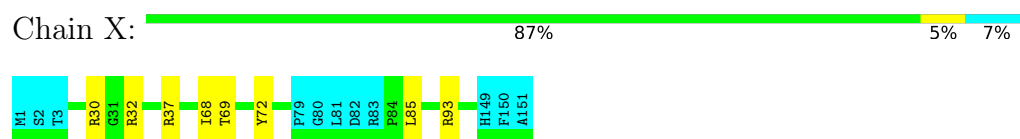
4.2.1 Score per residue for model 1

- Molecule 1: Ribosome maturation factor RimP



4.2.2 Score per residue for model 2

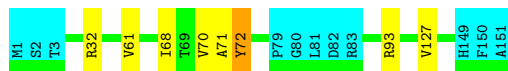
- Molecule 1: Ribosome maturation factor RimP



4.2.3 Score per residue for model 3

- Molecule 1: Ribosome maturation factor RimP

Chain X:  87% 5% • 7%



4.2.4 Score per residue for model 4

- Molecule 1: Ribosome maturation factor RimP

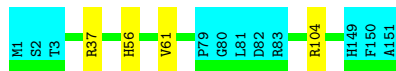
Chain X:  89% • 7%



4.2.5 Score per residue for model 5

- Molecule 1: Ribosome maturation factor RimP

Chain X:  90% • 7%



4.2.6 Score per residue for model 6

- Molecule 1: Ribosome maturation factor RimP

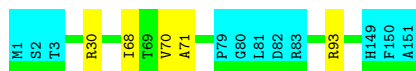
Chain X:  87% 5% • 7%



4.2.7 Score per residue for model 7

- Molecule 1: Ribosome maturation factor RimP

Chain X:  89% • 7%



4.2.8 Score per residue for model 8

- Molecule 1: Ribosome maturation factor RimP

Chain X:  90% • 7%



4.2.9 Score per residue for model 9

- Molecule 1: Ribosome maturation factor RimP

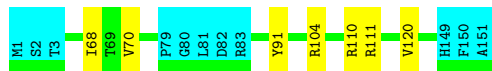
Chain X:  90% • 7%



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Ribosome maturation factor RimP

Chain X:  88% 5% 7%



4.2.11 Score per residue for model 11

- Molecule 1: Ribosome maturation factor RimP

Chain X:  89% • 7%



4.2.12 Score per residue for model 12

- Molecule 1: Ribosome maturation factor RimP

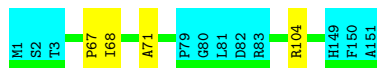
Chain X:  87% 6% 7%



4.2.13 Score per residue for model 13

- Molecule 1: Ribosome maturation factor RimP

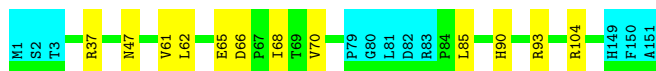
Chain X:  90% • 7%



4.2.14 Score per residue for model 14

- Molecule 1: Ribosome maturation factor RimP

Chain X:  85% 8% 7%



4.2.15 Score per residue for model 15

- Molecule 1: Ribosome maturation factor RimP

Chain X:  86% 7% 7%



4.2.16 Score per residue for model 16

- Molecule 1: Ribosome maturation factor RimP

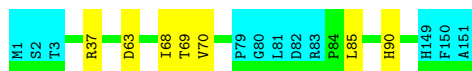
Chain X:  86% 7% 7%



4.2.17 Score per residue for model 17

- Molecule 1: Ribosome maturation factor RimP

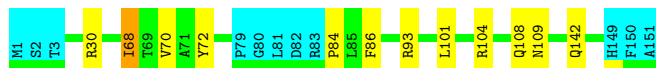
Chain X:  88% 5% 7%



4.2.18 Score per residue for model 18

- Molecule 1: Ribosome maturation factor RimP

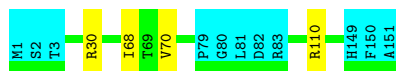
Chain X:  85% 7% • 7%



4.2.19 Score per residue for model 19

- Molecule 1: Ribosome maturation factor RimP

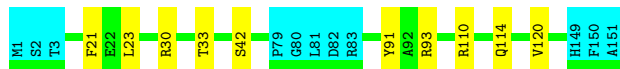
Chain X:  90% • 7%



4.2.20 Score per residue for model 20

- Molecule 1: Ribosome maturation factor RimP

Chain X:  86% 7% 7%



5 Refinement protocol and experimental data overview

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

Of the 120 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
X-PLOR NIH	structure calculation	
GROMACS	refinement	

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	1755
Number of shifts mapped to atoms	1755
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	X	0.92±0.01	0±0/1105 (0.0± 0.0%)	1.33±0.03	3±1/1503 (0.2± 0.1%)
All	All	0.92	0/22100 (0.0%)	1.33	51/30060 (0.2%)

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	X	0.0±0.0	0.3±0.5
All	All	0	7

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	X	30	ARG	NE-CZ-NH2	7.03	125.52	119.20	11	9
1	X	47	ASN	CA-CB-CG	6.90	119.50	112.60	14	1
1	X	93	ARG	NE-CZ-NH2	6.71	125.24	119.20	20	8
1	X	32	ARG	NE-CZ-NH2	6.55	125.10	119.20	15	2
1	X	110	ARG	NE-CZ-NH2	6.42	124.98	119.20	19	4
1	X	94	PHE	CA-CB-CG	6.21	120.01	113.80	15	1
1	X	37	ARG	NE-CZ-NH2	6.07	124.66	119.20	16	7
1	X	104	ARG	NE-CZ-NH2	5.96	124.56	119.20	14	8
1	X	90	HIS	CA-CB-CG	5.79	119.59	113.80	12	1
1	X	32	ARG	N-CA-C	-5.51	105.28	111.28	3	1
1	X	114	GLN	OE1-CD-NE2	-5.45	117.15	122.60	20	2
1	X	109	ASN	CA-CB-CG	5.35	117.95	112.60	12	1
1	X	111	ARG	NE-CZ-NH2	5.27	123.94	119.20	10	2
1	X	56	HIS	CB-CG-CD2	-5.14	124.52	131.20	8	2
1	X	90	HIS	CB-CG-CD2	-5.09	124.58	131.20	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	X	5	GLU	N-CA-C	-5.07	107.22	113.41	15	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	X	32	ARG	Peptide	3
1	X	72	TYR	Sidechain	1
1	X	111	ARG	Sidechain	1
1	X	108	GLN	Peptide	1
1	X	23	LEU	Peptide	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	X	1089	1092	1092	3±3
All	All	21780	21840	21840	55

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:X:66:ASP:OD1	1:X:68:ILE:O	1.10	1.66	6	1
1:X:68:ILE:HG23	1:X:71:ALA:HB3	1.08	1.23	7	1
1:X:68:ILE:CG2	1:X:71:ALA:HB3	1.01	1.86	7	2
1:X:68:ILE:CG2	1:X:71:ALA:CB	0.91	2.48	7	2
1:X:68:ILE:O	1:X:72:TYR:HB2	0.88	1.68	18	1
1:X:68:ILE:HG23	1:X:71:ALA:CB	0.88	1.98	7	1
1:X:61:VAL:O	1:X:65:GLU:HG2	0.87	1.69	14	1
1:X:68:ILE:HG22	1:X:71:ALA:HB3	0.76	1.57	15	1
1:X:69:THR:HG22	1:X:70:VAL:H	0.72	1.43	1	1
1:X:90:HIS:ND1	1:X:93:ARG:NH1	0.71	2.38	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:X:68:ILE:HD12	1:X:71:ALA:HB3	0.70	1.61	3	1
1:X:68:ILE:O	1:X:68:ILE:HG23	0.69	1.86	16	1
1:X:90:HIS:CE1	1:X:93:ARG:NH1	0.68	2.62	16	1
1:X:68:ILE:O	1:X:72:TYR:HD2	0.65	1.73	15	1
1:X:69:THR:HG22	1:X:70:VAL:N	0.64	2.08	1	1
1:X:68:ILE:HG21	1:X:71:ALA:CB	0.63	2.21	7	1
1:X:68:ILE:O	1:X:68:ILE:HG13	0.60	1.96	19	1
1:X:68:ILE:HG22	1:X:71:ALA:CB	0.60	2.24	15	1
1:X:104:ARG:HG2	1:X:142:GLN:HB2	0.60	1.72	18	1
1:X:90:HIS:CE1	1:X:93:ARG:HH12	0.59	2.15	16	1
1:X:68:ILE:HG21	1:X:71:ALA:HB2	0.58	1.75	7	1
1:X:91:TYR:HB3	1:X:120:VAL:HG21	0.56	1.75	10	3
1:X:68:ILE:CG1	1:X:71:ALA:HB3	0.56	2.31	16	1
1:X:68:ILE:CG2	1:X:70:VAL:CG1	0.54	2.85	6	1
1:X:63:ASP:O	1:X:69:THR:HG22	0.52	2.04	17	1
1:X:68:ILE:CG2	1:X:71:ALA:HB2	0.52	2.31	7	1
1:X:68:ILE:O	1:X:72:TYR:CD2	0.51	2.60	15	1
1:X:69:THR:HG23	1:X:72:TYR:HB2	0.51	1.82	2	1
1:X:68:ILE:HG12	1:X:71:ALA:CB	0.50	2.36	12	1
1:X:67:PRO:HB2	1:X:68:ILE:HD12	0.50	1.84	13	1
1:X:68:ILE:O	1:X:72:TYR:CB	0.49	2.54	18	1
1:X:68:ILE:O	1:X:68:ILE:CG2	0.49	2.58	16	1
1:X:68:ILE:HG13	1:X:71:ALA:HB3	0.46	1.86	16	1
1:X:120:VAL:HG22	1:X:125:ILE:HG23	0.46	1.88	9	1
1:X:68:ILE:HG23	1:X:68:ILE:O	0.46	2.10	7	1
1:X:125:ILE:CD1	1:X:138:LEU:HD23	0.45	2.41	6	1
1:X:68:ILE:HG22	1:X:71:ALA:H	0.45	1.71	13	2
1:X:62:LEU:HD12	1:X:66:ASP:OD1	0.45	2.11	14	1
1:X:68:ILE:CG2	1:X:70:VAL:HG13	0.45	2.42	6	1
1:X:68:ILE:HD11	1:X:72:TYR:CE1	0.44	2.46	3	1
1:X:68:ILE:HG22	1:X:68:ILE:O	0.44	2.11	15	1
1:X:85:LEU:HD11	1:X:90:HIS:HB3	0.44	1.88	14	2
1:X:21:PHE:CD1	1:X:42:SER:HB3	0.43	2.49	20	1
1:X:61:VAL:O	1:X:65:GLU:CG	0.42	2.58	14	1
1:X:62:LEU:CD1	1:X:66:ASP:OD1	0.42	2.67	14	1
1:X:108:GLN:O	1:X:109:ASN:C	0.42	2.61	18	1
1:X:68:ILE:CG2	1:X:70:VAL:HG12	0.42	2.45	6	1
1:X:84:PRO:HG2	1:X:86:PHE:CE1	0.42	2.50	18	1
1:X:8:LEU:HD13	1:X:65:GLU:HG2	0.41	1.93	11	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	140/151 (93%)	137±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	100	100
All	All	2800/3020 (93%)	2738 (98%)	62 (2%)	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	X	121/130 (93%)	120±1 (99±1%)	1±1 (1±1%)	61	94
All	All	2420/2600 (93%)	2392 (99%)	28 (1%)	61	94

All 10 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	X	70	VAL	11
1	X	68	ILE	6
1	X	61	VAL	3
1	X	85	LEU	2
1	X	127	VAL	1
1	X	64	VAL	1
1	X	69	THR	1
1	X	72	TYR	1
1	X	101	LEU	1
1	X	33	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1755
Number of shifts mapped to atoms	1755
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	-0.02 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	139	0.11 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	147	0.28 ± 0.13	None needed (< 0.5 ppm)
^{15}N	138	-0.01 ± 0.27	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1671 atoms were assigned a chemical shift out of a possible 1910. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	689/700 (98%)	279/284 (98%)	279/280 (100%)	131/136 (96%)
Sidechain	972/1107 (88%)	655/724 (90%)	310/347 (89%)	7/36 (19%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	10/103 (10%)	10/51 (20%)	0/49 (0%)	0/3 (0%)
Overall	1671/1910 (87%)	944/1059 (89%)	589/676 (87%)	138/175 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1755 atoms were assigned a chemical shift out of a possible 2054. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	728/754 (97%)	295/306 (96%)	295/302 (98%)	138/146 (95%)
Sidechain	1015/1180 (86%)	684/772 (89%)	324/369 (88%)	7/39 (18%)
Aromatic	12/120 (10%)	12/60 (20%)	0/56 (0%)	0/4 (0%)
Overall	1755/2054 (85%)	991/1138 (87%)	619/727 (85%)	145/189 (77%)

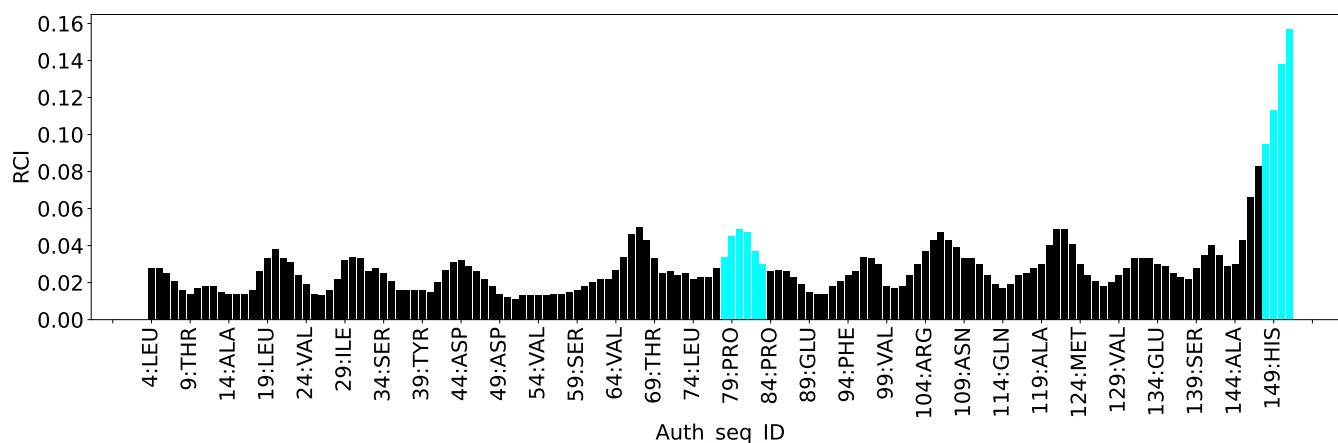
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain X:



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	2516
Intra-residue ($ i-j =0$)	731
Sequential ($ i-j =1$)	860
Medium range ($ i-j >1$ and $ i-j <5$)	394
Long range ($ i-j \geq 5$)	391
Inter-chain	0
Hydrogen bond restraints	140
Disulfide bond restraints	0
Total dihedral-angle restraints	264
Number of unmapped restraints	0
Number of restraints per residue	18.4
Number of long range restraints per residue ¹	3.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	44.0	0.2
0.2-0.5 (Medium)	58.3	0.5
>0.5 (Large)	31.1	4.78

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)	32.2	9.95
10.0-20.0 (Medium)	4.6	19.91
>20.0 (Large)	6.7	159.92

9 Distance violation analysis ⓘ

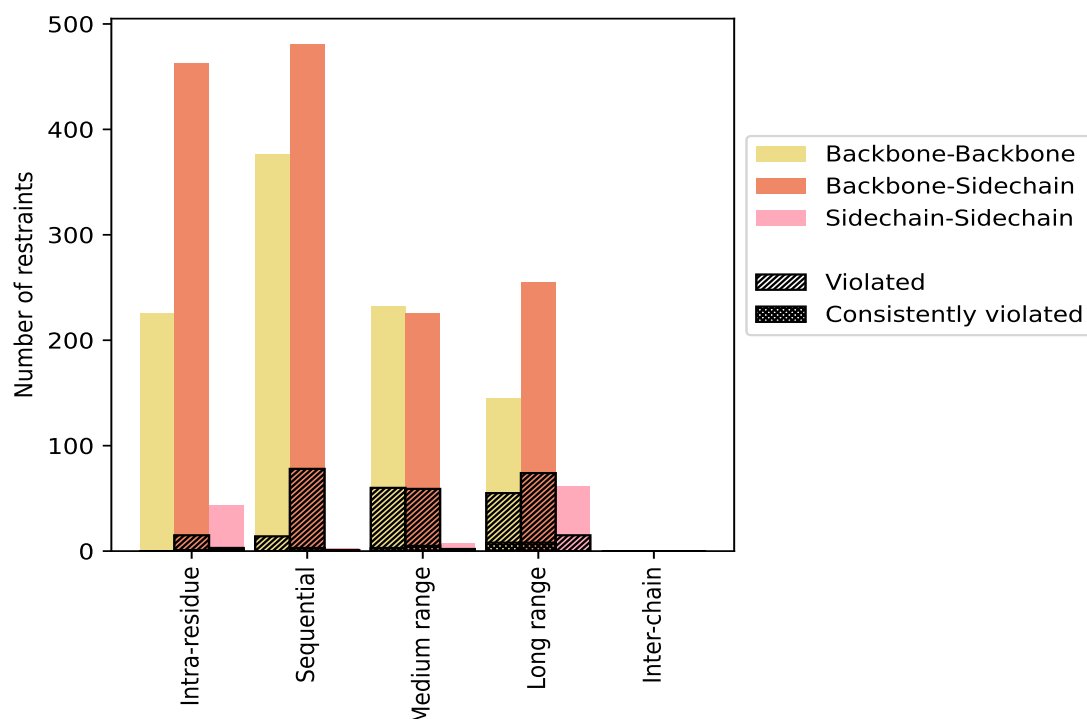
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	731	29.1	18	2.5	0.7	2	0.3	0.1
Backbone-Backbone	225	8.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	463	18.4	15	3.2	0.6	1	0.2	0.0
Sidechain-Sidechain	43	1.7	3	7.0	0.1	1	2.3	0.0
Sequential ($i-j =1$)	860	34.2	93	10.8	3.7	3	0.3	0.1
Backbone-Backbone	376	14.9	14	3.7	0.6	0	0.0	0.0
Backbone-Sidechain	481	19.1	78	16.2	3.1	3	0.6	0.1
Sidechain-Sidechain	3	0.1	1	33.3	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	394	15.7	87	22.1	3.5	6	1.5	0.2
Backbone-Backbone	232	9.2	60	25.9	2.4	3	1.3	0.1
Backbone-Sidechain	155	6.2	25	16.1	1.0	3	1.9	0.1
Sidechain-Sidechain	7	0.3	2	28.6	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	391	15.5	125	32.0	5.0	10	2.6	0.4
Backbone-Backbone	145	5.8	55	37.9	2.2	8	5.5	0.3
Backbone-Sidechain	185	7.4	55	29.7	2.2	2	1.1	0.1
Sidechain-Sidechain	61	2.4	15	24.6	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	140	5.6	53	37.9	2.1	8	5.7	0.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2516	100.0	376	14.9	14.9	29	1.2	1.2
Backbone-Backbone	978	38.9	129	13.2	5.1	11	1.1	0.4
Backbone-Sidechain	1424	56.6	226	15.9	9.0	17	1.2	0.7
Sidechain-Sidechain	114	4.5	21	18.4	0.8	1	0.9	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	9	29	54	55	0	147	0.42	2.46	0.35	0.32
2	9	28	57	54	0	148	0.4	2.1	0.31	0.3
3	8	28	45	56	0	137	0.38	1.51	0.29	0.28
4	6	28	54	53	0	141	0.35	2.26	0.28	0.24
5	8	26	44	76	0	154	0.4	1.85	0.31	0.3
6	8	29	35	50	0	122	0.36	2.38	0.32	0.29
7	5	22	43	48	0	118	0.41	1.61	0.32	0.3
8	7	22	45	38	0	112	0.36	1.62	0.27	0.28
9	8	31	52	52	0	143	0.42	1.74	0.33	0.32
10	7	28	62	50	0	147	0.42	2.27	0.38	0.3

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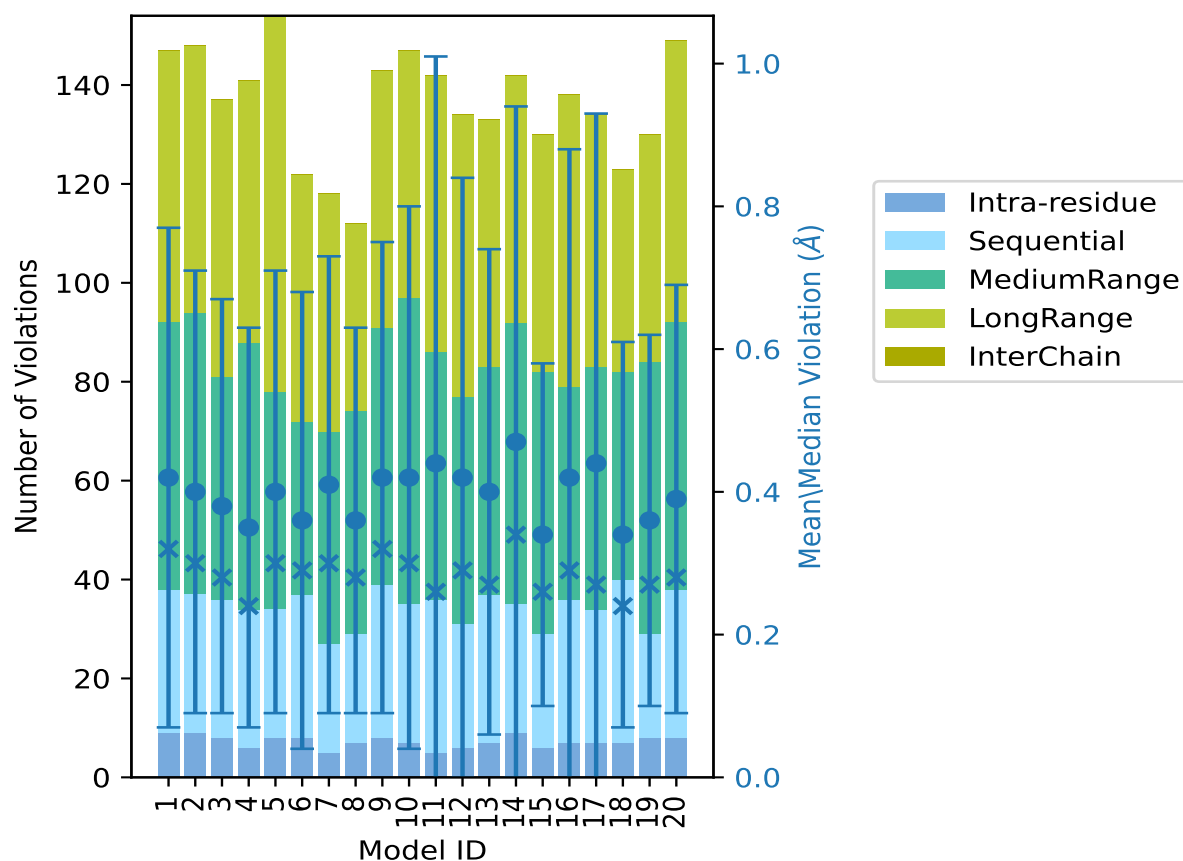
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	5	31	50	56	0	142	0.44	4.78	0.57	0.26
12	6	25	46	57	0	134	0.42	2.76	0.42	0.29
13	7	30	46	50	0	133	0.4	2.27	0.34	0.27
14	9	26	57	50	0	142	0.47	3.02	0.47	0.34
15	6	23	53	48	0	130	0.34	1.3	0.24	0.26
16	7	29	43	59	0	138	0.42	3.13	0.46	0.29
17	7	27	49	51	0	134	0.44	3.3	0.49	0.27
18	7	33	42	41	0	123	0.34	1.58	0.27	0.24
19	8	21	55	46	0	130	0.36	1.63	0.26	0.27
20	8	30	54	57	0	149	0.39	1.77	0.3	0.28

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

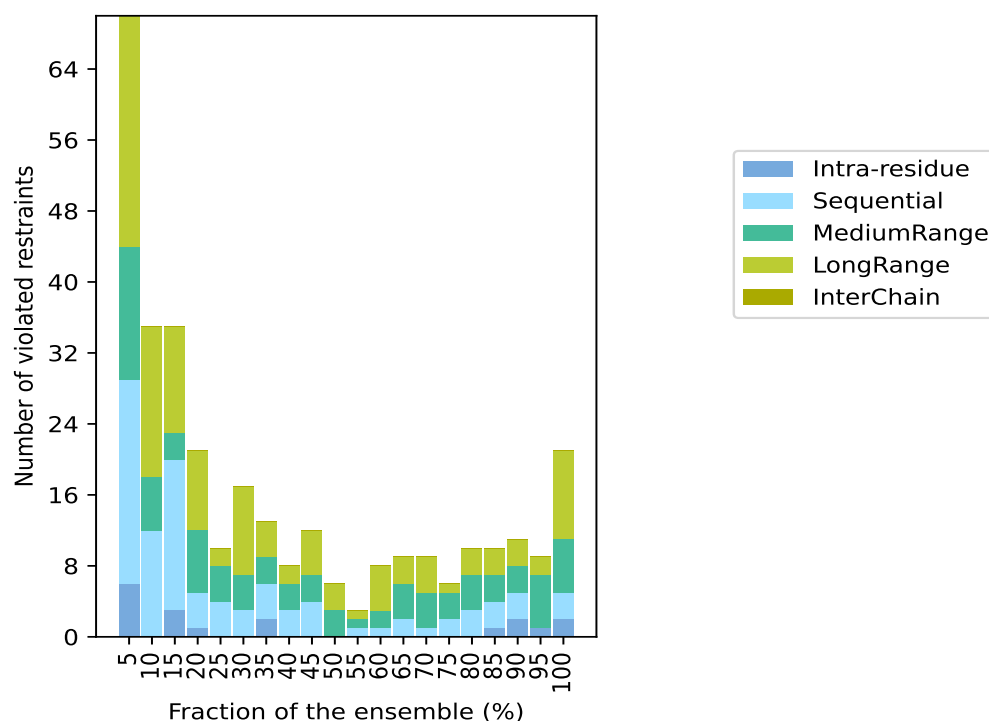
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2053(IR:713, SQ:767, MR:307, LR:266, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
6	23	15	26	0	70	1	5.0
0	12	6	17	0	35	2	10.0
3	17	3	12	0	35	3	15.0
1	4	7	9	0	21	4	20.0
0	4	4	2	0	10	5	25.0
0	3	4	10	0	17	6	30.0
2	4	3	4	0	13	7	35.0
0	3	3	2	0	8	8	40.0
0	4	3	5	0	12	9	45.0
0	0	3	3	0	6	10	50.0
0	1	1	1	0	3	11	55.0
0	1	2	5	0	8	12	60.0
0	2	4	3	0	9	13	65.0
0	1	4	4	0	9	14	70.0
0	2	3	1	0	6	15	75.0
0	3	4	3	0	10	16	80.0
1	3	3	3	0	10	17	85.0
2	3	3	3	0	11	18	90.0
1	0	6	2	0	9	19	95.0
2	3	6	10	0	21	20	100.0

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

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

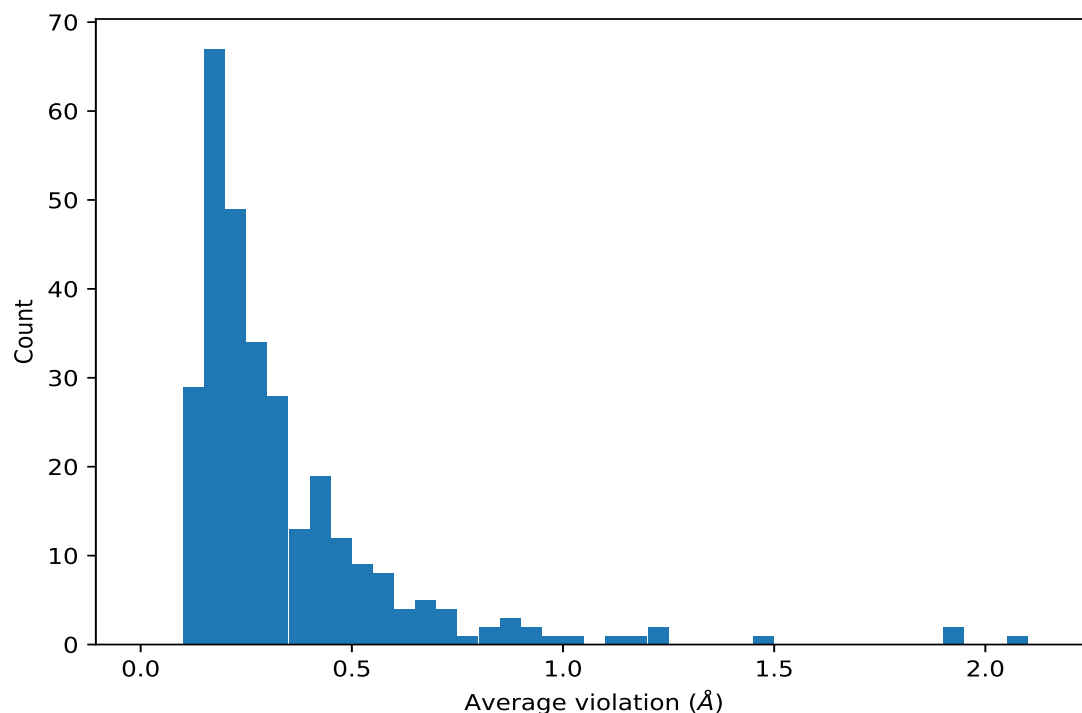
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	20	1.49	0.66	1.6
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	20	1.2	0.14	1.21
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	20	1.16	0.16	1.15
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	20	1.12	0.66	0.76
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	20	1.0	0.2	0.96
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	20	0.93	0.48	0.98
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	20	0.81	0.52	0.49
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	20	0.8	0.3	0.88
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	20	0.75	0.22	0.71
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	20	0.7	0.17	0.66
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	20	0.7	0.39	0.62
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	20	0.67	0.2	0.62
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	20	0.66	0.11	0.64
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	20	0.62	0.2	0.66
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	20	0.62	0.09	0.62
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	20	0.57	0.18	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	20	0.56	0.21	0.55
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	20	0.51	0.11	0.48
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	20	0.51	0.16	0.56
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	20	0.44	0.01	0.45
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	20	0.42	0.2	0.44
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	20	0.41	0.1	0.4
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	20	0.37	0.16	0.35
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	20	0.31	0.0	0.31
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	20	0.31	0.12	0.3
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	20	0.3	0.13	0.28
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	20	0.24	0.16	0.21
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	20	0.22	0.16	0.2
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	20	0.19	0.06	0.17
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	19	0.57	0.25	0.6
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	19	0.53	0.39	0.35
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	19	0.43	0.02	0.43
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	19	0.38	0.13	0.41
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	19	0.35	0.12	0.35
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	19	0.31	0.11	0.29
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	19	0.27	0.12	0.23
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	19	0.26	0.1	0.26
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	19	0.24	0.08	0.23
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	18	1.21	1.33	0.57
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	18	0.48	0.11	0.49
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	18	0.47	0.27	0.43
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	18	0.43	0.02	0.43
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	18	0.42	0.01	0.42
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	18	0.41	0.19	0.44
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	18	0.4	0.15	0.38
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	18	0.32	0.19	0.26
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	18	0.3	0.12	0.3
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	18	0.3	0.12	0.27
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	18	0.26	0.12	0.23
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	18	0.21	0.06	0.2
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	17	0.85	0.32	0.88
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	17	0.67	0.37	0.6
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	17	0.53	0.41	0.34
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	17	0.52	0.12	0.53
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	17	0.27	0.1	0.25
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	17	0.26	0.12	0.24
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	17	0.22	0.08	0.2
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	17	0.22	0.07	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	17	0.2	0.09	0.18
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	17	0.2	0.05	0.18
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	16	0.64	0.15	0.66
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	16	0.6	0.48	0.48
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	16	0.58	0.33	0.49
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	16	0.55	0.36	0.38
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	16	0.47	0.36	0.32
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	16	0.42	0.2	0.36
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	16	0.37	0.17	0.33
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	16	0.36	0.16	0.32
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	16	0.3	0.15	0.28
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	16	0.26	0.07	0.25
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	15	0.3	0.15	0.28
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	15	0.22	0.06	0.19
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	15	0.17	0.07	0.15
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	15	0.17	0.04	0.17
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	15	0.16	0.03	0.16
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	15	0.15	0.03	0.15
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	14	0.49	0.2	0.56
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	14	0.42	0.23	0.42
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	14	0.29	0.15	0.26
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	14	0.27	0.09	0.26
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	14	0.26	0.1	0.28
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	14	0.22	0.07	0.22
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	14	0.2	0.05	0.19
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	14	0.17	0.04	0.16
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	14	0.16	0.03	0.16
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	13	0.53	0.36	0.37
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	13	0.42	0.21	0.42
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	13	0.41	0.28	0.34
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	13	0.39	0.15	0.4
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	13	0.34	0.09	0.34
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	13	0.31	0.14	0.29
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	13	0.25	0.13	0.2
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	13	0.22	0.13	0.18
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	13	0.11	0.01	0.12
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	13	0.11	0.01	0.11
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	12	0.46	0.36	0.32
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	12	0.43	0.26	0.4
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	12	0.38	0.24	0.28
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	12	0.33	0.13	0.32
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	12	0.31	0.08	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	12	0.25	0.05	0.25
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	12	0.23	0.07	0.2
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	12	0.22	0.1	0.19
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	12	0.2	0.07	0.2
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	12	0.19	0.09	0.16
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	11	0.24	0.14	0.16
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	11	0.19	0.07	0.19
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	11	0.18	0.05	0.18
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	10	0.43	0.18	0.5
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	10	0.33	0.12	0.32
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	10	0.3	0.13	0.24
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	10	0.26	0.04	0.26
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	10	0.26	0.12	0.23
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	10	0.24	0.15	0.18
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	10	0.16	0.04	0.16
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	9	0.89	0.31	1.0
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	9	0.87	0.42	0.77
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	9	0.5	0.38	0.31
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	9	0.36	0.21	0.31
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	9	0.32	0.11	0.33
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	9	0.27	0.12	0.24
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	9	0.25	0.14	0.22
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	9	0.22	0.1	0.22
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	9	0.21	0.07	0.2
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	9	0.21	0.07	0.2
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	9	0.19	0.08	0.18
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	9	0.19	0.06	0.18
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	9	0.16	0.05	0.15
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	9	0.14	0.02	0.14
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	8	0.72	0.85	0.3
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	8	0.72	0.59	0.41
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	8	0.49	0.09	0.51
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	8	0.34	0.11	0.32
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	8	0.29	0.11	0.24
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	8	0.27	0.07	0.29
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	8	0.25	0.1	0.22
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	8	0.19	0.03	0.18
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	8	0.17	0.05	0.16
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	8	0.16	0.05	0.16
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	8	0.16	0.04	0.15
(2,4)	1:8:X:LEU:CD1	1:11:X:MET:CE	7	1.92	1.25	2.72
(2,4)	1:8:X:LEU:CD2	1:11:X:MET:CE	7	1.92	1.25	2.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,665)	1:78:X:SER:HA	1:40:X:ILE:H	7	0.94	0.86	0.29
(1,664)	1:77:X:SER:HB3	1:78:X:SER:H	7	0.47	0.11	0.51
(3,474)	1:68:X:ILE:N	1:68:X:ILE:CG2	7	0.42	0.02	0.43
(3,45)	1:11:X:MET:N	1:11:X:MET:CG	7	0.42	0.02	0.42
(3,130)	1:25:X:GLY:N	1:23:X:LEU:CG	7	0.28	0.11	0.22
(3,797)	1:121:X:ASP:N	1:120:X:VAL:CB	7	0.2	0.03	0.2
(5,12)	1:23:X:LEU:C	1:41:X:ASP:H	7	0.2	0.07	0.2
(5,39)	1:73:X:ASN:C	1:36:X:LEU:H	7	0.19	0.04	0.17
(1,164)	1:29:X:ILE:H	1:28:X:PHE:CZ	7	0.18	0.06	0.16
(1,467)	1:58:X:VAL:HB	1:56:X:HIS:H	7	0.17	0.08	0.13
(5,57)	1:119:X:ALA:C	1:126:X:THR:H	7	0.14	0.03	0.12
(3,189)	1:34:X:SER:N	1:33:X:THR:CB	7	0.12	0.02	0.12
(1,701)	1:87:X:THR:H	1:86:X:PHE:HB2	6	0.46	0.21	0.44
(1,756)	1:94:X:PHE:HA	1:97:X:GLU:H	6	0.35	0.12	0.34
(1,997)	1:124:X:MET:HG3	1:138:X:LEU:H	6	0.35	0.2	0.29
(3,333)	1:54:X:VAL:N	1:40:X:ILE:CD1	6	0.34	0.29	0.25
(3,610)	1:94:X:PHE:N	1:85:X:LEU:CD1	6	0.33	0.23	0.24
(3,663)	1:91:X:TYR:N	1:125:X:ILE:CD1	6	0.28	0.12	0.26
(1,500)	1:59:X:SER:H	1:62:X:LEU:HB3	6	0.26	0.08	0.28
(2,22)	1:16:X:VAL:CG1	1:54:X:VAL:CG2	6	0.23	0.09	0.2
(4,87)	1:89:X:GLU:O	1:93:X:ARG:H	6	0.22	0.1	0.16
(3,667)	1:95:X:VAL:N	1:117:X:ILE:CG2	6	0.2	0.09	0.17
(1,769)	1:95:X:VAL:HB	1:97:X:GLU:H	6	0.19	0.05	0.2
(1,561)	1:65:X:GLU:H	1:64:X:VAL:CB	6	0.19	0.08	0.16
(5,29)	1:52:X:ALA:C	1:56:X:HIS:H	6	0.17	0.05	0.15
(5,63)	1:128:X:THR:C	1:116:X:VAL:H	6	0.16	0.06	0.14
(5,18)	1:35:X:THR:C	1:29:X:ILE:H	6	0.16	0.03	0.15
(3,922)	1:141:X:ILE:N	1:140:X:ASN:CB	6	0.15	0.03	0.16
(5,61)	1:126:X:THR:C	1:118:X:LYS:H	6	0.15	0.04	0.14
(5,70)	1:145:X:ASN:C	1:100:X:THR:H	6	0.13	0.01	0.13
(3,587)	1:91:X:TYR:N	1:85:X:LEU:CD1	5	0.58	0.31	0.79
(5,58)	1:121:X:ASP:C	1:124:X:MET:H	5	0.5	0.06	0.5
(5,3)	1:6:X:GLN:C	1:10:X:GLU:H	5	0.39	0.25	0.37
(1,813)	1:99:X:VAL:H	1:117:X:ILE:HG12	5	0.35	0.07	0.4
(5,2)	1:5:X:GLU:C	1:9:X:THR:H	5	0.29	0.2	0.21
(4,65)	1:56:X:HIS:O	1:60:X:ALA:H	5	0.23	0.12	0.17
(1,243)	1:37:X:ARG:H	1:36:X:LEU:HB3	5	0.2	0.08	0.23
(4,67)	1:57:X:GLN:O	1:61:X:VAL:H	5	0.2	0.08	0.19
(3,556)	1:87:X:THR:N	1:86:X:PHE:CB	5	0.18	0.03	0.19
(1,51)	1:10:X:GLU:H	1:7:X:LYS:HA	5	0.17	0.03	0.16
(1,562)	1:65:X:GLU:HB2	1:64:X:VAL:H	5	0.17	0.05	0.15
(4,21)	1:15:X:PRO:O	1:19:X:LEU:H	5	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,200)	1:33:X:THR:H	1:32:X:ARG:HG2	5	0.14	0.03	0.15
(3,448)	1:65:X:GLU:N	1:11:X:MET:CE	4	2.07	0.61	1.8
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD1	4	0.45	0.21	0.5
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD2	4	0.45	0.21	0.5
(2,28)	1:29:X:ILE:CG2	1:29:X:ILE:CD1	4	0.43	0.01	0.43
(1,900)	1:108:X:GLN:HB2	1:109:X:ASN:H	4	0.34	0.09	0.31
(2,86)	1:91:X:TYR:CA	1:117:X:ILE:CD1	4	0.32	0.08	0.34
(2,107)	1:120:X:VAL:CG2	1:125:X:ILE:CD1	4	0.26	0.09	0.29
(1,1148)	1:141:X:ILE:HG13	1:137:X:ALA:H	4	0.24	0.05	0.25
(1,625)	1:74:X:LEU:HD21	1:39:X:TYR:H	4	0.24	0.09	0.22
(1,625)	1:74:X:LEU:HD22	1:39:X:TYR:H	4	0.24	0.09	0.22
(1,625)	1:74:X:LEU:HD23	1:39:X:TYR:H	4	0.24	0.09	0.22
(1,444)	1:56:X:HIS:HB3	1:55:X:SER:H	4	0.22	0.05	0.22
(1,5)	1:5:X:GLU:H	1:4:X:LEU:HG	4	0.2	0.04	0.2
(4,68)	1:57:X:GLN:O	1:61:X:VAL:N	4	0.2	0.08	0.18
(5,67)	1:136:X:PHE:C	1:125:X:ILE:H	4	0.19	0.04	0.2
(3,554)	1:85:X:LEU:CA	1:87:X:THR:N	4	0.18	0.03	0.18
(5,24)	1:47:X:ASN:C	1:50:X:ASP:H	4	0.18	0.07	0.14
(5,9)	1:13:X:THR:C	1:17:X:GLU:H	4	0.17	0.03	0.18
(3,666)	1:94:X:PHE:N	1:117:X:ILE:CG2	4	0.17	0.04	0.18
(2,121)	1:138:X:LEU:CD1	1:141:X:ILE:CD1	4	0.16	0.02	0.16
(1,96)	1:19:X:LEU:H	1:16:X:VAL:HA	4	0.16	0.03	0.16
(1,975)	1:122:X:GLY:H	1:124:X:MET:H	4	0.16	0.01	0.15
(3,749)	1:113:X:TRP:N	1:101:X:LEU:CD1	4	0.16	0.03	0.16
(5,56)	1:116:X:VAL:C	1:128:X:THR:H	4	0.16	0.03	0.16
(3,366)	1:56:X:HIS:N	1:57:X:GLN:CB	4	0.11	0.01	0.12
(1,890)	1:108:X:GLN:HE21	1:107:X:VAL:CB	3	0.96	0.08	0.99
(2,85)	1:85:X:LEU:CD2	1:117:X:ILE:CD1	3	0.66	0.15	0.7
(1,1001)	1:125:X:ILE:H	1:124:X:MET:HB3	3	0.57	0.02	0.57
(3,145)	1:27:X:GLU:N	1:26:X:ILE:CD1	3	0.56	0.31	0.73
(5,15)	1:29:X:ILE:C	1:35:X:THR:H	3	0.47	0.05	0.44
(3,479)	1:70:X:VAL:CG1	1:70:X:VAL:N	3	0.46	0.0	0.46
(1,190)	1:31:X:GLY:H	1:30:X:ARG:HG3	3	0.4	0.07	0.38
(3,464)	1:66:X:ASP:N	1:64:X:VAL:CG1	3	0.37	0.1	0.41
(1,217)	1:35:X:THR:H	1:34:X:SER:HB3	3	0.3	0.06	0.26
(1,755)	1:94:X:PHE:HB3	1:97:X:GLU:H	3	0.28	0.07	0.3
(5,49)	1:97:X:GLU:C	1:117:X:ILE:H	3	0.27	0.21	0.14
(4,54)	1:50:X:ASP:O	1:54:X:VAL:H	3	0.26	0.09	0.27
(3,765)	1:115:X:GLY:N	1:129:X:VAL:CG2	3	0.26	0.08	0.29
(1,581)	1:66:X:ASP:HB2	1:72:X:TYR:H	3	0.25	0.12	0.18
(3,823)	1:124:X:MET:CB	1:125:X:ILE:N	3	0.24	0.0	0.24
(4,53)	1:50:X:ASP:O	1:54:X:VAL:N	3	0.23	0.09	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,159)	1:29:X:ILE:N	1:28:X:PHE:CB	3	0.21	0.06	0.23
(3,484)	1:71:X:ALA:N	1:70:X:VAL:CB	3	0.2	0.07	0.16
(1,307)	1:44:X:ASP:H	1:43:X:GLU:HG2	3	0.19	0.05	0.17
(4,1)	1:4:X:LEU:O	1:8:X:LEU:H	3	0.19	0.08	0.15
(1,643)	1:76:X:VAL:HB	1:55:X:SER:H	3	0.18	0.05	0.16
(4,47)	1:47:X:ASN:O	1:50:X:ASP:H	3	0.17	0.04	0.17
(3,878)	1:133:X:ASP:N	1:128:X:THR:CG2	3	0.17	0.05	0.16
(3,197)	1:35:X:THR:N	1:34:X:SER:CB	3	0.16	0.02	0.15
(3,716)	1:104:X:ARG:N	1:105:X:MET:CB	3	0.16	0.03	0.17
(1,1149)	1:141:X:ILE:H	1:138:X:LEU:HA	3	0.15	0.01	0.15
(5,23)	1:41:X:ASP:C	1:23:X:LEU:H	3	0.15	0.04	0.15
(4,88)	1:89:X:GLU:O	1:93:X:ARG:N	3	0.15	0.04	0.14
(1,670)	1:78:X:SER:HB2	1:78:X:SER:H	3	0.15	0.03	0.17
(5,62)	1:127:X:VAL:C	1:134:X:GLU:H	3	0.15	0.01	0.15
(5,46)	1:115:X:GLY:C	1:99:X:VAL:H	3	0.14	0.02	0.15
(1,236)	1:37:X:ARG:H	1:27:X:GLU:HB2	3	0.14	0.02	0.13
(3,208)	1:36:X:LEU:N	1:37:X:ARG:CG	3	0.14	0.01	0.13
(5,40)	1:75:X:GLU:C	1:38:X:ILE:H	3	0.14	0.04	0.11
(3,534)	1:80:X:GLY:N	1:79:X:PRO:CB	3	0.12	0.02	0.13
(3,566)	1:88:X:ALA:N	1:89:X:GLU:CB	3	0.12	0.0	0.12
(3,92)	1:19:X:LEU:N	1:18:X:ALA:CB	3	0.12	0.01	0.12
(1,553)	1:64:X:VAL:HB	1:64:X:VAL:H	3	0.11	0.0	0.11
(1,584)	1:67:X:PRO:HA	1:68:X:ILE:H	3	0.11	0.01	0.11
(1,592)	1:69:X:THR:HA	1:70:X:VAL:H	3	0.11	0.01	0.11
(3,425)	1:62:X:LEU:N	1:61:X:VAL:CG2	2	0.68	0.56	0.68
(1,495)	1:59:X:SER:HB2	1:60:X:ALA:H	2	0.52	0.04	0.52
(1,685)	1:81:X:LEU:H	1:82:X:ASP:H	2	0.44	0.04	0.44
(1,223)	1:35:X:THR:HG21	1:75:X:GLU:H	2	0.34	0.01	0.34
(1,223)	1:35:X:THR:HG22	1:75:X:GLU:H	2	0.34	0.01	0.34
(1,223)	1:35:X:THR:HG23	1:75:X:GLU:H	2	0.34	0.01	0.34
(4,66)	1:56:X:HIS:O	1:60:X:ALA:N	2	0.3	0.05	0.3
(3,313)	1:52:X:ALA:N	1:40:X:ILE:CD1	2	0.3	0.1	0.3
(4,75)	1:71:X:ALA:O	1:34:X:SER:H	2	0.3	0.02	0.3
(1,172)	1:29:X:ILE:HB	1:35:X:THR:H	2	0.29	0.02	0.29
(1,214)	1:34:X:SER:H	1:73:X:ASN:H	2	0.29	0.18	0.29
(3,203)	1:36:X:LEU:N	1:35:X:THR:CG2	2	0.27	0.07	0.27
(1,1010)	1:125:X:ILE:H	1:136:X:PHE:H	2	0.26	0.01	0.26
(3,212)	1:37:X:ARG:N	1:27:X:GLU:CB	2	0.26	0.11	0.26
(1,841)	1:101:X:LEU:H	1:114:X:GLN:HB2	2	0.25	0.09	0.25
(1,596)	1:71:X:ALA:H	1:70:X:VAL:CB	2	0.24	0.08	0.24
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG21	2	0.24	0.08	0.24
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG22	2	0.24	0.08	0.24

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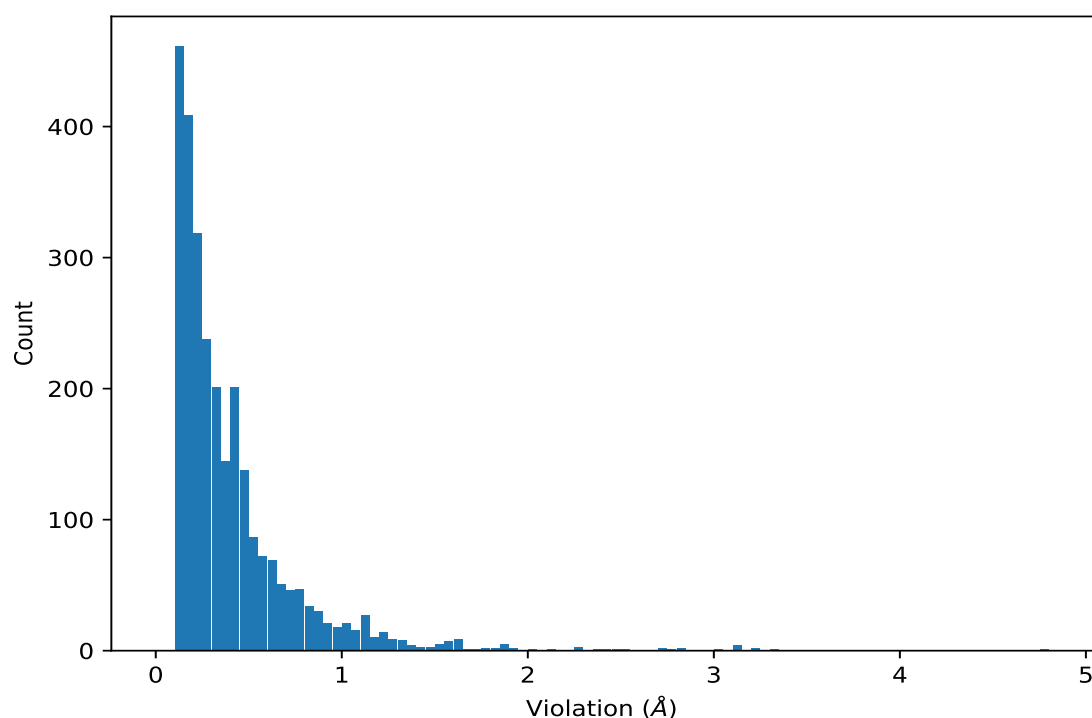
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG23	2	0.24	0.08	0.24
(1,342)	1:47:X:ASN:H	1:46:X:ILE:HG13	2	0.22	0.01	0.22
(3,661)	1:91:X:TYR:N	1:120:X:VAL:CG1	2	0.22	0.01	0.22
(4,2)	1:4:X:LEU:O	1:8:X:LEU:N	2	0.21	0.08	0.21
(4,76)	1:71:X:ALA:O	1:34:X:SER:N	2	0.21	0.08	0.21
(1,411)	1:54:X:VAL:H	1:51:X:CYS:HA	2	0.2	0.03	0.2
(3,847)	1:128:X:THR:CB	1:116:X:VAL:N	2	0.2	0.02	0.2
(1,603)	1:71:X:ALA:HB1	1:72:X:TYR:H	2	0.19	0.09	0.19
(1,603)	1:71:X:ALA:HB2	1:72:X:TYR:H	2	0.19	0.09	0.19
(1,603)	1:71:X:ALA:HB3	1:72:X:TYR:H	2	0.19	0.09	0.19
(1,1095)	1:134:X:GLU:H	1:127:X:VAL:H	2	0.18	0.02	0.18
(1,874)	1:106:X:ALA:HA	1:103:X:LEU:H	2	0.18	0.08	0.18
(3,371)	1:57:X:GLN:N	1:54:X:VAL:CG2	2	0.18	0.06	0.18
(5,19)	1:36:X:LEU:C	1:75:X:GLU:H	2	0.17	0.0	0.17
(4,71)	1:59:X:SER:O	1:63:X:ASP:H	2	0.16	0.04	0.16
(1,144)	1:25:X:GLY:H	1:39:X:TYR:HB2	2	0.16	0.04	0.16
(1,176)	1:29:X:ILE:H	1:36:X:LEU:H	2	0.16	0.04	0.16
(4,115)	1:121:X:ASP:O	1:124:X:MET:H	2	0.16	0.05	0.16
(1,520)	1:62:X:LEU:HB2	1:61:X:VAL:H	2	0.15	0.02	0.15
(3,124)	1:24:X:VAL:N	1:23:X:LEU:CD1	2	0.15	0.0	0.15
(1,985)	1:123:X:GLU:H	1:124:X:MET:HB2	2	0.14	0.0	0.14
(5,6)	1:9:X:THR:C	1:13:X:THR:H	2	0.14	0.01	0.14
(1,383)	1:50:X:ASP:HA	1:53:X:ASP:H	2	0.14	0.02	0.14
(3,239)	1:41:X:ASP:N	1:16:X:VAL:CG1	2	0.14	0.02	0.14
(1,943)	1:116:X:VAL:HB	1:128:X:THR:H	2	0.12	0.02	0.12
(2,29)	1:29:X:ILE:CD1	1:35:X:THR:CG2	2	0.12	0.02	0.12
(3,921)	1:141:X:ILE:N	1:101:X:LEU:CD2	2	0.12	0.02	0.12
(1,595)	1:71:X:ALA:H	1:70:X:VAL:HA	2	0.12	0.01	0.12
(1,521)	1:62:X:LEU:H	1:61:X:VAL:CB	2	0.12	0.0	0.12
(4,117)	1:124:X:MET:O	1:121:X:ASP:H	2	0.12	0.0	0.12
(3,315)	1:52:X:ALA:N	1:48:X:VAL:CA	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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)
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	11	4.78
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	17	3.3
(2,4)	1:8:X:LEU:CD1	1:11:X:MET:CE	17	3.23
(2,4)	1:8:X:LEU:CD2	1:11:X:MET:CE	17	3.23
(2,4)	1:8:X:LEU:CD1	1:11:X:MET:CE	16	3.13
(2,4)	1:8:X:LEU:CD2	1:11:X:MET:CE	16	3.13
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	16	3.11
(3,448)	1:65:X:GLU:N	1:11:X:MET:CE	11	3.11
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	14	3.02
(2,4)	1:8:X:LEU:CD1	1:11:X:MET:CE	11	2.82
(2,4)	1:8:X:LEU:CD2	1:11:X:MET:CE	11	2.82
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	12	2.76
(2,4)	1:8:X:LEU:CD1	1:11:X:MET:CE	14	2.72
(2,4)	1:8:X:LEU:CD2	1:11:X:MET:CE	14	2.72
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	11	2.53
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	1	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:78:X:SER:HA	1:40:X:ILE:H	12	2.44
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	6	2.38
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	13	2.27
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	10	2.27
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	4	2.26
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	2	2.1
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	12	2.03
(3,448)	1:65:X:GLU:N	1:11:X:MET:CE	17	1.94
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	10	1.9
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	1	1.88
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	14	1.88
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	14	1.87
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	6	1.86
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	5	1.85
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	17	1.82
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	13	1.8
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	14	1.79
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	20	1.77
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	9	1.74
(3,448)	1:65:X:GLU:N	1:11:X:MET:CE	14	1.65
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	1	1.64
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	10	1.64
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	20	1.64
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	19	1.63
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	16	1.62
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	8	1.62
(1,665)	1:78:X:SER:HA	1:40:X:ILE:H	16	1.62
(1,665)	1:78:X:SER:HA	1:40:X:ILE:H	7	1.61
(3,448)	1:65:X:GLU:N	1:11:X:MET:CE	16	1.6
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	10	1.59
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	10	1.59
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	17	1.59
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	12	1.58
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	18	1.58
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	9	1.57
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	1	1.56
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	5	1.53
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	17	1.52
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	3	1.51
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	5	1.5
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	5	1.5
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	1	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	3	1.45
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	7	1.45
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	14	1.44
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	14	1.42
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	10	1.41
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	3	1.39
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	12	1.37
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	9	1.36
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	14	1.36
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	13	1.33
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	10	1.33
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	3	1.32
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	7	1.32
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	2	1.32
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	4	1.31
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	8	1.31
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	15	1.3
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	13	1.28
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	16	1.28
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	17	1.27
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	15	1.26
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	13	1.25
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	10	1.25
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	12	1.25
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	7	1.25
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	9	1.25
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	1	1.24
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	19	1.24
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	6	1.24
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	12	1.24
(3,425)	1:62:X:LEU:N	1:61:X:VAL:CG2	2	1.24
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	10	1.24
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	7	1.24
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	18	1.22
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	11	1.22
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	12	1.21
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	2	1.21
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	19	1.21
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	13	1.21
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	16	1.2
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	11	1.18
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	8	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	9	1.18
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	7	1.17
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	6	1.15
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	20	1.15
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	12	1.15
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	16	1.15
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	10	1.15
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	11	1.15
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	7	1.14
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	5	1.14
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	1	1.14
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	14	1.14
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	3	1.14
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	16	1.13
(1,1146)	1:141:X:ILE:CG2	1:102:X:VAL:H	5	1.13
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	11	1.13
(1,913)	1:109:X:ASN:H	1:110:X:ARG:H	9	1.13
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	14	1.13
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	3	1.12
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	17	1.12
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	9	1.12
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	9	1.12
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	16	1.11
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	20	1.11
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	16	1.11
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	20	1.11
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	18	1.11
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	20	1.11
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	10	1.11
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	2	1.1
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	11	1.1
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	14	1.1
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	17	1.1
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	20	1.1
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	7	1.1
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	6	1.09
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	19	1.09
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	3	1.09
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	7	1.08
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	18	1.08
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	2	1.08
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	1	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	1	1.07
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	15	1.07
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	12	1.07
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	9	1.07
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	8	1.06
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	20	1.06
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	13	1.06
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	14	1.05
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	3	1.05
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	19	1.04
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	19	1.04
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	14	1.04
(1,890)	1:108:X:GLN:HE21	1:107:X:VAL:CB	11	1.04
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	4	1.03
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	5	1.03
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	18	1.03
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	18	1.03
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	17	1.03
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	16	1.02
(1,881)	1:106:X:ALA:HB1	1:110:X:ARG:H	9	1.02
(1,881)	1:106:X:ALA:HB2	1:110:X:ARG:H	9	1.02
(1,881)	1:106:X:ALA:HB3	1:110:X:ARG:H	9	1.02
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	13	1.01
(2,4)	1:8:X:LEU:CD1	1:11:X:MET:CE	2	1.01
(2,4)	1:8:X:LEU:CD2	1:11:X:MET:CE	2	1.01
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	18	1.01
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	12	1.0
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	10	1.0
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	17	1.0
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	2	1.0
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	2	0.99
(1,890)	1:108:X:GLN:HE21	1:107:X:VAL:CB	13	0.99
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	8	0.98
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	6	0.98
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	14	0.98
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	7	0.98
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	12	0.98
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	16	0.98
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	13	0.98
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	8	0.97
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	5	0.96
(3,333)	1:54:X:VAL:N	1:40:X:ILE:CD1	5	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	2	0.96
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	8	0.96
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	11	0.96
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	1	0.96
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	2	0.96
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	9	0.95
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	15	0.94
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	13	0.93
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	9	0.93
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	13	0.93
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	17	0.93
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	9	0.92
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	10	0.92
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	14	0.92
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	18	0.91
(5,47)	1:117:X:ILE:C	1:97:X:GLU:H	5	0.91
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	5	0.91
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	2	0.91
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	9	0.91
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	19	0.91
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	16	0.91
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	12	0.91
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	17	0.91
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	20	0.9
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	13	0.9
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	20	0.9
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	11	0.9
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	9	0.89
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	16	0.89
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	20	0.89
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	4	0.89
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	20	0.89
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	8	0.88
(5,48)	1:147:X:VAL:C	1:98:X:GLU:H	10	0.88
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	20	0.88
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	4	0.88
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	20	0.88
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	3	0.88
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	5	0.88
(1,701)	1:87:X:THR:H	1:86:X:PHE:HB2	5	0.88
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	9	0.88
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	7	0.87
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	1	0.87
(3,587)	1:91:X:TYR:N	1:85:X:LEU:CD1	12	0.87
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	4	0.87
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	4	0.86
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	11	0.86
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	14	0.86
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	13	0.86
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	11	0.86
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	10	0.86
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	3	0.86
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	15	0.86
(5,3)	1:6:X:GLN:C	1:10:X:GLU:H	2	0.85
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	2	0.85
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	10	0.85
(3,610)	1:94:X:PHE:N	1:85:X:LEU:CD1	5	0.84
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	4	0.84
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	19	0.84
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	2	0.84
(1,890)	1:108:X:GLN:HE21	1:107:X:VAL:CB	6	0.84
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	15	0.83
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	17	0.83
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	4	0.83
(3,145)	1:27:X:GLU:N	1:26:X:ILE:CD1	11	0.83
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	7	0.83
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	1	0.83
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	2	0.83
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	5	0.82
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	15	0.82
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	1	0.82
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	20	0.82
(2,85)	1:85:X:LEU:CD2	1:117:X:ILE:CD1	20	0.82
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	11	0.82
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	4	0.82
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	14	0.81
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	8	0.81
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	11	0.81
(3,587)	1:91:X:TYR:N	1:85:X:LEU:CD1	5	0.81
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	8	0.81
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	14	0.81
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	13	0.81
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	9	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	7	0.8
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	13	0.8
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	17	0.8
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	10	0.8
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	17	0.8
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	7	0.8
(1,557)	1:64:X:VAL:H	1:65:X:GLU:HB3	14	0.8
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	15	0.79
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	12	0.79
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	19	0.79
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	9	0.79
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	4	0.79
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	1	0.79
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	15	0.79
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	14	0.79
(3,587)	1:91:X:TYR:N	1:85:X:LEU:CD1	2	0.79
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	9	0.79
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	10	0.79
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	3	0.79
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	10	0.79
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	17	0.79
(1,8)	1:5:X:GLU:HG3	1:5:X:GLU:H	14	0.79
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	11	0.78
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	15	0.78
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	16	0.78
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	9	0.78
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	7	0.78
(1,997)	1:124:X:MET:HG3	1:138:X:LEU:H	9	0.78
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	2	0.77
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	1	0.77
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	2	0.77
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	15	0.77
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	1	0.77
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	13	0.77
(3,481)	1:70:X:VAL:N	1:72:X:TYR:CB	1	0.77
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	2	0.77
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	4	0.76
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	3	0.76
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	18	0.76
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	12	0.76
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	20	0.75
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	18	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	2	0.75
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	10	0.75
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	14	0.75
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	9	0.75
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	7	0.75
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	12	0.75
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	15	0.75
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	5	0.75
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	7	0.75
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	11	0.75
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	16	0.75
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	14	0.75
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	5	0.74
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	3	0.74
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	3	0.74
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	18	0.74
(4,94)	1:117:X:ILE:O	1:97:X:GLU:H	5	0.74
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	12	0.74
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	20	0.74
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	6	0.74
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	2	0.74
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	20	0.74
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	6	0.74
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	9	0.73
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	12	0.73
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	3	0.73
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	16	0.73
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	5	0.73
(3,145)	1:27:X:GLU:N	1:26:X:ILE:CD1	3	0.73
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	11	0.72
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	20	0.72
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	20	0.72
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	14	0.72
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	1	0.72
(1,916)	1:110:X:ARG:HG3	1:109:X:ASN:H	9	0.72
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	4	0.72
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	5	0.72
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	3	0.72
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	13	0.72
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	17	0.71
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	6	0.71
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	12	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	8	0.71
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	11	0.71
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	17	0.71
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	16	0.71
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	1	0.71
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	13	0.71
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	5	0.71
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	10	0.7
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	16	0.7
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	7	0.7
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	9	0.7
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	19	0.7
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	1	0.7
(2,85)	1:85:X:LEU:CD2	1:117:X:ILE:CD1	14	0.7
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	9	0.7
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	12	0.7
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	15	0.69
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	17	0.69
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	20	0.69
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	4	0.69
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	7	0.69
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	13	0.69
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	17	0.68
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	3	0.68
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	14	0.68
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	12	0.68
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	2	0.68
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	12	0.68
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	18	0.68
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	6	0.68
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	13	0.68
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	20	0.68
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	16	0.67
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	3	0.67
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	4	0.67
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	20	0.67
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	7	0.67
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	3	0.67
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	12	0.67
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	5	0.67
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	17	0.67
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	1	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	17	0.66
(5,2)	1:5:X:GLU:C	1:9:X:THR:H	2	0.66
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	20	0.66
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	11	0.66
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	15	0.66
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	13	0.66
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	11	0.66
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	3	0.66
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	20	0.66
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	14	0.66
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	16	0.66
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	19	0.66
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	1	0.65
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	6	0.65
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	17	0.65
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	18	0.65
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	5	0.65
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	10	0.65
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	2	0.65
(2,81)	1:85:X:LEU:CD2	1:99:X:VAL:CG1	5	0.65
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD1	2	0.65
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD2	2	0.65
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	17	0.65
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	17	0.65
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	3	0.65
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	18	0.64
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	14	0.64
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	12	0.64
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	20	0.64
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	8	0.64
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	16	0.64
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	17	0.64
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	19	0.64
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	7	0.64
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	11	0.64
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	4	0.64
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	18	0.64
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	9	0.64
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	8	0.64
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	17	0.64
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	9	0.63
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	20	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	15	0.63
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	12	0.63
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	3	0.63
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	15	0.63
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	1	0.63
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	2	0.63
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	4	0.63
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	5	0.63
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	1	0.63
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	1	0.62
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	10	0.62
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	4	0.62
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	7	0.62
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	1	0.62
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	5	0.62
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	4	0.62
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD1	9	0.62
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD2	9	0.62
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	14	0.62
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	1	0.62
(1,664)	1:77:X:SER:HB3	1:78:X:SER:H	6	0.62
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	15	0.61
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	14	0.61
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	1	0.61
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	9	0.61
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	8	0.61
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	13	0.61
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	13	0.61
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	10	0.61
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	10	0.61
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	18	0.61
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	19	0.61
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	5	0.61
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	18	0.61
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	15	0.61
(5,58)	1:121:X:ASP:C	1:124:X:MET:H	10	0.6
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	1	0.6
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	8	0.6
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	19	0.6
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	2	0.6
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	7	0.6
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	3	0.6
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	12	0.6
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	2	0.6
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	18	0.6
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	12	0.6
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	5	0.6
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	20	0.6
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	15	0.6
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	17	0.6
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	15	0.6
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	11	0.59
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	1	0.59
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	2	0.59
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	5	0.59
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	11	0.59
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	17	0.59
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	1	0.59
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	1	0.59
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	11	0.59
(1,1001)	1:125:X:ILE:H	1:124:X:MET:HB3	4	0.59
(1,892)	1:108:X:GLN:H	1:107:X:VAL:HB	18	0.59
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	20	0.59
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	2	0.59
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	1	0.58
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	7	0.58
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	14	0.58
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	8	0.58
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	19	0.58
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	14	0.58
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	16	0.58
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	6	0.58
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	19	0.58
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	4	0.58
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	5	0.58
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	20	0.58
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	1	0.58
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	9	0.58
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	10	0.58
(2,46)	1:38:X:ILE:CD1	1:76:X:VAL:CG1	16	0.58
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	13	0.58
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	6	0.58
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	16	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:94:X:PHE:HA	1:97:X:GLU:H	19	0.58
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	17	0.58
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	4	0.58
(5,49)	1:97:X:GLU:C	1:117:X:ILE:H	10	0.57
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	19	0.57
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	17	0.57
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	19	0.57
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	8	0.57
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	4	0.57
(1,1001)	1:125:X:ILE:H	1:124:X:MET:HB3	1	0.57
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	8	0.57
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	5	0.57
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	2	0.56
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	19	0.56
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	10	0.56
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	20	0.56
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	4	0.56
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	6	0.56
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	20	0.56
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	20	0.56
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	11	0.56
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	20	0.56
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	13	0.56
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	3	0.56
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	10	0.56
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	11	0.56
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	2	0.56
(1,495)	1:59:X:SER:HB2	1:60:X:ALA:H	16	0.56
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	12	0.56
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	6	0.56
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	7	0.55
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	11	0.55
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	5	0.55
(5,15)	1:29:X:ILE:C	1:35:X:THR:H	5	0.55
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	3	0.55
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	10	0.55
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	3	0.55
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	9	0.55
(1,1001)	1:125:X:ILE:H	1:124:X:MET:HB3	2	0.55
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	8	0.55
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	10	0.54
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	19	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	10	0.54
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	15	0.54
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	6	0.54
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	19	0.54
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	2	0.54
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	4	0.54
(4,4)	1:5:X:GLU:O	1:9:X:THR:H	2	0.54
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	15	0.54
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	14	0.54
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	20	0.54
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	13	0.54
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	1	0.54
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	5	0.54
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	7	0.54
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	19	0.54
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	15	0.54
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	3	0.53
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	4	0.53
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	15	0.53
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	9	0.53
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	2	0.53
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	14	0.53
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	7	0.53
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	15	0.53
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	10	0.53
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	10	0.53
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	1	0.53
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	8	0.53
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	11	0.53
(1,285)	1:40:X:ILE:CD1	1:54:X:VAL:H	5	0.53
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	10	0.53
(5,58)	1:121:X:ASP:C	1:124:X:MET:H	14	0.52
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	20	0.52
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	10	0.52
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	9	0.52
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	14	0.52
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	11	0.52
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	17	0.52
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	15	0.52
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	2	0.52
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	6	0.52
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	13	0.52
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	18	0.52
(3,130)	1:25:X:GLY:N	1:23:X:LEU:CG	9	0.52
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	16	0.52
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	9	0.52
(1,664)	1:77:X:SER:HB3	1:78:X:SER:H	5	0.52
(1,664)	1:77:X:SER:HB3	1:78:X:SER:H	10	0.52
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	8	0.51
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	19	0.51
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	5	0.51
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	3	0.51
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	12	0.51
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	6	0.51
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	15	0.51
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	15	0.51
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	2	0.51
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	3	0.51
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	9	0.51
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	1	0.51
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	14	0.51
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	7	0.51
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	19	0.51
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	3	0.51
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	2	0.51
(1,664)	1:77:X:SER:HB3	1:78:X:SER:H	13	0.51
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	6	0.51
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	2	0.51
(5,58)	1:121:X:ASP:C	1:124:X:MET:H	20	0.5
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	7	0.5
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	4	0.5
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	10	0.5
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	17	0.5
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	7	0.5
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	14	0.5
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	16	0.5
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	19	0.5
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	2	0.5
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	16	0.5
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	4	0.5
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	10	0.5
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	3	0.5
(1,190)	1:31:X:GLY:H	1:30:X:ARG:HG3	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	1	0.5
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	10	0.49
(5,58)	1:121:X:ASP:C	1:124:X:MET:H	9	0.49
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	1	0.49
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	4	0.49
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	5	0.49
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	8	0.49
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	9	0.49
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	19	0.49
(5,8)	1:12:X:ILE:C	1:16:X:VAL:H	16	0.49
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	14	0.49
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	8	0.49
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	19	0.49
(4,5)	1:6:X:GLN:O	1:10:X:GLU:H	2	0.49
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	4	0.49
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	6	0.49
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	18	0.49
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	12	0.49
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	20	0.49
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	7	0.49
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	5	0.49
(1,900)	1:108:X:GLN:HB2	1:109:X:ASN:H	9	0.49
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	9	0.49
(1,685)	1:81:X:LEU:H	1:82:X:ASP:H	13	0.49
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	5	0.49
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	9	0.49
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	2	0.49
(1,495)	1:59:X:SER:HB2	1:60:X:ALA:H	14	0.49
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	16	0.49
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	17	0.49
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	20	0.49
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	4	0.48
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	13	0.48
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	6	0.48
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	9	0.48
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	15	0.48
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	1	0.48
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	15	0.48
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	11	0.48
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	19	0.48
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	1	0.48
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	7	0.48
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	3	0.48
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	4	0.48
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	5	0.48
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	8	0.48
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	14	0.48
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	13	0.48
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	14	0.48
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	11	0.47
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	2	0.47
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	5	0.47
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	3	0.47
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	8	0.47
(3,663)	1:91:X:TYR:N	1:125:X:ILE:CD1	9	0.47
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	20	0.47
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	16	0.47
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	13	0.47
(2,85)	1:85:X:LEU:CD2	1:117:X:ILE:CD1	17	0.47
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	2	0.47
(1,701)	1:87:X:THR:H	1:86:X:PHE:HB2	6	0.47
(1,701)	1:87:X:THR:H	1:86:X:PHE:HB2	13	0.47
(1,214)	1:34:X:SER:H	1:73:X:ASN:H	14	0.47
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	5	0.47
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	11	0.46
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	17	0.46
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	2	0.46
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	17	0.46
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	7	0.46
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	12	0.46
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	15	0.46
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	7	0.46
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	16	0.46
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	4	0.46
(3,479)	1:70:X:VAL:CG1	1:70:X:VAL:N	1	0.46
(3,479)	1:70:X:VAL:CG1	1:70:X:VAL:N	2	0.46
(3,479)	1:70:X:VAL:CG1	1:70:X:VAL:N	13	0.46
(3,464)	1:66:X:ASP:N	1:64:X:VAL:CG1	20	0.46
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	10	0.46
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	11	0.46
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	2	0.46
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	8	0.46
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	18	0.46
(2,30)	1:33:X:THR:CG2	1:71:X:ALA:CB	5	0.46
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	6	0.46
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	14	0.46
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	10	0.46
(1,664)	1:77:X:SER:HB3	1:78:X:SER:H	18	0.46
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	4	0.46
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	7	0.46
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	13	0.46
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	4	0.46
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	20	0.46
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	8	0.46
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	18	0.46
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	16	0.46
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	14	0.46
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	1	0.45
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	12	0.45
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	16	0.45
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	3	0.45
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	20	0.45
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	16	0.45
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	7	0.45
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	2	0.45
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	8	0.45
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	2	0.45
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	9	0.45
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	18	0.45
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	12	0.45
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	6	0.45
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	11	0.45
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	7	0.45
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	9	0.45
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	19	0.45
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	6	0.45
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	19	0.45
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	3	0.45
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	4	0.45
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	5	0.45
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	6	0.45
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	7	0.45
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	10	0.45
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	11	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	19	0.45
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	17	0.45
(2,49)	1:40:X:ILE:CG2	1:40:X:ILE:CD1	5	0.45
(2,28)	1:29:X:ILE:CG2	1:29:X:ILE:CD1	8	0.45
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	16	0.45
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	1	0.45
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	10	0.45
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	11	0.45
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	7	0.45
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	15	0.45
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	18	0.45
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	10	0.45
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	19	0.45
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	1	0.44
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	15	0.44
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	16	0.44
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	8	0.44
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	12	0.44
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	19	0.44
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	4	0.44
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	15	0.44
(5,15)	1:29:X:ILE:C	1:35:X:THR:H	14	0.44
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	2	0.44
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	4	0.44
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	16	0.44
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	18	0.44
(4,65)	1:56:X:HIS:O	1:60:X:ALA:H	3	0.44
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	9	0.44
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	19	0.44
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	9	0.44
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	10	0.44
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	5	0.44
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	12	0.44
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	13	0.44
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	20	0.44
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	3	0.44
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	5	0.44
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	10	0.44
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	17	0.44
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	1	0.44
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	9	0.44
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	13	0.44
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	16	0.44
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	17	0.44
(3,474)	1:68:X:ILE:N	1:68:X:ILE:CG2	5	0.44
(3,474)	1:68:X:ILE:N	1:68:X:ILE:CG2	9	0.44
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	16	0.44
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	9	0.44
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	12	0.44
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	13	0.44
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	14	0.44
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	17	0.44
(3,45)	1:11:X:MET:N	1:11:X:MET:CG	2	0.44
(3,45)	1:11:X:MET:N	1:11:X:MET:CG	6	0.44
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	15	0.44
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	13	0.44
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	11	0.44
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	8	0.44
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	19	0.44
(1,674)	1:79:X:PRO:HB3	1:80:X:GLY:H	18	0.44
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	5	0.44
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	6	0.43
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	18	0.43
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	18	0.43
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	10	0.43
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	8	0.43
(5,15)	1:29:X:ILE:C	1:35:X:THR:H	1	0.43
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	20	0.43
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	17	0.43
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	10	0.43
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	20	0.43
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	6	0.43
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	14	0.43
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	16	0.43
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	17	0.43
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	7	0.43
(4,6)	1:6:X:GLN:O	1:10:X:GLU:N	2	0.43
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	11	0.43
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	3	0.43
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	10	0.43
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	11	0.43
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	17	0.43
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	19	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	9	0.43
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	13	0.43
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	15	0.43
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	19	0.43
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	4	0.43
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	5	0.43
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	8	0.43
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	11	0.43
(3,474)	1:68:X:ILE:N	1:68:X:ILE:CG2	6	0.43
(3,474)	1:68:X:ILE:N	1:68:X:ILE:CG2	13	0.43
(3,474)	1:68:X:ILE:N	1:68:X:ILE:CG2	15	0.43
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	4	0.43
(3,415)	1:61:X:VAL:N	1:61:X:VAL:CG1	2	0.43
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	1	0.43
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	1	0.43
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	12	0.43
(3,45)	1:11:X:MET:N	1:11:X:MET:CG	9	0.43
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	2	0.43
(2,28)	1:29:X:ILE:CG2	1:29:X:ILE:CD1	2	0.43
(2,28)	1:29:X:ILE:CG2	1:29:X:ILE:CD1	18	0.43
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	6	0.43
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	16	0.43
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	6	0.43
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	20	0.43
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	3	0.43
(1,62)	1:9:X:THR:HB	1:10:X:GLU:H	2	0.43
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	13	0.43
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	13	0.42
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	14	0.42
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	11	0.42
(4,97)	1:97:X:GLU:O	1:117:X:ILE:N	10	0.42
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	20	0.42
(4,87)	1:89:X:GLU:O	1:93:X:ARG:H	19	0.42
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	12	0.42
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	8	0.42
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	12	0.42
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	3	0.42
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	4	0.42
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	15	0.42
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	16	0.42
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	1	0.42
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	7	0.42
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	12	0.42
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	14	0.42
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	16	0.42
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	5	0.42
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	14	0.42
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	20	0.42
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	5	0.42
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	6	0.42
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	15	0.42
(3,45)	1:11:X:MET:N	1:11:X:MET:CG	3	0.42
(3,45)	1:11:X:MET:N	1:11:X:MET:CG	19	0.42
(2,86)	1:91:X:TYR:CA	1:117:X:ILE:CD1	9	0.42
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	3	0.42
(1,820)	1:100:X:THR:HA	1:115:X:GLY:H	18	0.42
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	12	0.42
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	17	0.42
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	9	0.42
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	6	0.42
(5,54)	1:102:X:VAL:C	1:143:X:LYS:H	7	0.41
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	10	0.41
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	20	0.41
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	11	0.41
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	1	0.41
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	14	0.41
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	13	0.41
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	8	0.41
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	17	0.41
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	20	0.41
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	6	0.41
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	10	0.41
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	12	0.41
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	15	0.41
(3,474)	1:68:X:ILE:N	1:68:X:ILE:CG2	20	0.41
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	7	0.41
(3,464)	1:66:X:ASP:N	1:64:X:VAL:CG1	13	0.41
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	19	0.41
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	2	0.41
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	8	0.41
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	5	0.41
(3,188)	1:33:X:THR:N	1:33:X:THR:CG2	20	0.41
(2,28)	1:29:X:ILE:CG2	1:29:X:ILE:CD1	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	5	0.41
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	9	0.41
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	12	0.41
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	18	0.41
(1,813)	1:99:X:VAL:H	1:117:X:ILE:HG12	11	0.41
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	14	0.41
(1,581)	1:66:X:ASP:HB2	1:72:X:TYR:H	20	0.41
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	1	0.41
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	18	0.41
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	15	0.41
(5,58)	1:121:X:ASP:C	1:124:X:MET:H	11	0.4
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	9	0.4
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	6	0.4
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	9	0.4
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	14	0.4
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	9	0.4
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	12	0.4
(5,3)	1:6:X:GLN:C	1:10:X:GLU:H	19	0.4
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	17	0.4
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	14	0.4
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	17	0.4
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	8	0.4
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	1	0.4
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	3	0.4
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	14	0.4
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	8	0.4
(3,667)	1:95:X:VAL:N	1:117:X:ILE:CG2	19	0.4
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	12	0.4
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	3	0.4
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	1	0.4
(3,574)	1:89:X:GLU:N	1:89:X:GLU:CG	3	0.4
(3,507)	1:75:X:GLU:N	1:75:X:GLU:CG	16	0.4
(3,313)	1:52:X:ALA:N	1:40:X:ILE:CD1	5	0.4
(3,45)	1:11:X:MET:N	1:11:X:MET:CG	1	0.4
(3,45)	1:11:X:MET:N	1:11:X:MET:CG	18	0.4
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	10	0.4
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	4	0.4
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	11	0.4
(1,813)	1:99:X:VAL:H	1:117:X:ILE:HG12	4	0.4
(1,813)	1:99:X:VAL:H	1:117:X:ILE:HG12	5	0.4
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	10	0.4
(1,701)	1:87:X:THR:H	1:86:X:PHE:HB2	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:81:X:LEU:H	1:82:X:ASP:H	7	0.4
(1,664)	1:77:X:SER:HB3	1:78:X:SER:H	16	0.4
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	4	0.4
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	13	0.4
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	3	0.39
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	13	0.39
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	12	0.39
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	16	0.39
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	20	0.39
(4,3)	1:5:X:GLU:O	1:9:X:THR:N	2	0.39
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	9	0.39
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	15	0.39
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	14	0.39
(3,721)	1:105:X:MET:N	1:105:X:MET:CG	6	0.39
(3,712)	1:104:X:ARG:N	1:104:X:ARG:CG	4	0.39
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	7	0.39
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	6	0.39
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	16	0.39
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	2	0.39
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	19	0.39
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	1	0.39
(3,5)	1:5:X:GLU:N	1:5:X:GLU:CG	14	0.39
(2,22)	1:16:X:VAL:CG1	1:54:X:VAL:CG2	3	0.39
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD1	12	0.39
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD2	12	0.39
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	1	0.39
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	11	0.39
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	13	0.39
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	1	0.39
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	14	0.39
(1,701)	1:87:X:THR:H	1:86:X:PHE:HB2	20	0.39
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	3	0.39
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	11	0.39
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	11	0.39
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	19	0.39
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	6	0.39
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	4	0.39
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	4	0.38
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	14	0.38
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	18	0.38
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	19	0.38
(4,98)	1:97:X:GLU:O	1:117:X:ILE:H	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	18	0.38
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	18	0.38
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	6	0.38
(3,663)	1:91:X:TYR:N	1:125:X:ILE:CD1	13	0.38
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	9	0.38
(3,474)	1:68:X:ILE:N	1:68:X:ILE:CG2	17	0.38
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	11	0.38
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	18	0.38
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	15	0.38
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	6	0.38
(1,756)	1:94:X:PHE:HA	1:97:X:GLU:H	4	0.38
(1,625)	1:74:X:LEU:HD21	1:39:X:TYR:H	1	0.38
(1,625)	1:74:X:LEU:HD22	1:39:X:TYR:H	1	0.38
(1,625)	1:74:X:LEU:HD23	1:39:X:TYR:H	1	0.38
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	4	0.38
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	5	0.38
(1,217)	1:35:X:THR:H	1:34:X:SER:HB3	5	0.38
(1,190)	1:31:X:GLY:H	1:30:X:ARG:HG3	1	0.38
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	19	0.38
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	6	0.37
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	19	0.37
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	5	0.37
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	5	0.37
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	7	0.37
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	13	0.37
(5,3)	1:6:X:GLN:C	1:10:X:GLU:H	9	0.37
(4,96)	1:147:X:VAL:O	1:98:X:GLU:H	10	0.37
(4,93)	1:117:X:ILE:O	1:97:X:GLU:N	5	0.37
(4,54)	1:50:X:ASP:O	1:54:X:VAL:H	10	0.37
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	10	0.37
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	19	0.37
(4,33)	1:34:X:SER:O	1:73:X:ASN:H	14	0.37
(4,31)	1:33:X:THR:O	1:31:X:GLY:H	18	0.37
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	3	0.37
(3,955)	1:147:X:VAL:N	1:146:X:LEU:CD1	9	0.37
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	2	0.37
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	16	0.37
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	6	0.37
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	7	0.37
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	15	0.37
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	18	0.37
(3,212)	1:37:X:ARG:N	1:27:X:GLU:CB	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	20	0.37
(1,756)	1:94:X:PHE:HA	1:97:X:GLU:H	20	0.37
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	6	0.37
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	16	0.37
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	11	0.37
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	18	0.37
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	14	0.37
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	1	0.37
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	14	0.36
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	9	0.36
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	12	0.36
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	13	0.36
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	11	0.36
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	16	0.36
(4,85)	1:88:X:ALA:O	1:92:X:ALA:H	1	0.36
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	14	0.36
(4,66)	1:56:X:HIS:O	1:60:X:ALA:N	3	0.36
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	1	0.36
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	18	0.36
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	16	0.36
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	13	0.36
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	15	0.36
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	14	0.36
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	6	0.36
(1,968)	1:121:X:ASP:H	1:125:X:ILE:CD1	16	0.36
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	9	0.36
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	12	0.36
(1,755)	1:94:X:PHE:HB3	1:97:X:GLU:H	19	0.36
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	10	0.36
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	19	0.36
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	4	0.36
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	6	0.36
(1,284)	1:40:X:ILE:CD1	1:51:X:CYS:H	5	0.36
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	16	0.36
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	13	0.35
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	9	0.35
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	1	0.35
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	1	0.35
(5,12)	1:23:X:LEU:C	1:41:X:ASP:H	13	0.35
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	20	0.35
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	14	0.35
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	17	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	7	0.35
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	10	0.35
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	8	0.35
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	6	0.35
(2,107)	1:120:X:VAL:CG2	1:125:X:ILE:CD1	7	0.35
(2,86)	1:91:X:TYR:CA	1:117:X:ILE:CD1	14	0.35
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	2	0.35
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	15	0.35
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	1	0.35
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	3	0.35
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	19	0.35
(1,561)	1:65:X:GLU:H	1:64:X:VAL:CB	20	0.35
(1,500)	1:59:X:SER:H	1:62:X:LEU:HB3	4	0.35
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	11	0.35
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	10	0.35
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	1	0.35
(1,223)	1:35:X:THR:HG21	1:75:X:GLU:H	14	0.35
(1,223)	1:35:X:THR:HG22	1:75:X:GLU:H	14	0.35
(1,223)	1:35:X:THR:HG23	1:75:X:GLU:H	14	0.35
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	14	0.35
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	2	0.35
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	17	0.35
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	11	0.35
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	4	0.34
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	18	0.34
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	3	0.34
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	17	0.34
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	18	0.34
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	2	0.34
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	10	0.34
(4,67)	1:57:X:GLN:O	1:61:X:VAL:H	7	0.34
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	3	0.34
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	19	0.34
(3,954)	1:147:X:VAL:N	1:146:X:LEU:CD2	11	0.34
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	17	0.34
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	13	0.34
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	14	0.34
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	5	0.34
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	7	0.34
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	8	0.34
(3,203)	1:36:X:LEU:N	1:35:X:THR:CG2	14	0.34
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	17	0.34
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	14	0.34
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	4	0.34
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	6	0.34
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	4	0.34
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	4	0.34
(1,841)	1:101:X:LEU:H	1:114:X:GLN:HB2	6	0.34
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	14	0.34
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	1	0.34
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	4	0.34
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	14	0.34
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	11	0.34
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	2	0.33
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	11	0.33
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	8	0.33
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	17	0.33
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	19	0.33
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	5	0.33
(4,68)	1:57:X:GLN:O	1:61:X:VAL:N	7	0.33
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	8	0.33
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	10	0.33
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	5	0.33
(3,894)	1:136:X:PHE:N	1:126:X:THR:CG2	20	0.33
(3,765)	1:115:X:GLY:N	1:129:X:VAL:CG2	17	0.33
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	5	0.33
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	3	0.33
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	5	0.33
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	5	0.33
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	17	0.33
(3,468)	1:66:X:ASP:N	1:67:X:PRO:CG	14	0.33
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	12	0.33
(2,86)	1:91:X:TYR:CA	1:117:X:ILE:CD1	20	0.33
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	8	0.33
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	7	0.33
(1,997)	1:124:X:MET:HG3	1:138:X:LEU:H	11	0.33
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	4	0.33
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	3	0.33
(1,900)	1:108:X:GLN:HB2	1:109:X:ASN:H	6	0.33
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	16	0.33
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	20	0.33
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	19	0.33
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:58:X:VAL:HB	1:56:X:HIS:H	10	0.33
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	16	0.33
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	15	0.33
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	9	0.33
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	18	0.32
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	18	0.32
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	7	0.32
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	6	0.32
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	3	0.32
(5,2)	1:5:X:GLU:C	1:9:X:THR:H	1	0.32
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	1	0.32
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	12	0.32
(4,75)	1:71:X:ALA:O	1:34:X:SER:H	5	0.32
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	14	0.32
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	9	0.32
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	12	0.32
(4,30)	1:29:X:ILE:O	1:35:X:THR:H	5	0.32
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	6	0.32
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	5	0.32
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	13	0.32
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	12	0.32
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	4	0.32
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	6	0.32
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	9	0.32
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	20	0.32
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	17	0.32
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	1	0.32
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	15	0.32
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	8	0.32
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	15	0.32
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	2	0.32
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	10	0.32
(1,596)	1:71:X:ALA:H	1:70:X:VAL:CB	1	0.32
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG21	1	0.32
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG22	1	0.32
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG23	1	0.32
(1,500)	1:59:X:SER:H	1:62:X:LEU:HB3	8	0.32
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	16	0.32
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	3	0.32
(1,223)	1:35:X:THR:HG21	1:75:X:GLU:H	1	0.32
(1,223)	1:35:X:THR:HG22	1:75:X:GLU:H	1	0.32
(1,223)	1:35:X:THR:HG23	1:75:X:GLU:H	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:31:X:GLY:H	1:30:X:ARG:HG3	14	0.32
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	7	0.31
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	13	0.31
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	6	0.31
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	20	0.31
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	18	0.31
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	8	0.31
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	4	0.31
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	5	0.31
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	8	0.31
(4,86)	1:88:X:ALA:O	1:92:X:ALA:N	1	0.31
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	2	0.31
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	20	0.31
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	19	0.31
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	15	0.31
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	20	0.31
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	10	0.31
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	14	0.31
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	5	0.31
(3,663)	1:91:X:TYR:N	1:125:X:ILE:CD1	10	0.31
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	18	0.31
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	3	0.31
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	12	0.31
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	16	0.31
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	18	0.31
(3,130)	1:25:X:GLY:N	1:23:X:LEU:CG	2	0.31
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	7	0.31
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	12	0.31
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	18	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	1	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	2	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	3	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	4	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	5	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	6	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	7	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	8	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	9	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	10	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	11	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	12	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	14	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	15	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	16	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	17	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	18	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	19	0.31
(1,933)	1:114:X:GLN:HE22	1:114:X:GLN:HE21	20	0.31
(1,756)	1:94:X:PHE:HA	1:97:X:GLU:H	17	0.31
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	6	0.31
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	1	0.31
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	11	0.31
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	2	0.31
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	12	0.31
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	12	0.31
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	9	0.31
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	11	0.31
(1,172)	1:29:X:ILE:HB	1:35:X:THR:H	19	0.31
(1,164)	1:29:X:ILE:H	1:28:X:PHE:CZ	12	0.31
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	15	0.31
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	16	0.31
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	10	0.3
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	1	0.3
(5,24)	1:47:X:ASN:C	1:50:X:ASP:H	3	0.3
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	7	0.3
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	11	0.3
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	1	0.3
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	5	0.3
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	8	0.3
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	10	0.3
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	7	0.3
(4,53)	1:50:X:ASP:O	1:54:X:VAL:N	10	0.3
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	1	0.3
(4,1)	1:4:X:LEU:O	1:8:X:LEU:H	15	0.3
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	3	0.3
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	7	0.3
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	16	0.3
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	10	0.3
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	6	0.3
(3,484)	1:71:X:ALA:N	1:70:X:VAL:CB	1	0.3
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	19	0.3
(3,333)	1:54:X:VAL:N	1:40:X:ILE:CD1	12	0.3
(2,107)	1:120:X:VAL:CG2	1:125:X:ILE:CD1	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:16:X:VAL:CG1	1:54:X:VAL:CG2	5	0.3
(1,1148)	1:141:X:ILE:HG13	1:137:X:ALA:H	14	0.3
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	18	0.3
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	16	0.3
(1,997)	1:124:X:MET:HG3	1:138:X:LEU:H	14	0.3
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	7	0.3
(1,755)	1:94:X:PHE:HB3	1:97:X:GLU:H	4	0.3
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	8	0.3
(1,576)	1:66:X:ASP:H	1:65:X:GLU:HB3	14	0.3
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	8	0.3
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	7	0.3
(1,243)	1:37:X:ARG:H	1:36:X:LEU:HB3	12	0.3
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	7	0.3
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	19	0.3
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	15	0.29
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	20	0.29
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	13	0.29
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	16	0.29
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	8	0.29
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	6	0.29
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	9	0.29
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	18	0.29
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	3	0.29
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	11	0.29
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	15	0.29
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	19	0.29
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	15	0.29
(4,76)	1:71:X:ALA:O	1:34:X:SER:N	5	0.29
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	1	0.29
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	15	0.29
(4,2)	1:4:X:LEU:O	1:8:X:LEU:N	15	0.29
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	10	0.29
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	13	0.29
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	5	0.29
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	17	0.29
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	18	0.29
(3,765)	1:115:X:GLY:N	1:129:X:VAL:CG2	20	0.29
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	3	0.29
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	17	0.29
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	6	0.29
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	15	0.29
(3,610)	1:94:X:PHE:N	1:85:X:LEU:CD1	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,587)	1:91:X:TYR:N	1:85:X:LEU:CD1	16	0.29
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	17	0.29
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	15	0.29
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	18	0.29
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	8	0.29
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	4	0.29
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	17	0.29
(3,130)	1:25:X:GLY:N	1:23:X:LEU:CG	16	0.29
(2,92)	1:101:X:LEU:CD2	1:141:X:ILE:CG2	5	0.29
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	19	0.29
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	17	0.29
(2,4)	1:8:X:LEU:CD1	1:11:X:MET:CE	20	0.29
(2,4)	1:8:X:LEU:CD2	1:11:X:MET:CE	20	0.29
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	3	0.29
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	6	0.29
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	16	0.29
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	3	0.29
(1,665)	1:78:X:SER:HA	1:40:X:ILE:H	15	0.29
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	13	0.29
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	19	0.29
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	12	0.29
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	12	0.29
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	5	0.28
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	20	0.28
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	20	0.28
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	5	0.28
(4,53)	1:50:X:ASP:O	1:54:X:VAL:N	15	0.28
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	1	0.28
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	4	0.28
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	12	0.28
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	20	0.28
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	19	0.28
(3,610)	1:94:X:PHE:N	1:85:X:LEU:CD1	13	0.28
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	8	0.28
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	18	0.28
(3,333)	1:54:X:VAL:N	1:40:X:ILE:CD1	3	0.28
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	5	0.28
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	2	0.28
(2,107)	1:120:X:VAL:CG2	1:125:X:ILE:CD1	10	0.28
(2,106)	1:117:X:ILE:CD1	1:125:X:ILE:CG2	5	0.28
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	14	0.28
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	6	0.28
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	7	0.28
(1,997)	1:124:X:MET:HG3	1:138:X:LEU:H	20	0.28
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	20	0.28
(1,900)	1:108:X:GLN:HB2	1:109:X:ASN:H	11	0.28
(1,900)	1:108:X:GLN:HB2	1:109:X:ASN:H	13	0.28
(1,756)	1:94:X:PHE:HA	1:97:X:GLU:H	15	0.28
(1,665)	1:78:X:SER:HA	1:40:X:ILE:H	18	0.28
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	20	0.28
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	20	0.28
(1,603)	1:71:X:ALA:HB1	1:72:X:TYR:H	11	0.28
(1,603)	1:71:X:ALA:HB2	1:72:X:TYR:H	11	0.28
(1,603)	1:71:X:ALA:HB3	1:72:X:TYR:H	11	0.28
(1,500)	1:59:X:SER:H	1:62:X:LEU:HB3	2	0.28
(1,444)	1:56:X:HIS:HB3	1:55:X:SER:H	3	0.28
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	13	0.28
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	14	0.28
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	16	0.28
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	7	0.28
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	7	0.27
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	5	0.27
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	1	0.27
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	3	0.27
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	14	0.27
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	19	0.27
(5,29)	1:52:X:ALA:C	1:56:X:HIS:H	10	0.27
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	11	0.27
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	12	0.27
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	13	0.27
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	18	0.27
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	2	0.27
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	13	0.27
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	6	0.27
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	2	0.27
(4,87)	1:89:X:GLU:O	1:93:X:ARG:H	3	0.27
(4,75)	1:71:X:ALA:O	1:34:X:SER:H	1	0.27
(4,65)	1:56:X:HIS:O	1:60:X:ALA:H	11	0.27
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	14	0.27
(4,54)	1:50:X:ASP:O	1:54:X:VAL:H	15	0.27
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	20	0.27
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	8	0.27
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	19	0.27
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	8	0.27
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	19	0.27
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	8	0.27
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	2	0.27
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	10	0.27
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	17	0.27
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	19	0.27
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	2	0.27
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	9	0.27
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	5	0.27
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	14	0.27
(1,1010)	1:125:X:ILE:H	1:136:X:PHE:H	1	0.27
(1,813)	1:99:X:VAL:H	1:117:X:ILE:HG12	2	0.27
(1,769)	1:95:X:VAL:HB	1:97:X:GLU:H	5	0.27
(1,500)	1:59:X:SER:H	1:62:X:LEU:HB3	5	0.27
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	13	0.27
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	17	0.27
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	2	0.27
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	1	0.27
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	20	0.27
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	19	0.27
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	16	0.27
(1,172)	1:29:X:ILE:HB	1:35:X:THR:H	18	0.27
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	4	0.27
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	12	0.27
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	17	0.27
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	10	0.27
(1,52)	1:10:X:GLU:H	1:7:X:LYS:H	2	0.27
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	3	0.26
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	16	0.26
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	20	0.26
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	16	0.26
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	1	0.26
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	16	0.26
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	13	0.26
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	7	0.26
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	1	0.26
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	13	0.26
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	15	0.26
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	20	0.26
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	15	0.26
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	20	0.26
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	4	0.26
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	12	0.26
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	19	0.26
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	5	0.26
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	9	0.26
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	3	0.26
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	1	0.26
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	13	0.26
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	14	0.26
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	17	0.26
(3,159)	1:29:X:ILE:N	1:28:X:PHE:CB	12	0.26
(1,1148)	1:141:X:ILE:HG13	1:137:X:ALA:H	17	0.26
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	15	0.26
(1,1010)	1:125:X:ILE:H	1:136:X:PHE:H	4	0.26
(1,874)	1:106:X:ALA:HA	1:103:X:LEU:H	12	0.26
(1,813)	1:99:X:VAL:H	1:117:X:ILE:HG12	3	0.26
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	19	0.26
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	9	0.26
(1,664)	1:77:X:SER:HB3	1:78:X:SER:H	19	0.26
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	8	0.26
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	5	0.26
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	4	0.26
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	2	0.26
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	11	0.26
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	19	0.26
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	20	0.26
(1,243)	1:37:X:ARG:H	1:36:X:LEU:HB3	11	0.26
(1,217)	1:35:X:THR:H	1:34:X:SER:HB3	13	0.26
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	12	0.26
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	6	0.26
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	6	0.26
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	17	0.26
(1,5)	1:5:X:GLU:H	1:4:X:LEU:HG	19	0.26
(5,63)	1:128:X:THR:C	1:116:X:VAL:H	11	0.25
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	12	0.25
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	8	0.25
(5,39)	1:73:X:ASN:C	1:36:X:LEU:H	11	0.25
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	20	0.25
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	19	0.25
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	7	0.25
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	17	0.25
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	15	0.25
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	4	0.25
(4,66)	1:56:X:HIS:O	1:60:X:ALA:N	11	0.25
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	3	0.25
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	7	0.25
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	20	0.25
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	3	0.25
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	9	0.25
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	7	0.25
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	17	0.25
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	8	0.25
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	12	0.25
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	19	0.25
(2,4)	1:8:X:LEU:CD1	1:11:X:MET:CE	13	0.25
(2,4)	1:8:X:LEU:CD2	1:11:X:MET:CE	13	0.25
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	7	0.25
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	13	0.25
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	2	0.25
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	14	0.25
(1,1012)	1:125:X:ILE:H	1:138:X:LEU:H	9	0.25
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	13	0.25
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	7	0.25
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	2	0.25
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	4	0.25
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	11	0.25
(1,643)	1:76:X:VAL:HB	1:55:X:SER:H	16	0.25
(1,621)	1:73:X:ASN:HB3	1:74:X:LEU:H	19	0.25
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	1	0.25
(1,307)	1:44:X:ASP:H	1:43:X:GLU:HG2	3	0.25
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	2	0.25
(1,217)	1:35:X:THR:H	1:34:X:SER:HB3	17	0.25
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	11	0.25
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	9	0.25
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	17	0.25
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	1	0.25
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	6	0.25
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	18	0.25
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	1	0.25
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	3	0.25
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	5	0.24
(5,67)	1:136:X:PHE:C	1:125:X:ILE:H	4	0.24
(5,63)	1:128:X:THR:C	1:116:X:VAL:H	5	0.24
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	1	0.24
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	14	0.24
(5,39)	1:73:X:ASN:C	1:36:X:LEU:H	3	0.24
(5,39)	1:73:X:ASN:C	1:36:X:LEU:H	20	0.24
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	13	0.24
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	7	0.24
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	13	0.24
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	11	0.24
(5,12)	1:23:X:LEU:C	1:41:X:ASP:H	5	0.24
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	15	0.24
(5,3)	1:6:X:GLN:C	1:10:X:GLU:H	10	0.24
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	15	0.24
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	8	0.24
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	10	0.24
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	2	0.24
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	17	0.24
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	7	0.24
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	10	0.24
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	4	0.24
(4,24)	1:23:X:LEU:O	1:41:X:ASP:H	13	0.24
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	8	0.24
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	5	0.24
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	17	0.24
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	12	0.24
(3,823)	1:124:X:MET:CB	1:125:X:ILE:N	1	0.24
(3,823)	1:124:X:MET:CB	1:125:X:ILE:N	2	0.24
(3,823)	1:124:X:MET:CB	1:125:X:ILE:N	4	0.24
(3,814)	1:124:X:MET:N	1:121:X:ASP:CB	16	0.24
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	18	0.24
(3,797)	1:121:X:ASP:N	1:120:X:VAL:CB	4	0.24
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	18	0.24
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	19	0.24
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	3	0.24
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	11	0.24
(3,371)	1:57:X:GLN:N	1:54:X:VAL:CG2	3	0.24
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	2	0.24
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	14	0.24
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	15	0.24
(1,1148)	1:141:X:ILE:HG13	1:137:X:ALA:H	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	9	0.24
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	4	0.24
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	1	0.24
(1,997)	1:124:X:MET:HG3	1:138:X:LEU:H	2	0.24
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	8	0.24
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	13	0.24
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	11	0.24
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	17	0.24
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	13	0.24
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	12	0.24
(1,562)	1:65:X:GLU:HB2	1:64:X:VAL:H	4	0.24
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	17	0.24
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	1	0.24
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	3	0.24
(1,281)	1:40:X:ILE:H	1:39:X:TYR:HB3	6	0.24
(1,146)	1:25:X:GLY:H	1:40:X:ILE:HG13	5	0.24
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	8	0.24
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	1	0.23
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	3	0.23
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	5	0.23
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	4	0.23
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	6	0.23
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	19	0.23
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	4	0.23
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	17	0.23
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	16	0.23
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	7	0.23
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	13	0.23
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	20	0.23
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	10	0.23
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	7	0.23
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	12	0.23
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	14	0.23
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	3	0.23
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	19	0.23
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	20	0.23
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	3	0.23
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	10	0.23
(3,878)	1:133:X:ASP:N	1:128:X:THR:CG2	10	0.23
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	12	0.23
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	18	0.23
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	15	0.23
(3,555)	1:87:X:THR:N	1:85:X:LEU:CD1	13	0.23
(3,464)	1:66:X:ASP:N	1:64:X:VAL:CG1	17	0.23
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	18	0.23
(3,159)	1:29:X:ILE:N	1:28:X:PHE:CB	11	0.23
(2,59)	1:54:X:VAL:CG2	1:40:X:ILE:CD1	14	0.23
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	6	0.23
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	15	0.23
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	19	0.23
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	9	0.23
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	13	0.23
(1,887)	1:107:X:VAL:H	1:110:X:ARG:H	9	0.23
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	10	0.23
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	7	0.23
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	6	0.23
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	20	0.23
(1,769)	1:95:X:VAL:HB	1:97:X:GLU:H	20	0.23
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	16	0.23
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	9	0.23
(1,561)	1:65:X:GLU:H	1:64:X:VAL:CB	17	0.23
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	5	0.23
(1,444)	1:56:X:HIS:HB3	1:55:X:SER:H	2	0.23
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	5	0.23
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	17	0.23
(1,411)	1:54:X:VAL:H	1:51:X:CYS:HA	3	0.23
(1,243)	1:37:X:ARG:H	1:36:X:LEU:HB3	16	0.23
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	2	0.23
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	19	0.23
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	18	0.23
(1,51)	1:10:X:GLU:H	1:7:X:LYS:HA	12	0.23
(5,61)	1:126:X:THR:C	1:118:X:LYS:H	4	0.22
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	8	0.22
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	12	0.22
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	10	0.22
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	13	0.22
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	13	0.22
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	7	0.22
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	20	0.22
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	13	0.22
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	17	0.22
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	4	0.22
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	12	0.22
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	2	0.22
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	20	0.22
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	13	0.22
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	19	0.22
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	9	0.22
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	9	0.22
(4,47)	1:47:X:ASN:O	1:50:X:ASP:H	3	0.22
(3,847)	1:128:X:THR:CB	1:116:X:VAL:N	11	0.22
(3,797)	1:121:X:ASP:N	1:120:X:VAL:CB	2	0.22
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	2	0.22
(3,746)	1:112:X:LYS:N	1:111:X:ARG:CB	9	0.22
(3,666)	1:94:X:PHE:N	1:117:X:ILE:CG2	11	0.22
(3,663)	1:91:X:TYR:N	1:125:X:ILE:CD1	20	0.22
(3,661)	1:91:X:TYR:N	1:120:X:VAL:CG1	15	0.22
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	8	0.22
(3,595)	1:92:X:ALA:N	1:85:X:LEU:CD1	8	0.22
(3,556)	1:87:X:THR:N	1:86:X:PHE:CB	13	0.22
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	18	0.22
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	8	0.22
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	12	0.22
(3,333)	1:54:X:VAL:N	1:40:X:ILE:CD1	16	0.22
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	19	0.22
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	10	0.22
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	13	0.22
(3,130)	1:25:X:GLY:N	1:23:X:LEU:CG	4	0.22
(3,130)	1:25:X:GLY:N	1:23:X:LEU:CG	15	0.22
(2,22)	1:16:X:VAL:CG1	1:54:X:VAL:CG2	16	0.22
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	3	0.22
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	13	0.22
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	10	0.22
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	7	0.22
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	6	0.22
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	6	0.22
(1,625)	1:74:X:LEU:HD21	1:39:X:TYR:H	14	0.22
(1,625)	1:74:X:LEU:HD22	1:39:X:TYR:H	14	0.22
(1,625)	1:74:X:LEU:HD23	1:39:X:TYR:H	14	0.22
(1,562)	1:65:X:GLU:HB2	1:64:X:VAL:H	8	0.22
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	5	0.22
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	4	0.22
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	20	0.22
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	19	0.22
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	14	0.22
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	2	0.22
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	19	0.22
(1,342)	1:47:X:ASN:H	1:46:X:ILE:HG13	20	0.22
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	16	0.22
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	4	0.22
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	11	0.22
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	11	0.22
(1,5)	1:5:X:GLU:H	1:4:X:LEU:HG	15	0.22
(5,67)	1:136:X:PHE:C	1:125:X:ILE:H	1	0.21
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	3	0.21
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	18	0.21
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	11	0.21
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	10	0.21
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	3	0.21
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	2	0.21
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	7	0.21
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	12	0.21
(5,18)	1:35:X:THR:C	1:29:X:ILE:H	7	0.21
(5,16)	1:33:X:THR:C	1:31:X:GLY:H	18	0.21
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	19	0.21
(5,9)	1:13:X:THR:C	1:17:X:GLU:H	13	0.21
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	9	0.21
(5,2)	1:5:X:GLU:C	1:9:X:THR:H	12	0.21
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	11	0.21
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	15	0.21
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	8	0.21
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	10	0.21
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	15	0.21
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	5	0.21
(4,60)	1:53:X:ASP:O	1:57:X:GLN:N	10	0.21
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	8	0.21
(4,21)	1:15:X:PRO:O	1:19:X:LEU:H	7	0.21
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	11	0.21
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	17	0.21
(3,940)	1:144:X:ALA:N	1:143:X:LYS:CG	5	0.21
(3,887)	1:135:X:VAL:CG2	1:125:X:ILE:N	4	0.21
(3,797)	1:121:X:ASP:N	1:120:X:VAL:CB	1	0.21
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	4	0.21
(3,661)	1:91:X:TYR:N	1:120:X:VAL:CG1	16	0.21
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	9	0.21
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	10	0.21
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	15	0.21
(3,462)	1:66:X:ASP:N	1:11:X:MET:CE	10	0.21
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	10	0.21
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	20	0.21
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	20	0.21
(3,130)	1:25:X:GLY:N	1:23:X:LEU:CG	19	0.21
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	12	0.21
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	5	0.21
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	16	0.21
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	2	0.21
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	15	0.21
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	20	0.21
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	5	0.21
(1,769)	1:95:X:VAL:HB	1:97:X:GLU:H	12	0.21
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	11	0.21
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	18	0.21
(1,625)	1:74:X:LEU:HD21	1:39:X:TYR:H	11	0.21
(1,625)	1:74:X:LEU:HD22	1:39:X:TYR:H	11	0.21
(1,625)	1:74:X:LEU:HD23	1:39:X:TYR:H	11	0.21
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	15	0.21
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	10	0.21
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	16	0.21
(1,444)	1:56:X:HIS:HB3	1:55:X:SER:H	7	0.21
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	18	0.21
(1,342)	1:47:X:ASN:H	1:46:X:ILE:HG13	16	0.21
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	16	0.21
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	3	0.21
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	20	0.21
(1,164)	1:29:X:ILE:H	1:28:X:PHE:CZ	4	0.21
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	3	0.21
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	20	0.21
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	11	0.21
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	12	0.21
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	18	0.2
(5,57)	1:119:X:ALA:C	1:126:X:THR:H	3	0.2
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	5	0.2
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	14	0.2
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	1	0.2
(5,40)	1:75:X:GLU:C	1:38:X:ILE:H	9	0.2
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	9	0.2
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	2	0.2
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	15	0.2
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	2	0.2
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	7	0.2
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	3	0.2
(5,23)	1:41:X:ASP:C	1:23:X:LEU:H	12	0.2
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	2	0.2
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	5	0.2
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	17	0.2
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	4	0.2
(5,12)	1:23:X:LEU:C	1:41:X:ASP:H	3	0.2
(5,12)	1:23:X:LEU:C	1:41:X:ASP:H	18	0.2
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	1	0.2
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	18	0.2
(5,9)	1:13:X:THR:C	1:17:X:GLU:H	10	0.2
(4,115)	1:121:X:ASP:O	1:124:X:MET:H	10	0.2
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	6	0.2
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	11	0.2
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	15	0.2
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	20	0.2
(4,88)	1:89:X:GLU:O	1:93:X:ARG:N	19	0.2
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	1	0.2
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	4	0.2
(4,71)	1:59:X:SER:O	1:63:X:ASP:H	4	0.2
(4,67)	1:57:X:GLN:O	1:61:X:VAL:H	9	0.2
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	10	0.2
(4,23)	1:23:X:LEU:O	1:41:X:ASP:N	13	0.2
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	5	0.2
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	11	0.2
(3,922)	1:141:X:ILE:N	1:140:X:ASN:CB	14	0.2
(3,797)	1:121:X:ASP:N	1:120:X:VAL:CB	10	0.2
(3,797)	1:121:X:ASP:N	1:120:X:VAL:CB	14	0.2
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	6	0.2
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	1	0.2
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	7	0.2
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	16	0.2
(3,666)	1:94:X:PHE:N	1:117:X:ILE:CG2	3	0.2
(3,610)	1:94:X:PHE:N	1:85:X:LEU:CD1	12	0.2
(3,554)	1:85:X:LEU:CA	1:87:X:THR:N	8	0.2
(3,554)	1:85:X:LEU:CA	1:87:X:THR:N	9	0.2
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	3	0.2
(3,313)	1:52:X:ALA:N	1:40:X:ILE:CD1	16	0.2
(3,203)	1:36:X:LEU:N	1:35:X:THR:CG2	1	0.2
(2,121)	1:138:X:LEU:CD1	1:141:X:ILE:CD1	6	0.2
(2,86)	1:91:X:TYR:CA	1:117:X:ILE:CD1	1	0.2
(2,37)	1:38:X:ILE:CG2	1:26:X:ILE:CD1	3	0.2
(1,1095)	1:134:X:GLU:H	1:127:X:VAL:H	16	0.2
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	14	0.2
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	4	0.2
(1,891)	1:108:X:GLN:H	1:107:X:VAL:CB	18	0.2
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	11	0.2
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	15	0.2
(1,769)	1:95:X:VAL:HB	1:97:X:GLU:H	13	0.2
(1,665)	1:78:X:SER:HA	1:40:X:ILE:H	20	0.2
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	10	0.2
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	17	0.2
(1,561)	1:65:X:GLU:H	1:64:X:VAL:CB	1	0.2
(1,467)	1:58:X:VAL:HB	1:56:X:HIS:H	2	0.2
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	5	0.2
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	12	0.2
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	4	0.2
(1,144)	1:25:X:GLY:H	1:39:X:TYR:HB2	7	0.2
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	7	0.2
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	10	0.2
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	10	0.2
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	4	0.19
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	12	0.19
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	16	0.19
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	14	0.19
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	15	0.19
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	15	0.19
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	10	0.19
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	14	0.19
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	19	0.19
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	15	0.19
(5,29)	1:52:X:ALA:C	1:56:X:HIS:H	4	0.19
(5,26)	1:49:X:ASP:C	1:53:X:ASP:H	4	0.19
(5,25)	1:48:X:VAL:C	1:52:X:ALA:H	8	0.19
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	20	0.19
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	4	0.19
(4,68)	1:57:X:GLN:O	1:61:X:VAL:N	9	0.19
(4,67)	1:57:X:GLN:O	1:61:X:VAL:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,21)	1:15:X:PRO:O	1:19:X:LEU:H	2	0.19
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	2	0.19
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	16	0.19
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	2	0.19
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	4	0.19
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	17	0.19
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	14	0.19
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	20	0.19
(3,797)	1:121:X:ASP:N	1:120:X:VAL:CB	11	0.19
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	16	0.19
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	1	0.19
(3,716)	1:104:X:ARG:N	1:105:X:MET:CB	7	0.19
(3,690)	1:101:X:LEU:CG	1:115:X:GLY:N	13	0.19
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	18	0.19
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	13	0.19
(3,610)	1:94:X:PHE:N	1:85:X:LEU:CD1	2	0.19
(3,556)	1:87:X:THR:N	1:86:X:PHE:CB	6	0.19
(3,556)	1:87:X:THR:N	1:86:X:PHE:CB	12	0.19
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	10	0.19
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	1	0.19
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	14	0.19
(3,356)	1:55:X:SER:N	1:76:X:VAL:CG1	16	0.19
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	17	0.19
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	11	0.19
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	11	0.19
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	5	0.19
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	17	0.19
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	15	0.19
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	8	0.19
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	17	0.19
(1,755)	1:94:X:PHE:HB3	1:97:X:GLU:H	11	0.19
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	2	0.19
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	8	0.19
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	16	0.19
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	4	0.19
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	18	0.19
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	1	0.19
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	4	0.19
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	12	0.19
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	7	0.19
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	18	0.19
(1,287)	1:41:X:ASP:H	1:21:X:PHE:HA	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	6	0.19
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	19	0.19
(1,176)	1:29:X:ILE:H	1:36:X:LEU:H	7	0.19
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	15	0.19
(1,96)	1:19:X:LEU:H	1:16:X:VAL:HA	9	0.19
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	3	0.18
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	9	0.18
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	10	0.18
(5,67)	1:136:X:PHE:C	1:125:X:ILE:H	12	0.18
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	2	0.18
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	7	0.18
(5,57)	1:119:X:ALA:C	1:126:X:THR:H	11	0.18
(5,56)	1:116:X:VAL:C	1:128:X:THR:H	5	0.18
(5,56)	1:116:X:VAL:C	1:128:X:THR:H	11	0.18
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	6	0.18
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	9	0.18
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	8	0.18
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	15	0.18
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	18	0.18
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	16	0.18
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	6	0.18
(5,41)	1:77:X:SER:C	1:40:X:ILE:H	14	0.18
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	5	0.18
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	9	0.18
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	20	0.18
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	9	0.18
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	14	0.18
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	8	0.18
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	10	0.18
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	2	0.18
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	15	0.18
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	4	0.18
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	5	0.18
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	12	0.18
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	19	0.18
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	19	0.18
(5,1)	1:4:X:LEU:C	1:8:X:LEU:H	17	0.18
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	16	0.18
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	6	0.18
(4,87)	1:89:X:GLU:O	1:93:X:ARG:H	10	0.18
(3,922)	1:141:X:ILE:N	1:140:X:ASN:CB	4	0.18
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,749)	1:113:X:TRP:N	1:101:X:LEU:CD1	1	0.18
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	7	0.18
(3,667)	1:95:X:VAL:N	1:117:X:ILE:CG2	3	0.18
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	14	0.18
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	13	0.18
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	14	0.18
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	6	0.18
(3,197)	1:35:X:THR:N	1:34:X:SER:CB	5	0.18
(2,22)	1:16:X:VAL:CG1	1:54:X:VAL:CG2	18	0.18
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	13	0.18
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	19	0.18
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	20	0.18
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	11	0.18
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	9	0.18
(1,975)	1:122:X:GLY:H	1:124:X:MET:H	10	0.18
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	5	0.18
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	19	0.18
(1,756)	1:94:X:PHE:HA	1:97:X:GLU:H	11	0.18
(1,741)	1:93:X:ARG:H	1:90:X:HIS:HA	12	0.18
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	11	0.18
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	20	0.18
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	11	0.18
(1,581)	1:66:X:ASP:HB2	1:72:X:TYR:H	19	0.18
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	6	0.18
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	18	0.18
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	13	0.18
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	7	0.18
(1,467)	1:58:X:VAL:HB	1:56:X:HIS:H	9	0.18
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	9	0.18
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	4	0.18
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	18	0.18
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	9	0.18
(1,215)	1:35:X:THR:H	1:28:X:PHE:HA	10	0.18
(1,96)	1:19:X:LEU:H	1:16:X:VAL:HA	6	0.18
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	6	0.18
(1,5)	1:5:X:GLU:H	1:4:X:LEU:HG	10	0.18
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	3	0.18
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	2	0.17
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	4	0.17
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	1	0.17
(5,61)	1:126:X:THR:C	1:118:X:LYS:H	15	0.17
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	6	0.17
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	14	0.17
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	19	0.17
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	11	0.17
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	5	0.17
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	11	0.17
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	19	0.17
(5,39)	1:73:X:ASN:C	1:36:X:LEU:H	4	0.17
(5,39)	1:73:X:ASN:C	1:36:X:LEU:H	7	0.17
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	18	0.17
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	1	0.17
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	20	0.17
(5,34)	1:57:X:GLN:C	1:61:X:VAL:H	14	0.17
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	4	0.17
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	6	0.17
(5,28)	1:51:X:CYS:C	1:55:X:SER:H	10	0.17
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	1	0.17
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	8	0.17
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	17	0.17
(5,19)	1:36:X:LEU:C	1:75:X:GLU:H	9	0.17
(5,19)	1:36:X:LEU:C	1:75:X:GLU:H	12	0.17
(5,18)	1:35:X:THR:C	1:29:X:ILE:H	4	0.17
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	19	0.17
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	11	0.17
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	1	0.17
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	7	0.17
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	12	0.17
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	7	0.17
(4,74)	1:60:X:ALA:O	1:64:X:VAL:N	16	0.17
(4,65)	1:56:X:HIS:O	1:60:X:ALA:H	5	0.17
(4,47)	1:47:X:ASN:O	1:50:X:ASP:H	5	0.17
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	2	0.17
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	19	0.17
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	5	0.17
(3,847)	1:128:X:THR:CB	1:116:X:VAL:N	3	0.17
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	9	0.17
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	11	0.17
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	7	0.17
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	12	0.17
(3,749)	1:113:X:TRP:N	1:101:X:LEU:CD1	8	0.17
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	4	0.17
(3,716)	1:104:X:ARG:N	1:105:X:MET:CB	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,667)	1:95:X:VAL:N	1:117:X:ILE:CG2	2	0.17
(3,667)	1:95:X:VAL:N	1:117:X:ILE:CG2	9	0.17
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	2	0.17
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	13	0.17
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	17	0.17
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	6	0.17
(3,435)	1:63:X:ASP:N	1:62:X:LEU:CD1	13	0.17
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	15	0.17
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	16	0.17
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	15	0.17
(3,175)	1:31:X:GLY:N	1:30:X:ARG:CD	13	0.17
(2,121)	1:138:X:LEU:CD1	1:141:X:ILE:CD1	15	0.17
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	4	0.17
(1,1149)	1:141:X:ILE:H	1:138:X:LEU:HA	11	0.17
(1,1095)	1:134:X:GLU:H	1:127:X:VAL:H	11	0.17
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	9	0.17
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	1	0.17
(1,701)	1:87:X:THR:H	1:86:X:PHE:HB2	19	0.17
(1,670)	1:78:X:SER:HB2	1:78:X:SER:H	3	0.17
(1,670)	1:78:X:SER:HB2	1:78:X:SER:H	14	0.17
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	16	0.17
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	20	0.17
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	3	0.17
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	18	0.17
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	1	0.17
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	7	0.17
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	15	0.17
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	17	0.17
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	11	0.17
(1,411)	1:54:X:VAL:H	1:51:X:CYS:HA	2	0.17
(1,326)	1:46:X:ILE:H	1:45:X:GLY:H	16	0.17
(1,307)	1:44:X:ASP:H	1:43:X:GLU:HG2	11	0.17
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	10	0.17
(1,236)	1:37:X:ARG:H	1:27:X:GLU:HB2	2	0.17
(1,200)	1:33:X:THR:H	1:32:X:ARG:HG2	9	0.17
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	4	0.17
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	17	0.17
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	2	0.17
(1,51)	1:10:X:GLU:H	1:7:X:LYS:HA	13	0.17
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	11	0.16
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	17	0.16
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	17	0.16
(5,62)	1:127:X:VAL:C	1:134:X:GLU:H	18	0.16
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	3	0.16
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	17	0.16
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	2	0.16
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	17	0.16
(5,46)	1:115:X:GLY:C	1:99:X:VAL:H	5	0.16
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	6	0.16
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	8	0.16
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	17	0.16
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	17	0.16
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	6	0.16
(5,12)	1:23:X:LEU:C	1:41:X:ASP:H	4	0.16
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	2	0.16
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	7	0.16
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	13	0.16
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	17	0.16
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	16	0.16
(4,68)	1:57:X:GLN:O	1:61:X:VAL:N	8	0.16
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	12	0.16
(4,43)	1:39:X:TYR:O	1:25:X:GLY:H	13	0.16
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	7	0.16
(3,922)	1:141:X:ILE:N	1:140:X:ASN:CB	17	0.16
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	19	0.16
(3,878)	1:133:X:ASP:N	1:128:X:THR:CG2	17	0.16
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	4	0.16
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	10	0.16
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	14	0.16
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	17	0.16
(3,749)	1:113:X:TRP:N	1:101:X:LEU:CD1	19	0.16
(3,667)	1:95:X:VAL:N	1:117:X:ILE:CG2	20	0.16
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	4	0.16
(3,610)	1:94:X:PHE:N	1:85:X:LEU:CD1	14	0.16
(3,556)	1:87:X:THR:N	1:86:X:PHE:CB	20	0.16
(3,554)	1:85:X:LEU:CA	1:87:X:THR:N	4	0.16
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	11	0.16
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	20	0.16
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	1	0.16
(3,484)	1:71:X:ALA:N	1:70:X:VAL:CB	5	0.16
(3,304)	1:51:X:CYS:N	1:40:X:ILE:CD1	5	0.16
(3,266)	1:45:X:GLY:N	1:43:X:GLU:CG	15	0.16
(3,239)	1:41:X:ASP:N	1:16:X:VAL:CG1	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,130)	1:25:X:GLY:N	1:23:X:LEU:CG	1	0.16
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	6	0.16
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	7	0.16
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	19	0.16
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	20	0.16
(1,1015)	1:125:X:ILE:H	1:138:X:LEU:HG	19	0.16
(1,997)	1:124:X:MET:HG3	1:138:X:LEU:H	10	0.16
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	5	0.16
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	18	0.16
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	13	0.16
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	19	0.16
(1,841)	1:101:X:LEU:H	1:114:X:GLN:HB2	10	0.16
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	13	0.16
(1,643)	1:76:X:VAL:HB	1:55:X:SER:H	4	0.16
(1,609)	1:73:X:ASN:H	1:36:X:LEU:HB2	18	0.16
(1,596)	1:71:X:ALA:H	1:70:X:VAL:CB	20	0.16
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG21	20	0.16
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG22	20	0.16
(1,596)	1:71:X:ALA:H	1:70:X:VAL:HG23	20	0.16
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	2	0.16
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	6	0.16
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	15	0.16
(1,520)	1:62:X:LEU:HB2	1:61:X:VAL:H	11	0.16
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	2	0.16
(1,500)	1:59:X:SER:H	1:62:X:LEU:HB3	12	0.16
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	11	0.16
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	18	0.16
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	11	0.16
(1,383)	1:50:X:ASP:HA	1:53:X:ASP:H	19	0.16
(1,241)	1:37:X:ARG:H	1:29:X:ILE:H	1	0.16
(1,200)	1:33:X:THR:H	1:32:X:ARG:HG2	4	0.16
(1,174)	1:29:X:ILE:HA	1:35:X:THR:H	5	0.16
(1,164)	1:29:X:ILE:H	1:28:X:PHE:CZ	8	0.16
(1,164)	1:29:X:ILE:H	1:28:X:PHE:CZ	17	0.16
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	9	0.16
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	11	0.16
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	16	0.16
(1,51)	1:10:X:GLU:H	1:7:X:LYS:HA	2	0.16
(1,51)	1:10:X:GLU:H	1:7:X:LYS:HA	3	0.16
(5,70)	1:145:X:ASN:C	1:100:X:THR:H	3	0.15
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	1	0.15
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	11	0.15
(5,62)	1:127:X:VAL:C	1:134:X:GLU:H	10	0.15
(5,61)	1:126:X:THR:C	1:118:X:LYS:H	12	0.15
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	20	0.15
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	17	0.15
(5,52)	1:100:X:THR:C	1:145:X:ASN:H	6	0.15
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	11	0.15
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	18	0.15
(5,46)	1:115:X:GLY:C	1:99:X:VAL:H	4	0.15
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	5	0.15
(5,39)	1:73:X:ASN:C	1:36:X:LEU:H	1	0.15
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	2	0.15
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	5	0.15
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	15	0.15
(5,29)	1:52:X:ALA:C	1:56:X:HIS:H	8	0.15
(5,29)	1:52:X:ALA:C	1:56:X:HIS:H	17	0.15
(5,29)	1:52:X:ALA:C	1:56:X:HIS:H	20	0.15
(5,23)	1:41:X:ASP:C	1:23:X:LEU:H	6	0.15
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	14	0.15
(5,18)	1:35:X:THR:C	1:29:X:ILE:H	12	0.15
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	5	0.15
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	14	0.15
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	14	0.15
(5,9)	1:13:X:THR:C	1:17:X:GLU:H	20	0.15
(5,6)	1:9:X:THR:C	1:13:X:THR:H	19	0.15
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	18	0.15
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	1	0.15
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	12	0.15
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	17	0.15
(4,87)	1:89:X:GLU:O	1:93:X:ARG:H	8	0.15
(4,87)	1:89:X:GLU:O	1:93:X:ARG:H	18	0.15
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	17	0.15
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	1	0.15
(4,73)	1:60:X:ALA:O	1:64:X:VAL:H	16	0.15
(4,72)	1:59:X:SER:O	1:63:X:ASP:N	4	0.15
(4,21)	1:15:X:PRO:O	1:19:X:LEU:H	11	0.15
(4,21)	1:15:X:PRO:O	1:19:X:LEU:H	18	0.15
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	19	0.15
(4,1)	1:4:X:LEU:O	1:8:X:LEU:H	6	0.15
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	20	0.15
(3,922)	1:141:X:ILE:N	1:140:X:ASN:CB	20	0.15
(3,921)	1:141:X:ILE:N	1:101:X:LEU:CD2	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	1	0.15
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	7	0.15
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	9	0.15
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	12	0.15
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	2	0.15
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	9	0.15
(3,765)	1:115:X:GLY:N	1:129:X:VAL:CG2	5	0.15
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	16	0.15
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	2	0.15
(3,666)	1:94:X:PHE:N	1:117:X:ILE:CG2	4	0.15
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	4	0.15
(3,663)	1:91:X:TYR:N	1:125:X:ILE:CD1	7	0.15
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	3	0.15
(3,563)	1:88:X:ALA:N	1:87:X:THR:CG2	13	0.15
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	17	0.15
(3,484)	1:71:X:ALA:N	1:70:X:VAL:CB	20	0.15
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	9	0.15
(3,212)	1:37:X:ARG:N	1:27:X:GLU:CB	1	0.15
(3,209)	1:36:X:LEU:N	1:74:X:LEU:CD2	20	0.15
(3,208)	1:36:X:LEU:N	1:37:X:ARG:CG	3	0.15
(3,197)	1:35:X:THR:N	1:34:X:SER:CB	13	0.15
(3,189)	1:34:X:SER:N	1:33:X:THR:CB	3	0.15
(3,124)	1:24:X:VAL:N	1:23:X:LEU:CD1	15	0.15
(2,121)	1:138:X:LEU:CD1	1:141:X:ILE:CD1	5	0.15
(2,29)	1:29:X:ILE:CD1	1:35:X:THR:CG2	15	0.15
(2,23)	1:16:X:VAL:CG2	1:54:X:VAL:CG2	5	0.15
(1,1149)	1:141:X:ILE:H	1:138:X:LEU:HA	14	0.15
(1,1148)	1:141:X:ILE:HG13	1:137:X:ALA:H	4	0.15
(1,1072)	1:130:X:GLU:HB2	1:132:X:LYS:H	12	0.15
(1,1053)	1:128:X:THR:HA	1:134:X:GLU:H	9	0.15
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	6	0.15
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	8	0.15
(1,995)	1:124:X:MET:H	1:138:X:LEU:HG	15	0.15
(1,975)	1:122:X:GLY:H	1:124:X:MET:H	9	0.15
(1,975)	1:122:X:GLY:H	1:124:X:MET:H	14	0.15
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	15	0.15
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	16	0.15
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	16	0.15
(1,943)	1:116:X:VAL:HB	1:128:X:THR:H	13	0.15
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	11	0.15
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	15	0.15
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	4	0.15
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	9	0.15
(1,581)	1:66:X:ASP:HB2	1:72:X:TYR:H	3	0.15
(1,562)	1:65:X:GLU:HB2	1:64:X:VAL:H	19	0.15
(1,500)	1:59:X:SER:H	1:62:X:LEU:HB3	3	0.15
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	14	0.15
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	16	0.15
(1,482)	1:58:X:VAL:CB	1:60:X:ALA:H	13	0.15
(1,444)	1:56:X:HIS:HB3	1:55:X:SER:H	18	0.15
(1,200)	1:33:X:THR:H	1:32:X:ARG:HG2	11	0.15
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	7	0.15
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	5	0.15
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	1	0.15
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	10	0.15
(5,70)	1:145:X:ASN:C	1:100:X:THR:H	6	0.14
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	6	0.14
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	5	0.14
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	19	0.14
(5,63)	1:128:X:THR:C	1:116:X:VAL:H	13	0.14
(5,63)	1:128:X:THR:C	1:116:X:VAL:H	19	0.14
(5,59)	1:124:X:MET:C	1:121:X:ASP:H	13	0.14
(5,56)	1:116:X:VAL:C	1:128:X:THR:H	15	0.14
(5,49)	1:97:X:GLU:C	1:117:X:ILE:H	17	0.14
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	11	0.14
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	12	0.14
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	11	0.14
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	18	0.14
(5,39)	1:73:X:ASN:C	1:36:X:LEU:H	19	0.14
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	3	0.14
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	8	0.14
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	16	0.14
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	8	0.14
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	10	0.14
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	18	0.14
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	2	0.14
(5,24)	1:47:X:ASN:C	1:50:X:ASP:H	11	0.14
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	9	0.14
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	1	0.14
(5,18)	1:35:X:THR:C	1:29:X:ILE:H	3	0.14
(5,12)	1:23:X:LEU:C	1:41:X:ASP:H	8	0.14
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	1	0.14
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	10	0.14
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	3	0.14
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	6	0.14
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	14	0.14
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	13	0.14
(4,88)	1:89:X:GLU:O	1:93:X:ARG:N	10	0.14
(4,67)	1:57:X:GLN:O	1:61:X:VAL:H	4	0.14
(4,65)	1:56:X:HIS:O	1:60:X:ALA:H	9	0.14
(4,59)	1:53:X:ASP:O	1:57:X:GLN:H	2	0.14
(4,54)	1:50:X:ASP:O	1:54:X:VAL:H	5	0.14
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	14	0.14
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	6	0.14
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	10	0.14
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	15	0.14
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	20	0.14
(3,906)	1:137:X:ALA:N	1:141:X:ILE:CD1	16	0.14
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	5	0.14
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	3	0.14
(3,632)	1:97:X:GLU:N	1:94:X:PHE:CA	7	0.14
(3,554)	1:85:X:LEU:CA	1:87:X:THR:N	10	0.14
(3,545)	1:81:X:LEU:CD1	1:82:X:ASP:N	10	0.14
(3,534)	1:80:X:GLY:N	1:79:X:PRO:CB	11	0.14
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	12	0.14
(3,476)	1:68:X:ILE:N	1:68:X:ILE:CD1	5	0.14
(3,333)	1:54:X:VAL:N	1:40:X:ILE:CD1	20	0.14
(3,197)	1:35:X:THR:N	1:34:X:SER:CB	17	0.14
(3,189)	1:34:X:SER:N	1:33:X:THR:CB	5	0.14
(3,124)	1:24:X:VAL:N	1:23:X:LEU:CD1	1	0.14
(2,121)	1:138:X:LEU:CD1	1:141:X:ILE:CD1	9	0.14
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	1	0.14
(2,22)	1:16:X:VAL:CG1	1:54:X:VAL:CG2	4	0.14
(1,1149)	1:141:X:ILE:H	1:138:X:LEU:HA	17	0.14
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	16	0.14
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	2	0.14
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	3	0.14
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	15	0.14
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	18	0.14
(1,985)	1:123:X:GLU:H	1:124:X:MET:HB2	10	0.14
(1,985)	1:123:X:GLU:H	1:124:X:MET:HB2	20	0.14
(1,975)	1:122:X:GLY:H	1:124:X:MET:H	20	0.14
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	16	0.14
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	20	0.14
(1,871)	1:105:X:MET:HA	1:106:X:ALA:H	18	0.14
(1,796)	1:146:X:LEU:H	1:85:X:LEU:H	16	0.14
(1,769)	1:95:X:VAL:HB	1:97:X:GLU:H	8	0.14
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	18	0.14
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	16	0.14
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	3	0.14
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	7	0.14
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	16	0.14
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	19	0.14
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	10	0.14
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	14	0.14
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	15	0.14
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	20	0.14
(1,307)	1:44:X:ASP:H	1:43:X:GLU:HG2	15	0.14
(1,288)	1:41:X:ASP:H	1:22:X:GLU:HB3	6	0.14
(1,170)	1:29:X:ILE:H	1:35:X:THR:H	3	0.14
(1,164)	1:29:X:ILE:H	1:28:X:PHE:CZ	18	0.14
(1,96)	1:19:X:LEU:H	1:16:X:VAL:HA	2	0.14
(1,80)	1:14:X:ALA:H	1:11:X:MET:HA	15	0.14
(1,59)	1:12:X:ILE:H	1:9:X:THR:HA	4	0.14
(1,58)	1:12:X:ILE:H	1:9:X:THR:H	14	0.14
(1,51)	1:10:X:GLU:H	1:7:X:LYS:HA	10	0.14
(1,5)	1:5:X:GLU:H	1:4:X:LEU:HG	1	0.14
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	4	0.14
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	15	0.14
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	19	0.14
(5,70)	1:145:X:ASN:C	1:100:X:THR:H	14	0.13
(5,70)	1:145:X:ASN:C	1:100:X:THR:H	16	0.13
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	8	0.13
(5,68)	1:137:X:ALA:C	1:140:X:ASN:H	20	0.13
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	15	0.13
(5,62)	1:127:X:VAL:C	1:134:X:GLU:H	5	0.13
(5,61)	1:126:X:THR:C	1:118:X:LYS:H	20	0.13
(5,57)	1:119:X:ALA:C	1:126:X:THR:H	15	0.13
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	20	0.13
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	12	0.13
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	14	0.13
(5,27)	1:50:X:ASP:C	1:54:X:VAL:H	13	0.13
(5,24)	1:47:X:ASN:C	1:50:X:ASP:H	5	0.13
(5,24)	1:47:X:ASN:C	1:50:X:ASP:H	12	0.13
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	8	0.13
(5,20)	1:37:X:ARG:C	1:27:X:GLU:H	10	0.13
(5,18)	1:35:X:THR:C	1:29:X:ILE:H	9	0.13
(5,18)	1:35:X:THR:C	1:29:X:ILE:H	15	0.13
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	9	0.13
(5,10)	1:14:X:ALA:C	1:18:X:ALA:H	7	0.13
(5,9)	1:13:X:THR:C	1:17:X:GLU:H	15	0.13
(5,6)	1:9:X:THR:C	1:13:X:THR:H	13	0.13
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	11	0.13
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	14	0.13
(5,2)	1:5:X:GLU:C	1:9:X:THR:H	16	0.13
(4,108)	1:102:X:VAL:O	1:143:X:LYS:N	18	0.13
(4,89)	1:90:X:HIS:O	1:94:X:PHE:H	7	0.13
(4,87)	1:89:X:GLU:O	1:93:X:ARG:H	17	0.13
(4,82)	1:77:X:SER:O	1:40:X:ILE:N	9	0.13
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	18	0.13
(4,76)	1:71:X:ALA:O	1:34:X:SER:N	1	0.13
(4,71)	1:59:X:SER:O	1:63:X:ASP:H	20	0.13
(4,51)	1:49:X:ASP:O	1:53:X:ASP:N	20	0.13
(4,47)	1:47:X:ASN:O	1:50:X:ASP:H	11	0.13
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	16	0.13
(4,2)	1:4:X:LEU:O	1:8:X:LEU:N	19	0.13
(3,930)	1:142:X:GLN:N	1:141:X:ILE:CG2	18	0.13
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	6	0.13
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	16	0.13
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	17	0.13
(3,797)	1:121:X:ASP:N	1:120:X:VAL:CB	9	0.13
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	20	0.13
(3,663)	1:91:X:TYR:N	1:125:X:ILE:CD1	11	0.13
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	8	0.13
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	17	0.13
(3,651)	1:115:X:GLY:N	1:99:X:VAL:CG2	5	0.13
(3,587)	1:91:X:TYR:N	1:85:X:LEU:CD1	14	0.13
(3,566)	1:88:X:ALA:N	1:89:X:GLU:CB	9	0.13
(3,544)	1:81:X:LEU:CB	1:82:X:ASP:N	2	0.13
(3,534)	1:80:X:GLY:N	1:79:X:PRO:CB	14	0.13
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	8	0.13
(3,452)	1:65:X:GLU:N	1:64:X:VAL:CB	20	0.13
(3,386)	1:58:X:VAL:N	1:60:X:ALA:CB	6	0.13
(3,208)	1:36:X:LEU:N	1:37:X:ARG:CG	13	0.13
(3,208)	1:36:X:LEU:N	1:37:X:ARG:CG	14	0.13
(3,159)	1:29:X:ILE:N	1:28:X:PHE:CB	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,145)	1:27:X:GLU:N	1:26:X:ILE:CD1	12	0.13
(3,92)	1:19:X:LEU:N	1:18:X:ALA:CB	20	0.13
(2,22)	1:16:X:VAL:CG1	1:54:X:VAL:CG2	12	0.13
(1,1096)	1:134:X:GLU:H	1:127:X:VAL:HB	16	0.13
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	19	0.13
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	17	0.13
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	6	0.13
(1,959)	1:120:X:VAL:HA	1:124:X:MET:H	17	0.13
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	13	0.13
(1,665)	1:78:X:SER:HA	1:40:X:ILE:H	2	0.13
(1,625)	1:74:X:LEU:HD21	1:39:X:TYR:H	16	0.13
(1,625)	1:74:X:LEU:HD22	1:39:X:TYR:H	16	0.13
(1,625)	1:74:X:LEU:HD23	1:39:X:TYR:H	16	0.13
(1,595)	1:71:X:ALA:H	1:70:X:VAL:HA	16	0.13
(1,588)	1:68:X:ILE:HG12	1:68:X:ILE:H	18	0.13
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	18	0.13
(1,562)	1:65:X:GLU:HB2	1:64:X:VAL:H	18	0.13
(1,561)	1:65:X:GLU:H	1:64:X:VAL:CB	10	0.13
(1,520)	1:62:X:LEU:HB2	1:61:X:VAL:H	18	0.13
(1,485)	1:58:X:VAL:HA	1:61:X:VAL:H	6	0.13
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	7	0.13
(1,467)	1:58:X:VAL:HB	1:56:X:HIS:H	15	0.13
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	15	0.13
(1,355)	1:48:X:VAL:HA	1:51:X:CYS:H	4	0.13
(1,236)	1:37:X:ARG:H	1:27:X:GLU:HB2	12	0.13
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	19	0.13
(1,164)	1:29:X:ILE:H	1:28:X:PHE:CZ	16	0.13
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	15	0.13
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	5	0.13
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	13	0.13
(1,122)	1:23:X:LEU:CG	1:24:X:VAL:H	14	0.13
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	20	0.13
(5,69)	1:143:X:LYS:C	1:102:X:VAL:H	12	0.12
(5,67)	1:136:X:PHE:C	1:125:X:ILE:H	2	0.12
(5,63)	1:128:X:THR:C	1:116:X:VAL:H	2	0.12
(5,61)	1:126:X:THR:C	1:118:X:LYS:H	1	0.12
(5,57)	1:119:X:ALA:C	1:126:X:THR:H	12	0.12
(5,57)	1:119:X:ALA:C	1:126:X:THR:H	16	0.12
(5,56)	1:116:X:VAL:C	1:128:X:THR:H	6	0.12
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	14	0.12
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	19	0.12
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	13	0.12
(5,42)	1:87:X:THR:C	1:91:X:TYR:H	9	0.12
(5,38)	1:71:X:ALA:C	1:34:X:SER:H	19	0.12
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	3	0.12
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	10	0.12
(5,36)	1:59:X:SER:C	1:63:X:ASP:H	12	0.12
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	2	0.12
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	18	0.12
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	12	0.12
(5,31)	1:54:X:VAL:C	1:58:X:VAL:H	2	0.12
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	6	0.12
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	16	0.12
(5,17)	1:34:X:SER:C	1:73:X:ASN:H	16	0.12
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	4	0.12
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	9	0.12
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	12	0.12
(4,117)	1:124:X:MET:O	1:121:X:ASP:H	1	0.12
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	14	0.12
(4,81)	1:77:X:SER:O	1:40:X:ILE:H	11	0.12
(4,67)	1:57:X:GLN:O	1:61:X:VAL:H	3	0.12
(4,52)	1:49:X:ASP:O	1:53:X:ASP:H	11	0.12
(4,44)	1:39:X:TYR:O	1:25:X:GLY:N	13	0.12
(4,29)	1:29:X:ILE:O	1:35:X:THR:N	5	0.12
(4,21)	1:15:X:PRO:O	1:19:X:LEU:H	20	0.12
(4,16)	1:12:X:ILE:O	1:16:X:VAL:H	16	0.12
(4,15)	1:12:X:ILE:O	1:16:X:VAL:N	9	0.12
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	18	0.12
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	8	0.12
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	4	0.12
(3,717)	1:105:X:MET:N	1:104:X:ARG:CD	20	0.12
(3,665)	1:92:X:ALA:N	1:125:X:ILE:CD1	2	0.12
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	7	0.12
(3,652)	1:117:X:ILE:CD1	1:96:X:GLY:N	12	0.12
(3,566)	1:88:X:ALA:N	1:89:X:GLU:CB	6	0.12
(3,566)	1:88:X:ALA:N	1:89:X:GLU:CB	18	0.12
(3,556)	1:87:X:THR:N	1:86:X:PHE:CB	5	0.12
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	14	0.12
(3,502)	1:75:X:GLU:N	1:74:X:LEU:CG	6	0.12
(3,482)	1:71:X:ALA:N	1:70:X:VAL:CG2	16	0.12
(3,425)	1:62:X:LEU:N	1:61:X:VAL:CG2	13	0.12
(3,371)	1:57:X:GLN:N	1:54:X:VAL:CG2	12	0.12
(3,366)	1:56:X:HIS:N	1:57:X:GLN:CB	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,366)	1:56:X:HIS:N	1:57:X:GLN:CB	10	0.12
(3,289)	1:49:X:ASP:N	1:46:X:ILE:CG2	10	0.12
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	3	0.12
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	12	0.12
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	16	0.12
(3,189)	1:34:X:SER:N	1:33:X:THR:CB	1	0.12
(3,189)	1:34:X:SER:N	1:33:X:THR:CB	10	0.12
(3,151)	1:27:X:GLU:N	1:37:X:ARG:CB	1	0.12
(3,92)	1:19:X:LEU:N	1:18:X:ALA:CB	11	0.12
(2,107)	1:120:X:VAL:CG2	1:125:X:ILE:CD1	11	0.12
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD1	5	0.12
(2,15)	1:12:X:ILE:CD1	1:62:X:LEU:CD2	5	0.12
(2,6)	1:8:X:LEU:CG	1:26:X:ILE:CD1	8	0.12
(1,1121)	1:137:X:ALA:HA	1:125:X:ILE:H	5	0.12
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	10	0.12
(1,1045)	1:127:X:VAL:H	1:136:X:PHE:H	18	0.12
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	18	0.12
(1,987)	1:123:X:GLU:HA	1:138:X:LEU:H	6	0.12
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	8	0.12
(1,967)	1:121:X:ASP:H	1:124:X:MET:H	17	0.12
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	16	0.12
(1,800)	1:85:X:LEU:H	1:145:X:ASN:HA	6	0.12
(1,790)	1:117:X:ILE:HB	1:96:X:GLY:H	18	0.12
(1,769)	1:95:X:VAL:HB	1:97:X:GLU:H	7	0.12
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	2	0.12
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	6	0.12
(1,643)	1:76:X:VAL:HB	1:55:X:SER:H	12	0.12
(1,592)	1:69:X:THR:HA	1:70:X:VAL:H	20	0.12
(1,584)	1:67:X:PRO:HA	1:68:X:ILE:H	2	0.12
(1,582)	1:67:X:PRO:HD2	1:66:X:ASP:H	8	0.12
(1,561)	1:65:X:GLU:H	1:64:X:VAL:CB	14	0.12
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	4	0.12
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	5	0.12
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	7	0.12
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	9	0.12
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	12	0.12
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	15	0.12
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	16	0.12
(1,521)	1:62:X:LEU:H	1:61:X:VAL:CB	4	0.12
(1,512)	1:61:X:VAL:HA	1:64:X:VAL:H	14	0.12
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	2	0.12
(1,402)	1:52:X:ALA:HA	1:55:X:SER:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:45:X:GLY:H	1:42:X:SER:H	6	0.12
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	1	0.12
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	3	0.12
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	5	0.12
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	8	0.12
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	16	0.12
(1,200)	1:33:X:THR:H	1:32:X:ARG:HG2	12	0.12
(1,176)	1:29:X:ILE:H	1:36:X:LEU:H	9	0.12
(1,164)	1:29:X:ILE:H	1:28:X:PHE:CZ	3	0.12
(1,144)	1:25:X:GLY:H	1:39:X:TYR:HB2	8	0.12
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	1	0.12
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	7	0.12
(1,125)	1:23:X:LEU:H	1:25:X:GLY:H	20	0.12
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	14	0.12
(5,70)	1:145:X:ASN:C	1:100:X:THR:H	5	0.11
(5,70)	1:145:X:ASN:C	1:100:X:THR:H	20	0.11
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	3	0.11
(5,66)	1:134:X:GLU:C	1:127:X:VAL:H	10	0.11
(5,61)	1:126:X:THR:C	1:118:X:LYS:H	17	0.11
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	2	0.11
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	16	0.11
(5,60)	1:125:X:ILE:C	1:136:X:PHE:H	18	0.11
(5,57)	1:119:X:ALA:C	1:126:X:THR:H	6	0.11
(5,57)	1:119:X:ALA:C	1:126:X:THR:H	10	0.11
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	10	0.11
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	15	0.11
(5,49)	1:97:X:GLU:C	1:117:X:ILE:H	3	0.11
(5,46)	1:115:X:GLY:C	1:99:X:VAL:H	11	0.11
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	17	0.11
(5,44)	1:89:X:GLU:C	1:93:X:ARG:H	4	0.11
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	4	0.11
(5,43)	1:88:X:ALA:C	1:92:X:ALA:H	15	0.11
(5,40)	1:75:X:GLU:C	1:38:X:ILE:H	10	0.11
(5,37)	1:60:X:ALA:C	1:64:X:VAL:H	2	0.11
(5,35)	1:58:X:VAL:C	1:62:X:LEU:H	7	0.11
(5,30)	1:53:X:ASP:C	1:57:X:GLN:H	4	0.11
(5,29)	1:52:X:ALA:C	1:56:X:HIS:H	9	0.11
(5,23)	1:41:X:ASP:C	1:23:X:LEU:H	11	0.11
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	19	0.11
(5,21)	1:38:X:ILE:C	1:77:X:SER:H	16	0.11
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	15	0.11
(5,7)	1:10:X:GLU:C	1:14:X:ALA:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,5)	1:8:X:LEU:C	1:12:X:ILE:H	18	0.11
(5,4)	1:7:X:LYS:C	1:11:X:MET:H	16	0.11
(5,3)	1:6:X:GLN:C	1:10:X:GLU:H	18	0.11
(5,2)	1:5:X:GLU:C	1:9:X:THR:H	6	0.11
(4,118)	1:124:X:MET:O	1:121:X:ASP:N	1	0.11
(4,117)	1:124:X:MET:O	1:121:X:ASP:H	10	0.11
(4,115)	1:121:X:ASP:O	1:124:X:MET:H	14	0.11
(4,107)	1:102:X:VAL:O	1:143:X:LYS:H	18	0.11
(4,95)	1:147:X:VAL:O	1:98:X:GLU:N	10	0.11
(4,88)	1:89:X:GLU:O	1:93:X:ARG:N	3	0.11
(4,68)	1:57:X:GLN:O	1:61:X:VAL:N	4	0.11
(4,65)	1:56:X:HIS:O	1:60:X:ALA:H	18	0.11
(4,1)	1:4:X:LEU:O	1:8:X:LEU:H	19	0.11
(3,922)	1:141:X:ILE:N	1:140:X:ASN:CB	1	0.11
(3,922)	1:141:X:ILE:N	1:140:X:ASN:CB	2	0.11
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	8	0.11
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	10	0.11
(3,909)	1:138:X:LEU:N	1:137:X:ALA:CB	11	0.11
(3,878)	1:133:X:ASP:N	1:128:X:THR:CG2	13	0.11
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	19	0.11
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	2	0.11
(3,806)	1:122:X:GLY:N	1:121:X:ASP:CB	13	0.11
(3,804)	1:121:X:ASP:N	1:125:X:ILE:CD1	3	0.11
(3,760)	1:115:X:GLY:N	1:100:X:THR:CG2	18	0.11
(3,749)	1:113:X:TRP:N	1:101:X:LEU:CD1	5	0.11
(3,716)	1:104:X:ARG:N	1:105:X:MET:CB	3	0.11
(3,667)	1:95:X:VAL:N	1:117:X:ILE:CG2	4	0.11
(3,666)	1:94:X:PHE:N	1:117:X:ILE:CG2	19	0.11
(3,664)	1:92:X:ALA:N	1:120:X:VAL:CG1	12	0.11
(3,583)	1:90:X:HIS:N	1:89:X:GLU:CB	18	0.11
(3,366)	1:56:X:HIS:N	1:57:X:GLN:CB	17	0.11
(3,333)	1:54:X:VAL:N	1:40:X:ILE:CD1	15	0.11
(3,315)	1:52:X:ALA:N	1:48:X:VAL:CA	4	0.11
(3,315)	1:52:X:ALA:N	1:48:X:VAL:CA	15	0.11
(3,272)	1:46:X:ILE:N	1:44:X:ASP:CB	4	0.11
(3,239)	1:41:X:ASP:N	1:16:X:VAL:CG1	13	0.11
(3,92)	1:19:X:LEU:N	1:18:X:ALA:CB	1	0.11
(2,64)	1:61:X:VAL:CG1	1:15:X:PRO:CD	17	0.11
(1,1043)	1:127:X:VAL:H	1:135:X:VAL:HA	19	0.11
(1,1025)	1:126:X:THR:H	1:125:X:ILE:CD1	16	0.11
(1,983)	1:123:X:GLU:H	1:124:X:MET:HA	9	0.11
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,962)	1:121:X:ASP:H	1:120:X:VAL:CB	12	0.11
(1,904)	1:109:X:ASN:H	1:107:X:VAL:H	13	0.11
(1,899)	1:108:X:GLN:HA	1:109:X:ASN:H	9	0.11
(1,647)	1:76:X:VAL:H	1:75:X:GLU:HG3	9	0.11
(1,595)	1:71:X:ALA:H	1:70:X:VAL:HA	2	0.11
(1,592)	1:69:X:THR:HA	1:70:X:VAL:H	10	0.11
(1,584)	1:67:X:PRO:HA	1:68:X:ILE:H	6	0.11
(1,561)	1:65:X:GLU:H	1:64:X:VAL:CB	13	0.11
(1,553)	1:64:X:VAL:HB	1:64:X:VAL:H	1	0.11
(1,553)	1:64:X:VAL:HB	1:64:X:VAL:H	10	0.11
(1,553)	1:64:X:VAL:HB	1:64:X:VAL:H	20	0.11
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	3	0.11
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	6	0.11
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	8	0.11
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	19	0.11
(1,521)	1:62:X:LEU:H	1:61:X:VAL:CB	18	0.11
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	17	0.11
(1,467)	1:58:X:VAL:HB	1:56:X:HIS:H	11	0.11
(1,467)	1:58:X:VAL:HB	1:56:X:HIS:H	14	0.11
(1,432)	1:55:X:SER:H	1:53:X:ASP:HB3	3	0.11
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	17	0.11
(1,383)	1:50:X:ASP:HA	1:53:X:ASP:H	5	0.11
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	9	0.11
(1,243)	1:37:X:ARG:H	1:36:X:LEU:HB3	4	0.11
(1,243)	1:37:X:ARG:H	1:36:X:LEU:HB3	5	0.11
(1,236)	1:37:X:ARG:H	1:27:X:GLU:HB2	9	0.11
(1,214)	1:34:X:SER:H	1:73:X:ASN:H	1	0.11
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	1	0.11
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	2	0.11
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	6	0.11
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	10	0.11
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	14	0.11
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	17	0.11
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	18	0.11
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	19	0.11
(1,194)	1:31:X:GLY:H	1:30:X:ARG:HD2	12	0.11
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	9	0.11
(1,96)	1:19:X:LEU:H	1:16:X:VAL:HA	7	0.11
(1,25)	1:6:X:GLN:HA	1:7:X:LYS:H	3	0.11
(1,2)	1:4:X:LEU:CG	1:5:X:GLU:H	17	0.11
(5,63)	1:128:X:THR:C	1:116:X:VAL:H	9	0.1
(5,53)	1:101:X:LEU:C	1:113:X:TRP:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	7	0.1
(5,51)	1:99:X:VAL:C	1:115:X:GLY:H	8	0.1
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	9	0.1
(5,45)	1:90:X:HIS:C	1:94:X:PHE:H	14	0.1
(5,40)	1:75:X:GLU:C	1:38:X:ILE:H	13	0.1
(5,33)	1:56:X:HIS:C	1:60:X:ALA:H	13	0.1
(5,22)	1:39:X:TYR:C	1:25:X:GLY:H	11	0.1
(5,12)	1:23:X:LEU:C	1:41:X:ASP:H	11	0.1
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	4	0.1
(5,11)	1:15:X:PRO:C	1:19:X:LEU:H	12	0.1
(4,53)	1:50:X:ASP:O	1:54:X:VAL:N	5	0.1
(4,32)	1:33:X:THR:O	1:31:X:GLY:N	12	0.1
(3,921)	1:141:X:ILE:N	1:101:X:LEU:CD2	17	0.1
(3,813)	1:124:X:MET:N	1:120:X:VAL:CG2	7	0.1
(3,778)	1:118:X:LYS:N	1:117:X:ILE:CG2	11	0.1
(3,577)	1:89:X:GLU:N	1:90:X:HIS:CB	17	0.1
(3,534)	1:80:X:GLY:N	1:79:X:PRO:CB	10	0.1
(3,531)	1:79:X:PRO:CD	1:40:X:ILE:N	8	0.1
(3,366)	1:56:X:HIS:N	1:57:X:GLN:CB	15	0.1
(3,243)	1:41:X:ASP:N	1:22:X:GLU:CG	4	0.1
(3,241)	1:41:X:ASP:N	1:21:X:PHE:CB	3	0.1
(3,189)	1:34:X:SER:N	1:33:X:THR:CB	13	0.1
(3,189)	1:34:X:SER:N	1:33:X:THR:CB	14	0.1
(3,189)	1:34:X:SER:N	1:33:X:THR:CB	17	0.1
(3,178)	1:31:X:GLY:N	1:30:X:ARG:CB	5	0.1
(2,29)	1:29:X:ILE:CD1	1:35:X:THR:CG2	13	0.1
(1,998)	1:124:X:MET:HA	1:138:X:LEU:H	19	0.1
(1,951)	1:118:X:LYS:H	1:128:X:THR:H	20	0.1
(1,943)	1:116:X:VAL:HB	1:128:X:THR:H	11	0.1
(1,921)	1:112:X:LYS:HA	1:103:X:LEU:H	16	0.1
(1,874)	1:106:X:ALA:HA	1:103:X:LEU:H	15	0.1
(1,866)	1:105:X:MET:H	1:104:X:ARG:HA	9	0.1
(1,678)	1:81:X:LEU:H	1:80:X:GLY:HA3	17	0.1
(1,670)	1:78:X:SER:HB2	1:78:X:SER:H	19	0.1
(1,659)	1:77:X:SER:H	1:76:X:VAL:CB	1	0.1
(1,656)	1:77:X:SER:H	1:39:X:TYR:HA	8	0.1
(1,603)	1:71:X:ALA:HB1	1:72:X:TYR:H	2	0.1
(1,603)	1:71:X:ALA:HB2	1:72:X:TYR:H	2	0.1
(1,603)	1:71:X:ALA:HB3	1:72:X:TYR:H	2	0.1
(1,592)	1:69:X:THR:HA	1:70:X:VAL:H	8	0.1
(1,584)	1:67:X:PRO:HA	1:68:X:ILE:H	3	0.1
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,571)	1:66:X:ASP:H	1:63:X:ASP:HA	15	0.1
(1,562)	1:65:X:GLU:HB2	1:64:X:VAL:H	12	0.1
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	2	0.1
(1,547)	1:63:X:ASP:HA	1:64:X:VAL:H	18	0.1
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	12	0.1
(1,483)	1:58:X:VAL:HB	1:60:X:ALA:H	13	0.1
(1,467)	1:58:X:VAL:HB	1:56:X:HIS:H	20	0.1
(1,440)	1:56:X:HIS:H	1:53:X:ASP:HA	9	0.1
(1,391)	1:52:X:ALA:H	1:48:X:VAL:CB	9	0.1
(1,275)	1:39:X:TYR:H	1:27:X:GLU:H	14	0.1
(1,202)	1:33:X:THR:H	1:32:X:ARG:HA	13	0.1
(1,200)	1:33:X:THR:H	1:32:X:ARG:HG2	8	0.1
(1,180)	1:30:X:ARG:H	1:29:X:ILE:CG2	12	0.1

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

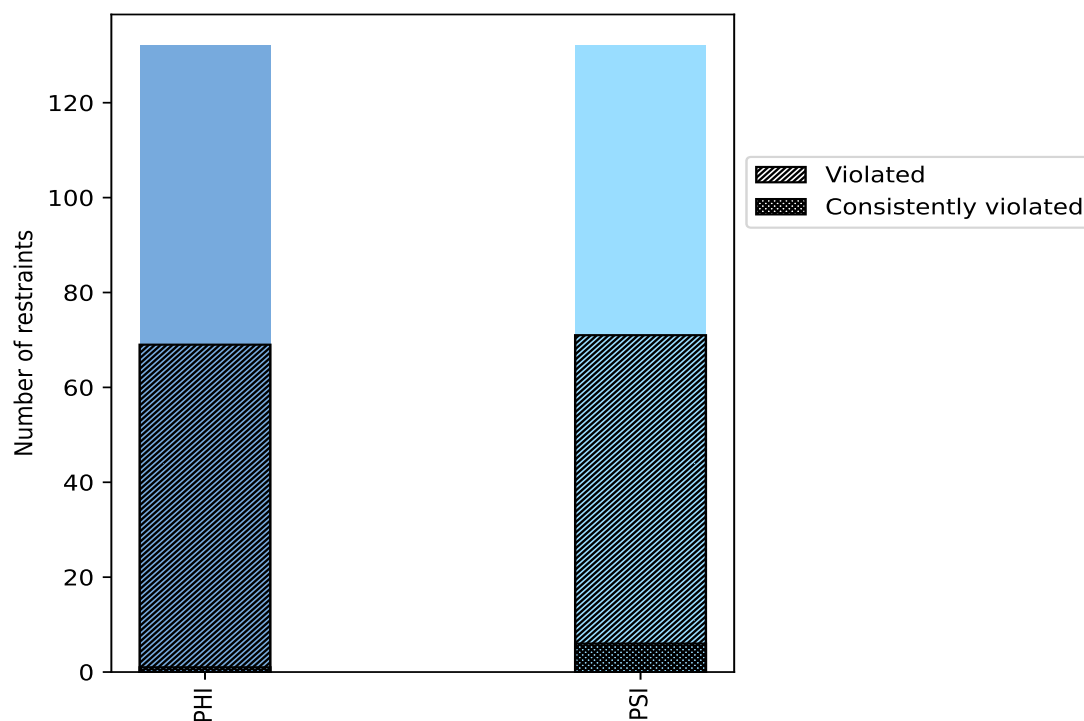
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	132	50.0	69	52.3	26.1	1	0.8	0.4
PSI	132	50.0	71	53.8	26.9	6	4.5	2.3
Total	264	100.0	140	53.0	53.0	7	2.7	2.7

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](#)



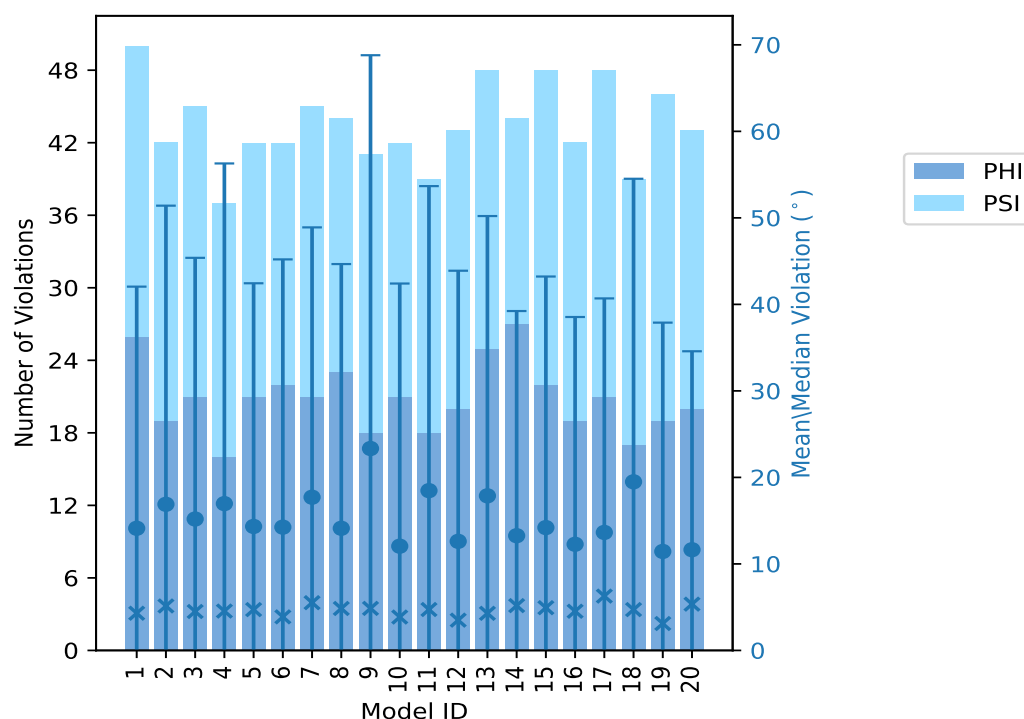
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	26	24	50	14.12	119.39	27.93	4.3
2	19	23	42	16.89	154.83	34.52	5.14
3	21	24	45	15.19	158.63	30.19	4.5
4	16	21	37	16.97	159.5	39.32	4.55
5	21	21	42	14.33	135.93	28.11	4.72
6	22	20	42	14.25	157.48	30.95	3.88
7	21	24	45	17.71	158.23	31.19	5.52
8	23	21	44	14.12	158.62	30.54	4.85
9	18	23	41	23.34	159.92	45.46	4.86
10	21	21	42	12.05	159.08	30.36	3.86
11	18	21	39	18.47	157.02	35.2	4.73
12	20	23	43	12.61	158.16	31.28	3.5
13	25	23	48	17.87	156.88	32.34	4.29
14	27	17	44	13.26	159.24	25.97	5.18
15	22	26	48	14.2	159.06	29.02	4.94
16	19	23	42	12.27	158.31	26.27	4.53
17	21	27	48	13.64	157.64	27.05	6.28
18	17	22	39	19.49	159.06	35.03	4.72
19	19	27	46	11.44	159.9	26.45	3.11
20	20	23	43	11.64	145.95	22.94	5.35

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
18	19	37	1	5.0
9	8	17	2	10.0
5	8	13	3	15.0
5	2	7	4	20.0
3	4	7	5	25.0
4	4	8	6	30.0
3	4	7	7	35.0
4	3	7	8	40.0
2	3	5	9	45.0
2	2	4	10	50.0
1	0	1	11	55.0

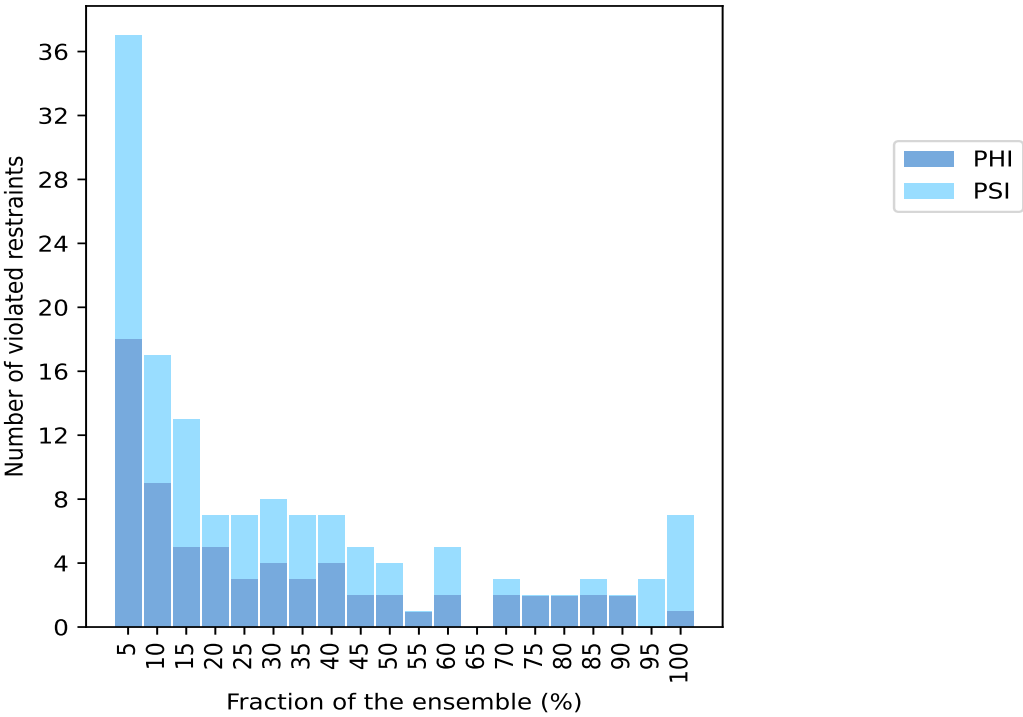
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
2	3	5	12	60.0
0	0	0	13	65.0
2	1	3	14	70.0
2	0	2	15	75.0
2	0	2	16	80.0
2	1	3	17	85.0
2	0	2	18	90.0
0	3	3	19	95.0
1	6	7	20	100.0

¹ Number of models with violations

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

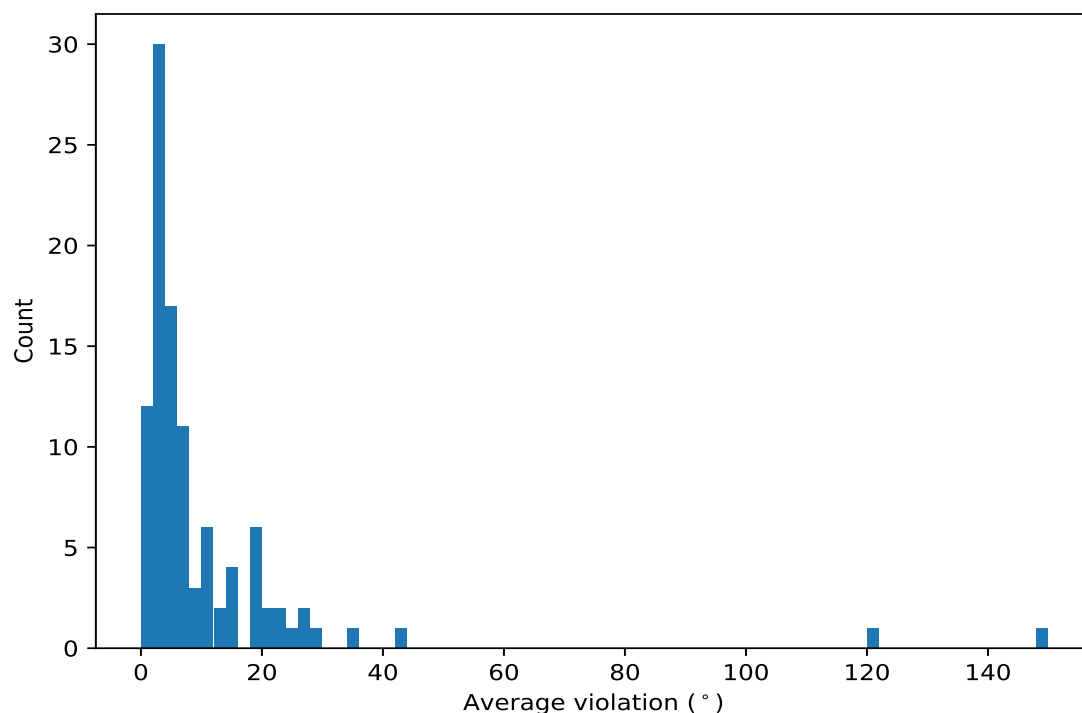


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 [i](#)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	20	149.36	24.96	158.27
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	20	22.39	13.53	25.3
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	20	20.65	7.79	19.66
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	20	18.54	13.61	18.61
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	20	18.1	26.99	9.48
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	20	10.36	4.96	10.24
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	20	3.8	2.11	3.36
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	19	120.31	22.56	131.83
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	19	4.59	1.83	4.26
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	19	4.56	1.4	4.44
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	18	5.71	2.27	5.68
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	18	4.93	2.67	5.66
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	17	13.0	32.76	3.9
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	17	5.1	3.72	4.27
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	17	3.8	1.92	3.19
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	16	5.69	6.47	3.44
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	16	5.26	2.59	5.65
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	15	10.39	1.05	10.33
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	15	6.48	4.42	4.35
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	14	29.39	46.15	9.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	14	6.69	10.49	4.05
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	14	2.41	0.83	2.2
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	12	27.34	28.88	18.02
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	12	19.36	14.96	20.64
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	12	5.64	2.26	5.6
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	12	5.14	3.47	4.56
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	12	1.89	0.73	1.71
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	11	3.47	1.45	2.66
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	10	15.04	8.07	16.47
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	10	3.16	1.74	2.88
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	10	2.85	1.26	2.46
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	10	2.65	0.53	2.74
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	9	24.56	43.08	2.48
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	9	18.72	12.13	18.62
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	9	15.03	17.25	3.36
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	9	6.73	4.45	4.95
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	9	2.43	2.49	1.43
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	8	23.53	32.69	10.98
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	8	15.58	11.77	14.51
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	8	6.71	6.0	3.51
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	8	6.09	2.88	4.49
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	8	5.62	3.35	4.8
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	8	5.13	2.54	4.53
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	8	2.66	0.91	2.6
(1,120)	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1:70:X:VAL:N	7	35.82	41.54	8.49
(1,122)	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	1:72:X:TYR:N	7	13.6	12.5	9.69
(1,149)	1:86:X:PHE:C	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	7	8.84	2.52	9.18
(1,113)	1:65:X:GLU:C	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	7	8.51	5.96	9.17
(1,135)	1:77:X:SER:C	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	7	6.18	6.73	4.27
(1,184)	1:104:X:ARG:N	1:104:X:ARG:CA	1:104:X:ARG:C	1:105:X:MET:N	7	3.66	2.06	3.15
(1,36)	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1:24:X:VAL:N	7	3.02	0.97	2.71
(1,119)	1:68:X:ILE:C	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	6	42.75	50.7	8.18
(1,215)	1:123:X:GLU:C	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	6	19.34	8.48	21.77
(1,136)	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	1:79:X:PRO:N	6	7.94	10.74	3.36
(1,144)	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	1:84:X:PRO:N	6	4.9	3.19	4.57
(1,213)	1:120:X:VAL:C	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	6	4.08	2.74	3.78
(1,51)	1:33:X:THR:C	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	6	4.01	2.96	2.57
(1,198)	1:113:X:TRP:N	1:113:X:TRP:CA	1:113:X:TRP:C	1:114:X:GLN:N	6	3.45	0.96	3.26
(1,126)	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	1:74:X:LEU:N	6	1.57	0.57	1.31
(1,124)	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	1:73:X:ASN:N	5	26.64	21.43	33.21
(1,125)	1:72:X:TYR:C	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	5	21.54	16.46	17.19
(1,109)	1:63:X:ASP:C	1:64:X:VAL:N	1:64:X:VAL:CA	1:64:X:VAL:C	5	3.75	0.85	3.83
(1,214)	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	1:122:X:GLY:N	5	3.34	0.93	3.19
(1,14)	1:11:X:MET:N	1:11:X:MET:CA	1:11:X:MET:C	1:12:X:ILE:N	5	2.7	1.09	2.87
(1,92)	1:55:X:SER:N	1:55:X:SER:CA	1:55:X:SER:C	1:56:X:HIS:N	5	2.58	1.07	3.01
(1,203)	1:115:X:GLY:C	1:116:X:VAL:N	1:116:X:VAL:CA	1:116:X:VAL:C	5	1.94	0.58	1.62
(1,47)	1:29:X:ILE:C	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	4	11.86	9.1	10.93
(1,71)	1:43:X:GLU:C	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	4	11.35	7.82	11.43
(1,161)	1:92:X:ALA:C	1:93:X:ARG:N	1:93:X:ARG:CA	1:93:X:ARG:C	4	4.13	3.24	2.48
(1,67)	1:41:X:ASP:C	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	4	2.2	1.22	1.76
(1,244)	1:138:X:LEU:N	1:138:X:LEU:CA	1:138:X:LEU:C	1:139:X:SER:N	4	2.07	1.35	1.44

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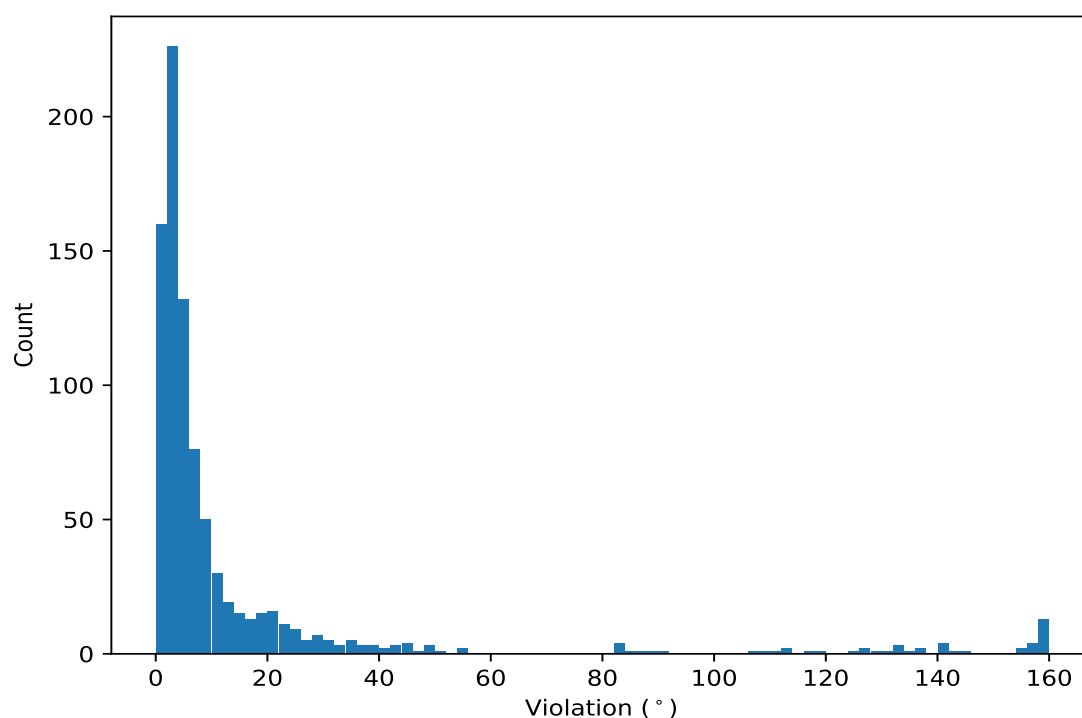
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,168)	1:96:X:GLY:N	1:96:X:GLY:CA	1:96:X:GLY:C	1:97:X:GLU:N	4	1.96	0.41	2.0
(1,181)	1:102:X:VAL:C	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	4	1.68	0.32	1.68
(1,217)	1:124:X:MET:C	1:125:X:ILE:N	1:125:X:ILE:CA	1:125:X:ILE:C	3	19.04	6.47	22.8
(1,72)	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	1:45:X:GLY:N	3	11.11	5.74	13.65
(1,52)	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	1:35:X:THR:N	3	10.41	2.17	9.59
(1,53)	1:34:X:SER:C	1:35:X:THR:N	1:35:X:THR:CA	1:35:X:THR:C	3	7.02	4.47	6.82
(1,146)	1:84:X:PRO:N	1:84:X:PRO:CA	1:84:X:PRO:C	1:85:X:LEU:N	3	6.23	3.19	5.49
(1,236)	1:134:X:GLU:N	1:134:X:GLU:CA	1:134:X:GLU:C	1:135:X:VAL:N	3	3.01	0.87	3.43
(1,196)	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	1:113:X:TRP:N	3	2.78	1.52	2.61
(1,78)	1:48:X:VAL:N	1:48:X:VAL:CA	1:48:X:VAL:C	1:49:X:ASP:N	3	2.69	0.75	2.75
(1,221)	1:126:X:THR:C	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	3	2.45	0.79	2.91
(1,56)	1:36:X:LEU:N	1:36:X:LEU:CA	1:36:X:LEU:C	1:37:X:ARG:N	3	1.94	0.74	1.8
(1,45)	1:28:X:PHE:C	1:29:X:ILE:N	1:29:X:ILE:CA	1:29:X:ILE:C	3	1.91	0.27	2.01
(1,86)	1:52:X:ALA:N	1:52:X:ALA:CA	1:52:X:ALA:C	1:53:X:ASP:N	3	1.79	0.79	1.3
(1,207)	1:117:X:ILE:C	1:118:X:LYS:N	1:118:X:LYS:CA	1:118:X:LYS:C	3	1.32	0.22	1.43
(1,171)	1:97:X:GLU:C	1:98:X:GLU:N	1:98:X:GLU:CA	1:98:X:GLU:C	2	14.12	2.3	14.12
(1,1)	1:4:X:LEU:C	1:5:X:GLU:N	1:5:X:GLU:CA	1:5:X:GLU:C	2	9.59	5.68	9.59
(1,262)	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	1:148:X:PRO:N	2	6.74	2.17	6.74
(1,192)	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	1:111:X:ARG:N	2	6.31	3.64	6.31
(1,219)	1:125:X:ILE:C	1:126:X:THR:N	1:126:X:THR:CA	1:126:X:THR:C	2	5.44	1.98	5.44
(1,131)	1:75:X:GLU:C	1:76:X:VAL:N	1:76:X:VAL:CA	1:76:X:VAL:C	2	4.19	0.89	4.19
(1,147)	1:84:X:PRO:C	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	2	3.96	0.63	3.96
(1,55)	1:35:X:THR:C	1:36:X:LEU:N	1:36:X:LEU:CA	1:36:X:LEU:C	2	2.94	1.83	2.94
(1,133)	1:76:X:VAL:C	1:77:X:SER:N	1:77:X:SER:CA	1:77:X:SER:C	2	2.88	0.06	2.88
(1,199)	1:113:X:TRP:C	1:114:X:GLN:N	1:114:X:GLN:CA	1:114:X:GLN:C	2	2.69	0.79	2.69
(1,231)	1:131:X:GLY:C	1:132:X:LYS:N	1:132:X:LYS:CA	1:132:X:LYS:C	2	2.63	0.11	2.63
(1,66)	1:41:X:ASP:N	1:41:X:ASP:CA	1:41:X:ASP:C	1:42:X:SER:N	2	2.56	1.4	2.56
(1,246)	1:139:X:SER:N	1:139:X:SER:CA	1:139:X:SER:C	1:140:X:ASN:N	2	2.24	0.8	2.24
(1,34)	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	1:22:X:GLU:N	2	2.21	0.94	2.21
(1,130)	1:75:X:GLU:N	1:75:X:GLU:CA	1:75:X:GLU:C	1:76:X:VAL:N	2	1.74	0.02	1.74
(1,224)	1:128:X:THR:N	1:128:X:THR:CA	1:128:X:THR:C	1:129:X:VAL:N	2	1.16	0.16	1.16
(1,42)	1:27:X:GLU:N	1:27:X:GLU:CA	1:27:X:GLU:C	1:28:X:PHE:N	2	1.14	0.12	1.14

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,188)	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	1:109:X:ASN:N	9	159.92
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	19	159.9
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	4	159.5
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	14	159.24
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	9	159.17
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	10	159.08
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	15	159.06
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	18	159.06
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	3	158.63
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	8	158.62
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	16	158.31
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	7	158.23
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	12	158.16
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	17	157.64
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	6	157.48
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	11	157.02
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	13	156.88
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	2	154.83
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	4	154.73
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	20	145.95
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	18	143.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	8	141.64
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	9	141.59
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	2	141.39
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	12	141.18
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	13	137.7
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	3	136.39
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	5	135.93
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	9	132.86
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	6	132.76
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	10	132.0
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	5	131.83
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	4	128.4
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	11	127.82
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	7	127.4
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	9	124.37
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	1	119.39
(1,119)	1:68:X:ILE:C	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	11	117.21
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	17	113.65
(1,120)	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1:70:X:VAL:N	2	112.57
(1,119)	1:68:X:ILE:C	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1	111.56
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	15	108.13
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	1	106.3
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	13	90.32
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	15	88.03
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	19	86.35
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	18	84.29
(1,120)	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1:70:X:VAL:N	1	83.11
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	16	82.66
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	7	82.08
(1,118)	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1:69:X:THR:N	14	82.04
(1,124)	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	1:73:X:ASN:N	7	54.78
(1,116)	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1:68:X:ILE:N	20	54.23
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	13	51.16
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	19	49.19
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	2	48.09
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	18	48.01
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	6	46.8
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	13	44.75
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	5	44.54
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	13	44.38
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	18	44.21
(1,125)	1:72:X:TYR:C	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	7	42.75
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	3	42.74
(1,122)	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	1:72:X:TYR:N	11	42.58
(1,124)	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	1:73:X:ASN:N	13	41.64
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	18	40.4
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	1	39.38
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	13	39.13
(1,125)	1:72:X:TYR:C	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	13	38.86
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	18	37.29
(1,120)	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1:70:X:VAL:N	11	37.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	11	36.13
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	15	35.54
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	12	35.47
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	17	35.36
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	3	34.51
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	12	34.46
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	3	33.46
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	6	33.37
(1,124)	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	1:73:X:ASN:N	15	33.21
(1,136)	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	1:79:X:PRO:N	17	31.81
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	14	31.34
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	7	30.51
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	8	30.25
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	17	30.23
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	6	29.84
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	5	29.44
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	20	29.32
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	7	28.56
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	15	28.45
(1,215)	1:123:X:GLU:C	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	11	28.19
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	14	28.0
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	13	27.79
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	6	27.62
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	14	26.54
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	3	26.16
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	3	26.02
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	2	25.55
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	8	25.04
(1,115)	1:66:X:ASP:C	1:67:X:PRO:N	1:67:X:PRO:CA	1:67:X:PRO:C	1	24.66
(1,217)	1:124:X:MET:C	1:125:X:ILE:N	1:125:X:ILE:CA	1:125:X:ILE:C	4	24.39
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	7	24.33
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	5	24.33
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	9	24.29
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	5	24.27
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	16	24.21
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	13	23.55
(1,47)	1:29:X:ILE:C	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	14	23.25
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	19	23.0
(1,217)	1:124:X:MET:C	1:125:X:ILE:N	1:125:X:ILE:CA	1:125:X:ILE:C	1	22.8
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	18	22.74
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	19	22.6
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	7	22.58
(1,135)	1:77:X:SER:C	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	17	22.43
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	8	22.34
(1,215)	1:123:X:GLU:C	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	10	22.22
(1,215)	1:123:X:GLU:C	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	14	22.09
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	2	21.96
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	2	21.7
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	16	21.65
(1,215)	1:123:X:GLU:C	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	9	21.45
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	20	21.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	8	21.14
(1,215)	1:123:X:GLU:C	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	20	20.91
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	18	20.68
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	6	20.67
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	12	20.64
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	19	20.57
(1,71)	1:43:X:GLU:C	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	20	20.53
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	17	20.45
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	7	20.12
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	10	20.05
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	4	20.05
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	11	19.91
(1,113)	1:65:X:GLU:C	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	20	19.68
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	12	19.56
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	15	19.42
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	16	19.05
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	3	18.94
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	11	18.73
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	8	18.73
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	4	18.71
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	18	18.65
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	14	18.62
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	9	18.33
(1,47)	1:29:X:ILE:C	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1	18.32
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	8	18.23
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	17	18.17
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	5	17.95
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	3	17.88
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	16	17.85
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	7	17.69
(1,71)	1:43:X:GLU:C	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	16	17.47
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	19	17.32
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	9	17.32
(1,125)	1:72:X:TYR:C	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	15	17.19
(1,72)	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	1:45:X:GLY:N	16	16.52
(1,122)	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	1:72:X:TYR:N	2	16.44
(1,171)	1:97:X:GLU:C	1:98:X:GLU:N	1:98:X:GLU:CA	1:98:X:GLU:C	10	16.43
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	20	16.13
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	20	16.1
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	3	15.94
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	19	15.69
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	8	15.41
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	13	15.32
(1,1)	1:4:X:LEU:C	1:5:X:GLU:N	1:5:X:GLU:CA	1:5:X:GLU:C	15	15.27
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	9	15.1
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	20	14.84
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	14	14.75
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	7	14.73
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	16	14.71
(1,180)	1:102:X:VAL:N	1:102:X:VAL:CA	1:102:X:VAL:C	1:103:X:LEU:N	9	14.62
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	17	14.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	14	14.52
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	5	14.42
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	9	14.4
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	14	13.93
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	5	13.87
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	3	13.73
(1,72)	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	1:45:X:GLY:N	20	13.65
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	6	13.5
(1,149)	1:86:X:PHE:C	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	5	13.49
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	7	13.38
(1,52)	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	1:35:X:THR:N	5	13.38
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	16	13.34
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	18	13.13
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	17	13.01
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	17	12.69
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	15	12.65
(1,53)	1:34:X:SER:C	1:35:X:THR:N	1:35:X:THR:CA	1:35:X:THR:C	5	12.59
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	3	12.5
(1,113)	1:65:X:GLU:C	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	13	12.49
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	19	12.47
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	2	12.39
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	18	12.39
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	15	11.99
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	17	11.96
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	19	11.89
(1,171)	1:97:X:GLU:C	1:98:X:GLU:N	1:98:X:GLU:CA	1:98:X:GLU:C	17	11.82
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	5	11.82
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	2	11.68
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	2	11.66
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	19	11.58
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	11	11.54
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	18	11.53
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	8	11.51
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	7	11.44
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	17	11.43
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	8	11.38
(1,122)	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	1:72:X:TYR:N	18	11.36
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	10	11.33
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	6	11.11
(1,144)	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	1:84:X:PRO:N	15	11.03
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	9	11.01
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	7	10.99
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	15	10.79
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	3	10.77
(1,149)	1:86:X:PHE:C	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	7	10.62
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	15	10.54
(1,146)	1:84:X:PRO:N	1:84:X:PRO:CA	1:84:X:PRO:C	1:85:X:LEU:N	11	10.45
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	17	10.38
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	16	10.33
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	4	10.27
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	20	10.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	13	10.08
(1,192)	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	1:111:X:ARG:N	3	9.95
(1,217)	1:124:X:MET:C	1:125:X:ILE:N	1:125:X:ILE:CA	1:125:X:ILE:C	2	9.94
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	8	9.89
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	11	9.86
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	12	9.82
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	18	9.79
(1,161)	1:92:X:ALA:C	1:93:X:ARG:N	1:93:X:ARG:CA	1:93:X:ARG:C	17	9.71
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	10	9.71
(1,122)	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	1:72:X:TYR:N	3	9.69
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	7	9.69
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	8	9.62
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1	9.6
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	15	9.6
(1,52)	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	1:35:X:THR:N	13	9.59
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	1	9.55
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	14	9.51
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	12	9.47
(1,113)	1:65:X:GLU:C	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	11	9.47
(1,149)	1:86:X:PHE:C	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	2	9.46
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	9	9.38
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	8	9.35
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	7	9.29
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	2	9.24
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	1	9.23
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1	9.19
(1,149)	1:86:X:PHE:C	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	12	9.18
(1,113)	1:65:X:GLU:C	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	6	9.17
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	10	9.14
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	20	9.06
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	7	9.06
(1,213)	1:120:X:VAL:C	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	8	9.03
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	14	8.93
(1,262)	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	1:148:X:PRO:N	8	8.91
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	12	8.84
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	6	8.84
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	16	8.7
(1,120)	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1:70:X:VAL:N	10	8.49
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	16	8.47
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	7	8.44
(1,119)	1:68:X:ILE:C	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	8	8.44
(1,112)	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	1:66:X:ASP:N	10	8.41
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	5	8.38
(1,51)	1:33:X:THR:C	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	14	8.36
(1,52)	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	1:35:X:THR:N	17	8.25
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	6	8.24
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	17	8.18
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	2	8.16
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	14	8.15
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	15	8.11
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	14	8.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	1:64:X:VAL:C	1:65:X:GLU:N	1:65:X:GLU:CA	1:65:X:GLU:C	4	7.99
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	10	7.93
(1,119)	1:68:X:ILE:C	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	2	7.92
(1,184)	1:104:X:ARG:N	1:104:X:ARG:CA	1:104:X:ARG:C	1:105:X:MET:N	7	7.88
(1,51)	1:33:X:THR:C	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	1	7.88
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	7	7.87
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	8	7.84
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	17	7.83
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	20	7.8
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	5	7.72
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	1	7.71
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	1	7.7
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	12	7.69
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	4	7.67
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	2	7.66
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	11	7.66
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	3	7.64
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	9	7.63
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	14	7.62
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	13	7.55
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	14	7.52
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	3	7.47
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	3	7.45
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	17	7.43
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	13	7.43
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	9	7.42
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	15	7.41
(1,219)	1:125:X:ILE:C	1:126:X:THR:N	1:126:X:THR:CA	1:126:X:THR:C	20	7.41
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	17	7.34
(1,127)	1:73:X:ASN:C	1:74:X:LEU:N	1:74:X:LEU:CA	1:74:X:LEU:C	1	7.34
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	20	7.27
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	4	7.24
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	15	7.21
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	8	7.17
(1,149)	1:86:X:PHE:C	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	17	7.14
(1,119)	1:68:X:ILE:C	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	3	7.11
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	13	7.07
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	4	7.05
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	5	6.93
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	8	6.92
(1,122)	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	1:72:X:TYR:N	1	6.92
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	6	6.87
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	18	6.87
(1,53)	1:34:X:SER:C	1:35:X:THR:N	1:35:X:THR:CA	1:35:X:THR:C	17	6.82
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	10	6.77
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	2	6.76
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	15	6.67
(1,210)	1:119:X:ALA:N	1:119:X:ALA:CA	1:119:X:ALA:C	1:120:X:VAL:N	9	6.65
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	16	6.63
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	18	6.63
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	17	6.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,137)	1:78:X:SER:C	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	11	6.57
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	3	6.56
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	20	6.56
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	5	6.51
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	6	6.49
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	16	6.49
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	13	6.45
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	4	6.41
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	6	6.39
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	11	6.34
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	18	6.33
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	16	6.32
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	2	6.31
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	15	6.29
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	15	6.27
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	3	6.25
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	1	6.25
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	14	6.23
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	20	6.14
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	11	6.14
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	5	6.09
(1,149)	1:86:X:PHE:C	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	16	6.08
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	18	6.08
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	19	6.07
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	16	6.01
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	16	5.97
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	10	5.97
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	17	5.96
(1,144)	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	1:84:X:PRO:N	20	5.93
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	10	5.92
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	20	5.91
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	17	5.9
(1,149)	1:86:X:PHE:C	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	14	5.88
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	2	5.87
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	1	5.84
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	20	5.84
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	1	5.84
(1,113)	1:65:X:GLU:C	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	2	5.83
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	10	5.81
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	12	5.77
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	13	5.7
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	12	5.62
(1,213)	1:120:X:VAL:C	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	13	5.57
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	7	5.52
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	19	5.52
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	17	5.51
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	9	5.49
(1,146)	1:84:X:PRO:N	1:84:X:PRO:CA	1:84:X:PRO:C	1:85:X:LEU:N	4	5.49
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	15	5.45
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	8	5.44
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	4	5.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,71)	1:43:X:GLU:C	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	5	5.39
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	7	5.37
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	20	5.35
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	10	5.35
(1,144)	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	1:84:X:PRO:N	9	5.31
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	14	5.31
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	8	5.3
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	11	5.3
(1,136)	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	1:79:X:PRO:N	11	5.3
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	6	5.26
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1	5.24
(1,125)	1:72:X:TYR:C	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	14	5.19
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	12	5.18
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	14	5.16
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	10	5.14
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	15	5.13
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	6	5.13
(1,198)	1:113:X:TRP:N	1:113:X:TRP:CA	1:113:X:TRP:C	1:114:X:GLN:N	10	5.1
(1,121)	1:70:X:VAL:C	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	16	5.08
(1,135)	1:77:X:SER:C	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	7	5.07
(1,131)	1:75:X:GLU:C	1:76:X:VAL:N	1:76:X:VAL:CA	1:76:X:VAL:C	16	5.07
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	6	5.05
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	13	5.03
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	12	5.01
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	15	4.99
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	20	4.95
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	19	4.95
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	9	4.95
(1,109)	1:63:X:ASP:C	1:64:X:VAL:N	1:64:X:VAL:CA	1:64:X:VAL:C	1	4.95
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	15	4.9
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	9	4.86
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	5	4.83
(1,184)	1:104:X:ARG:N	1:104:X:ARG:CA	1:104:X:ARG:C	1:105:X:MET:N	9	4.8
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	4	4.79
(1,55)	1:35:X:THR:C	1:36:X:LEU:N	1:36:X:LEU:CA	1:36:X:LEU:C	14	4.77
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	4	4.74
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	5	4.73
(1,196)	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	1:113:X:TRP:N	11	4.73
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	13	4.73
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	6	4.73
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	18	4.72
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	18	4.72
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	14	4.71
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	5	4.7
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	4	4.68
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	9	4.65
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	18	4.63
(1,214)	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	1:122:X:GLY:N	7	4.61
(1,147)	1:84:X:PRO:C	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	3	4.6
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	5	4.59
(1,262)	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	1:148:X:PRO:N	4	4.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	7	4.56
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	4	4.55
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	15	4.54
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	1	4.54
(1,135)	1:77:X:SER:C	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	14	4.51
(1,213)	1:120:X:VAL:C	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	3	4.5
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	5	4.5
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	10	4.48
(1,14)	1:11:X:MET:N	1:11:X:MET:CA	1:11:X:MET:C	1:12:X:ILE:N	5	4.47
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	2	4.44
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	1	4.43
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	1	4.42
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	4	4.42
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	8	4.4
(1,36)	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1:24:X:VAL:N	8	4.4
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	17	4.4
(1,244)	1:138:X:LEU:N	1:138:X:LEU:CA	1:138:X:LEU:C	1:139:X:SER:N	19	4.39
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	20	4.35
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	3	4.32
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	17	4.31
(1,160)	1:92:X:ALA:N	1:92:X:ALA:CA	1:92:X:ALA:C	1:93:X:ARG:N	19	4.31
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	13	4.31
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	14	4.27
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	13	4.27
(1,135)	1:77:X:SER:C	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	3	4.27
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	8	4.26
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	2	4.26
(1,36)	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1:24:X:VAL:N	14	4.25
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	11	4.24
(1,119)	1:68:X:ILE:C	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	12	4.24
(1,109)	1:63:X:ASP:C	1:64:X:VAL:N	1:64:X:VAL:CA	1:64:X:VAL:C	10	4.24
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	19	4.23
(1,67)	1:41:X:ASP:C	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	3	4.23
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	8	4.21
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	9	4.21
(1,122)	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	1:72:X:TYR:N	19	4.21
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	2	4.21
(1,197)	1:112:X:LYS:C	1:113:X:TRP:N	1:113:X:TRP:CA	1:113:X:TRP:C	1	4.19
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	6	4.18
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	17	4.16
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	12	4.15
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	12	4.14
(1,184)	1:104:X:ARG:N	1:104:X:ARG:CA	1:104:X:ARG:C	1:105:X:MET:N	3	4.11
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	15	4.11
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	12	4.11
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	6	4.1
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	14	4.1
(1,120)	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1:70:X:VAL:N	8	4.09
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	18	4.07
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	7	4.07
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	9	4.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,142)	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	1:83:X:ARG:N	17	4.06
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	3	4.03
(1,198)	1:113:X:TRP:N	1:113:X:TRP:CA	1:113:X:TRP:C	1:114:X:GLN:N	11	4.02
(1,92)	1:55:X:SER:N	1:55:X:SER:CA	1:55:X:SER:C	1:56:X:HIS:N	7	4.01
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	3	3.98
(1,122)	1:71:X:ALA:N	1:71:X:ALA:CA	1:71:X:ALA:C	1:72:X:TYR:N	16	3.98
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	11	3.97
(1,214)	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	1:122:X:GLY:N	16	3.96
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	5	3.96
(1,66)	1:41:X:ASP:N	1:41:X:ASP:CA	1:41:X:ASP:C	1:42:X:SER:N	7	3.96
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	19	3.95
(1,251)	1:141:X:ILE:C	1:142:X:GLN:N	1:142:X:GLN:CA	1:142:X:GLN:C	5	3.94
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	14	3.92
(1,1)	1:4:X:LEU:C	1:5:X:GLU:N	1:5:X:GLU:CA	1:5:X:GLU:C	19	3.92
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	10	3.9
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	19	3.87
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	3	3.86
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	1	3.83
(1,144)	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	1:84:X:PRO:N	16	3.83
(1,109)	1:63:X:ASP:C	1:64:X:VAL:N	1:64:X:VAL:CA	1:64:X:VAL:C	17	3.83
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	10	3.82
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	2	3.81
(1,236)	1:134:X:GLU:N	1:134:X:GLU:CA	1:134:X:GLU:C	1:135:X:VAL:N	1	3.8
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	8	3.78
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	5	3.74
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	18	3.73
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	20	3.71
(1,125)	1:72:X:TYR:C	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	5	3.71
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	11	3.7
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	12	3.69
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	1	3.69
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	6	3.66
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	14	3.66
(1,164)	1:94:X:PHE:N	1:94:X:PHE:CA	1:94:X:PHE:C	1:95:X:VAL:N	12	3.65
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	7	3.61
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	13	3.59
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	2	3.58
(1,78)	1:48:X:VAL:N	1:48:X:VAL:CA	1:48:X:VAL:C	1:49:X:ASP:N	17	3.58
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	5	3.57
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	1	3.56
(1,47)	1:29:X:ILE:C	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	18	3.54
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	10	3.53
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	13	3.53
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	10	3.52
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	16	3.51
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	1	3.5
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	12	3.5
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	13	3.49
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	19	3.49
(1,199)	1:113:X:TRP:C	1:114:X:GLN:N	1:114:X:GLN:CA	1:114:X:GLN:C	1	3.48
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	9	3.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	4	3.47
(1,139)	1:80:X:GLY:C	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	6	3.47
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	1	3.47
(1,219)	1:125:X:ILE:C	1:126:X:THR:N	1:126:X:THR:CA	1:126:X:THR:C	10	3.46
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	8	3.45
(1,136)	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	1:79:X:PRO:N	18	3.45
(1,236)	1:134:X:GLU:N	1:134:X:GLU:CA	1:134:X:GLU:C	1:135:X:VAL:N	7	3.43
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	20	3.43
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	1	3.41
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	18	3.4
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	13	3.38
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	17	3.38
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	16	3.36
(1,198)	1:113:X:TRP:N	1:113:X:TRP:CA	1:113:X:TRP:C	1:114:X:GLN:N	6	3.35
(1,36)	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1:24:X:VAL:N	5	3.35
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	1	3.33
(1,147)	1:84:X:PRO:C	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	12	3.33
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	10	3.32
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	6	3.32
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	17	3.3
(1,131)	1:75:X:GLU:C	1:76:X:VAL:N	1:76:X:VAL:CA	1:76:X:VAL:C	13	3.3
(1,109)	1:63:X:ASP:C	1:64:X:VAL:N	1:64:X:VAL:CA	1:64:X:VAL:C	20	3.3
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	3	3.3
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	4	3.28
(1,136)	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	1:79:X:PRO:N	16	3.28
(1,120)	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1:70:X:VAL:N	12	3.25
(1,82)	1:50:X:ASP:N	1:50:X:ASP:CA	1:50:X:ASP:C	1:51:X:CYS:N	6	3.24
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	2	3.22
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	13	3.21
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	3	3.2
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	19	3.19
(1,214)	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	1:122:X:GLY:N	18	3.19
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	8	3.18
(1,92)	1:55:X:SER:N	1:55:X:SER:CA	1:55:X:SER:C	1:56:X:HIS:N	3	3.18
(1,72)	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	1:45:X:GLY:N	11	3.17
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	11	3.17
(1,198)	1:113:X:TRP:N	1:113:X:TRP:CA	1:113:X:TRP:C	1:114:X:GLN:N	7	3.16
(1,184)	1:104:X:ARG:N	1:104:X:ARG:CA	1:104:X:ARG:C	1:105:X:MET:N	16	3.15
(1,34)	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	1:22:X:GLU:N	11	3.15
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	3	3.14
(1,198)	1:113:X:TRP:N	1:113:X:TRP:CA	1:113:X:TRP:C	1:114:X:GLN:N	13	3.13
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	5	3.12
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	11	3.11
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	9	3.11
(1,221)	1:126:X:THR:C	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	13	3.1
(1,214)	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	1:122:X:GLY:N	6	3.1
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	7	3.09
(1,54)	1:35:X:THR:N	1:35:X:THR:CA	1:35:X:THR:C	1:36:X:LEU:N	14	3.09
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	16	3.08
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	14	3.08
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	13	3.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	1:91:X:TYR:C	1:92:X:ALA:N	1:92:X:ALA:CA	1:92:X:ALA:C	20	3.07
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	9	3.07
(1,213)	1:120:X:VAL:C	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	18	3.06
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	8	3.05
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	18	3.04
(1,246)	1:139:X:SER:N	1:139:X:SER:CA	1:139:X:SER:C	1:140:X:ASN:N	19	3.03
(1,203)	1:115:X:GLY:C	1:116:X:VAL:N	1:116:X:VAL:CA	1:116:X:VAL:C	2	3.03
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	2	3.03
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	12	3.03
(1,51)	1:33:X:THR:C	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	7	3.03
(1,92)	1:55:X:SER:N	1:55:X:SER:CA	1:55:X:SER:C	1:56:X:HIS:N	8	3.01
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	7	3.01
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	7	3.01
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	4	3.0
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	8	2.98
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	6	2.98
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	5	2.98
(1,138)	1:79:X:PRO:N	1:79:X:PRO:CA	1:79:X:PRO:C	1:80:X:GLY:N	20	2.97
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	15	2.97
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	7	2.96
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	16	2.96
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	10	2.95
(1,135)	1:77:X:SER:C	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	6	2.95
(1,133)	1:76:X:VAL:C	1:77:X:SER:N	1:77:X:SER:CA	1:77:X:SER:C	14	2.94
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	2	2.92
(1,221)	1:126:X:THR:C	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	6	2.91
(1,86)	1:52:X:ALA:N	1:52:X:ALA:CA	1:52:X:ALA:C	1:53:X:ASP:N	1	2.9
(1,56)	1:36:X:LEU:N	1:36:X:LEU:CA	1:36:X:LEU:C	1:37:X:ARG:N	1	2.9
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	3	2.89
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	11	2.89
(1,14)	1:11:X:MET:N	1:11:X:MET:CA	1:11:X:MET:C	1:12:X:ILE:N	15	2.89
(1,14)	1:11:X:MET:N	1:11:X:MET:CA	1:11:X:MET:C	1:12:X:ILE:N	20	2.87
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	14	2.85
(1,161)	1:92:X:ALA:C	1:93:X:ARG:N	1:93:X:ARG:CA	1:93:X:ARG:C	15	2.82
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	19	2.81
(1,133)	1:76:X:VAL:C	1:77:X:SER:N	1:77:X:SER:CA	1:77:X:SER:C	13	2.81
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	15	2.8
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	11	2.78
(1,114)	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	1:67:X:PRO:N	10	2.78
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	16	2.77
(1,126)	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	1:74:X:LEU:N	3	2.77
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	8	2.76
(1,146)	1:84:X:PRO:N	1:84:X:PRO:CA	1:84:X:PRO:C	1:85:X:LEU:N	18	2.75
(1,78)	1:48:X:VAL:N	1:48:X:VAL:CA	1:48:X:VAL:C	1:49:X:ASP:N	3	2.75
(1,231)	1:131:X:GLY:C	1:132:X:LYS:N	1:132:X:LYS:CA	1:132:X:LYS:C	10	2.74
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	20	2.72
(1,36)	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1:24:X:VAL:N	17	2.71
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	14	2.68
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	15	2.67
(1,192)	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	1:111:X:ARG:N	12	2.67
(1,81)	1:49:X:ASP:C	1:50:X:ASP:N	1:50:X:ASP:CA	1:50:X:ASP:C	9	2.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	3	2.66
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	20	2.66
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	11	2.64
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	13	2.64
(1,196)	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	1:113:X:TRP:N	6	2.61
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	1	2.61
(1,184)	1:104:X:ARG:N	1:104:X:ARG:CA	1:104:X:ARG:C	1:105:X:MET:N	19	2.6
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	3	2.6
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	6	2.58
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	2	2.57
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	7	2.55
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	19	2.55
(1,36)	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1:24:X:VAL:N	2	2.54
(1,231)	1:131:X:GLY:C	1:132:X:LYS:N	1:132:X:LYS:CA	1:132:X:LYS:C	16	2.52
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	19	2.49
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	16	2.48
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	12	2.47
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	19	2.46
(1,109)	1:63:X:ASP:C	1:64:X:VAL:N	1:64:X:VAL:CA	1:64:X:VAL:C	14	2.45
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	11	2.44
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	2	2.44
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	4	2.43
(1,168)	1:96:X:GLY:N	1:96:X:GLY:CA	1:96:X:GLY:C	1:97:X:GLU:N	11	2.43
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	4	2.43
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	10	2.42
(1,135)	1:77:X:SER:C	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	4	2.42
(1,36)	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1:24:X:VAL:N	20	2.42
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	15	2.41
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	13	2.39
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	17	2.38
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	13	2.36
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	17	2.36
(1,136)	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	1:79:X:PRO:N	12	2.33
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1	2.33
(1,47)	1:29:X:ILE:C	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	16	2.33
(1,208)	1:118:X:LYS:N	1:118:X:LYS:CA	1:118:X:LYS:C	1:119:X:ALA:N	15	2.32
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	15	2.32
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	6	2.3
(1,186)	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	1:108:X:GLN:N	5	2.29
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	19	2.29
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	5	2.29
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	5	2.28
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	18	2.27
(1,168)	1:96:X:GLY:N	1:96:X:GLY:CA	1:96:X:GLY:C	1:97:X:GLU:N	4	2.27
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	13	2.26
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	11	2.25
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	9	2.24
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	5	2.24
(1,152)	1:88:X:ALA:N	1:88:X:ALA:CA	1:88:X:ALA:C	1:89:X:GLU:N	6	2.21
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	14	2.2
(1,45)	1:28:X:PHE:C	1:29:X:ILE:N	1:29:X:ILE:CA	1:29:X:ILE:C	16	2.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	4	2.18
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	13	2.18
(1,124)	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	1:73:X:ASN:N	2	2.18
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	10	2.17
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	19	2.15
(1,161)	1:92:X:ALA:C	1:93:X:ARG:N	1:93:X:ARG:CA	1:93:X:ARG:C	9	2.15
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	10	2.15
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	8	2.14
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	10	2.14
(1,120)	1:69:X:THR:N	1:69:X:THR:CA	1:69:X:THR:C	1:70:X:VAL:N	20	2.14
(1,14)	1:11:X:MET:N	1:11:X:MET:CA	1:11:X:MET:C	1:12:X:ILE:N	10	2.13
(1,181)	1:102:X:VAL:C	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	9	2.12
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	2	2.11
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	4	2.11
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	4	2.11
(1,51)	1:33:X:THR:C	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	16	2.11
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	6	2.09
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	20	2.08
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	7	2.08
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	14	2.06
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	3	2.03
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	1	2.02
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	7	2.01
(1,48)	1:30:X:ARG:N	1:30:X:ARG:CA	1:30:X:ARG:C	1:31:X:GLY:N	9	2.01
(1,45)	1:28:X:PHE:C	1:29:X:ILE:N	1:29:X:ILE:CA	1:29:X:ILE:C	19	2.01
(1,71)	1:43:X:GLU:C	1:44:X:ASP:N	1:44:X:ASP:CA	1:44:X:ASP:C	6	2.0
(1,203)	1:115:X:GLY:C	1:116:X:VAL:N	1:116:X:VAL:CA	1:116:X:VAL:C	14	1.99
(1,140)	1:81:X:LEU:N	1:81:X:LEU:CA	1:81:X:LEU:C	1:82:X:ASP:N	10	1.99
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	15	1.98
(1,67)	1:41:X:ASP:C	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	4	1.96
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	11	1.96
(1,154)	1:89:X:GLU:N	1:89:X:GLU:CA	1:89:X:GLU:C	1:90:X:HIS:N	18	1.95
(1,198)	1:113:X:TRP:N	1:113:X:TRP:CA	1:113:X:TRP:C	1:114:X:GLN:N	5	1.94
(1,148)	1:85:X:LEU:N	1:85:X:LEU:CA	1:85:X:LEU:C	1:86:X:PHE:N	9	1.94
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	9	1.93
(1,178)	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	1:102:X:VAL:N	16	1.92
(1,194)	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	1:112:X:LYS:N	16	1.91
(1,199)	1:113:X:TRP:C	1:114:X:GLN:N	1:114:X:GLN:CA	1:114:X:GLN:C	3	1.9
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	1	1.88
(1,29)	1:18:X:ALA:C	1:19:X:LEU:N	1:19:X:LEU:CA	1:19:X:LEU:C	8	1.86
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	5	1.85
(1,214)	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	1:122:X:GLY:N	17	1.85
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	14	1.85
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	13	1.83
(1,161)	1:92:X:ALA:C	1:93:X:ARG:N	1:93:X:ARG:CA	1:93:X:ARG:C	19	1.83
(1,144)	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	1:84:X:PRO:N	1	1.82
(1,181)	1:102:X:VAL:C	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	13	1.8
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	15	1.8
(1,56)	1:36:X:LEU:N	1:36:X:LEU:CA	1:36:X:LEU:C	1:37:X:ARG:N	19	1.8
(1,236)	1:134:X:GLU:N	1:134:X:GLU:CA	1:134:X:GLU:C	1:135:X:VAL:N	20	1.79
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	4	1.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:75:X:GLU:N	1:75:X:GLU:CA	1:75:X:GLU:C	1:76:X:VAL:N	14	1.76
(1,184)	1:104:X:ARG:N	1:104:X:ARG:CA	1:104:X:ARG:C	1:105:X:MET:N	15	1.75
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	9	1.75
(1,168)	1:96:X:GLY:N	1:96:X:GLY:CA	1:96:X:GLY:C	1:97:X:GLU:N	12	1.74
(1,78)	1:48:X:VAL:N	1:48:X:VAL:CA	1:48:X:VAL:C	1:49:X:ASP:N	8	1.74
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	2	1.73
(1,41)	1:26:X:ILE:C	1:27:X:GLU:N	1:27:X:GLU:CA	1:27:X:GLU:C	11	1.73
(1,187)	1:107:X:VAL:C	1:108:X:GLN:N	1:108:X:GLN:CA	1:108:X:GLN:C	4	1.72
(1,130)	1:75:X:GLU:N	1:75:X:GLU:CA	1:75:X:GLU:C	1:76:X:VAL:N	19	1.72
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	19	1.72
(1,75)	1:46:X:ILE:C	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	18	1.71
(1,126)	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	1:74:X:LEU:N	12	1.7
(1,113)	1:65:X:GLU:C	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	12	1.68
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	16	1.67
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	6	1.67
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	8	1.67
(1,226)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:GLU:N	17	1.65
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	1	1.65
(1,53)	1:34:X:SER:C	1:35:X:THR:N	1:35:X:THR:CA	1:35:X:THR:C	13	1.64
(1,135)	1:77:X:SER:C	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	15	1.63
(1,31)	1:19:X:LEU:C	1:20:X:GLY:N	1:20:X:GLY:CA	1:20:X:GLY:C	8	1.63
(1,203)	1:115:X:GLY:C	1:116:X:VAL:N	1:116:X:VAL:CA	1:116:X:VAL:C	12	1.62
(1,203)	1:115:X:GLY:C	1:116:X:VAL:N	1:116:X:VAL:CA	1:116:X:VAL:C	19	1.62
(1,2)	1:5:X:GLU:N	1:5:X:GLU:CA	1:5:X:GLU:C	1:6:X:GLN:N	4	1.62
(1,37)	1:24:X:VAL:C	1:25:X:GLY:N	1:25:X:GLY:CA	1:25:X:GLY:C	10	1.61
(1,238)	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	1:136:X:PHE:N	12	1.6
(1,143)	1:82:X:ASP:C	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	6	1.6
(1,51)	1:33:X:THR:C	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	8	1.6
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	17	1.59
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1	1.58
(1,67)	1:41:X:ASP:C	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	11	1.57
(1,181)	1:102:X:VAL:C	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	11	1.56
(1,76)	1:47:X:ASN:N	1:47:X:ASN:CA	1:47:X:ASN:C	1:48:X:VAL:N	17	1.56
(1,92)	1:55:X:SER:N	1:55:X:SER:CA	1:55:X:SER:C	1:56:X:HIS:N	19	1.55
(1,244)	1:138:X:LEU:N	1:138:X:LEU:CA	1:138:X:LEU:C	1:139:X:SER:N	13	1.54
(1,45)	1:28:X:PHE:C	1:29:X:ILE:N	1:29:X:ILE:CA	1:29:X:ILE:C	12	1.54
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	9	1.52
(1,117)	1:67:X:PRO:C	1:68:X:ILE:N	1:68:X:ILE:CA	1:68:X:ILE:C	19	1.52
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	15	1.52
(1,216)	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	1:125:X:ILE:N	7	1.51
(1,207)	1:117:X:ILE:C	1:118:X:LYS:N	1:118:X:LYS:CA	1:118:X:LYS:C	1	1.51
(1,191)	1:109:X:ASN:C	1:110:X:ARG:N	1:110:X:ARG:CA	1:110:X:ARG:C	6	1.51
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1	1.51
(1,144)	1:83:X:ARG:N	1:83:X:ARG:CA	1:83:X:ARG:C	1:84:X:PRO:N	19	1.49
(1,141)	1:81:X:LEU:C	1:82:X:ASP:N	1:82:X:ASP:CA	1:82:X:ASP:C	10	1.49
(1,136)	1:78:X:SER:N	1:78:X:SER:CA	1:78:X:SER:C	1:79:X:PRO:N	2	1.49
(1,36)	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	1:24:X:VAL:N	10	1.49
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	18	1.48
(1,73)	1:45:X:GLY:C	1:46:X:ILE:N	1:46:X:ILE:CA	1:46:X:ILE:C	8	1.48
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	3	1.48
(1,69)	1:42:X:SER:C	1:43:X:GLU:N	1:43:X:GLU:CA	1:43:X:GLU:C	2	1.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,33)	1:20:X:GLY:C	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	12	1.47
(1,169)	1:96:X:GLY:C	1:97:X:GLU:N	1:97:X:GLU:CA	1:97:X:GLU:C	11	1.46
(1,150)	1:87:X:THR:N	1:87:X:THR:CA	1:87:X:THR:C	1:88:X:ALA:N	9	1.45
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	19	1.44
(1,246)	1:139:X:SER:N	1:139:X:SER:CA	1:139:X:SER:C	1:140:X:ASN:N	3	1.44
(1,190)	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	1:110:X:ARG:N	12	1.44
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	13	1.44
(1,207)	1:117:X:ILE:C	1:118:X:LYS:N	1:118:X:LYS:CA	1:118:X:LYS:C	17	1.43
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	19	1.43
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	17	1.42
(1,203)	1:115:X:GLY:C	1:116:X:VAL:N	1:116:X:VAL:CA	1:116:X:VAL:C	18	1.42
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	12	1.42
(1,261)	1:146:X:LEU:C	1:147:X:VAL:N	1:147:X:VAL:CA	1:147:X:VAL:C	12	1.41
(1,168)	1:96:X:GLY:N	1:96:X:GLY:CA	1:96:X:GLY:C	1:97:X:GLU:N	15	1.41
(1,80)	1:49:X:ASP:N	1:49:X:ASP:CA	1:49:X:ASP:C	1:50:X:ASP:N	4	1.41
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	10	1.39
(1,124)	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	1:73:X:ASN:N	10	1.39
(1,195)	1:111:X:ARG:C	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	5	1.38
(1,145)	1:83:X:ARG:C	1:84:X:PRO:N	1:84:X:PRO:CA	1:84:X:PRO:C	18	1.38
(1,134)	1:77:X:SER:N	1:77:X:SER:CA	1:77:X:SER:C	1:78:X:SER:N	1	1.38
(1,212)	1:120:X:VAL:N	1:120:X:VAL:CA	1:120:X:VAL:C	1:121:X:ASP:N	4	1.35
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	15	1.35
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	15	1.35
(1,221)	1:126:X:THR:C	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	7	1.34
(1,244)	1:138:X:LEU:N	1:138:X:LEU:CA	1:138:X:LEU:C	1:139:X:SER:N	9	1.33
(1,224)	1:128:X:THR:N	1:128:X:THR:CA	1:128:X:THR:C	1:129:X:VAL:N	7	1.32
(1,184)	1:104:X:ARG:N	1:104:X:ARG:CA	1:104:X:ARG:C	1:105:X:MET:N	20	1.32
(1,126)	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	1:74:X:LEU:N	16	1.32
(1,126)	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	1:74:X:LEU:N	17	1.3
(1,86)	1:52:X:ALA:N	1:52:X:ALA:CA	1:52:X:ALA:C	1:53:X:ASP:N	12	1.3
(1,237)	1:134:X:GLU:C	1:135:X:VAL:N	1:135:X:VAL:CA	1:135:X:VAL:C	5	1.29
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	3	1.29
(1,126)	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	1:74:X:LEU:N	19	1.27
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	1	1.27
(1,34)	1:21:X:PHE:N	1:21:X:PHE:CA	1:21:X:PHE:C	1:22:X:GLU:N	2	1.27
(1,181)	1:102:X:VAL:C	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	12	1.26
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	5	1.26
(1,42)	1:27:X:GLU:N	1:27:X:GLU:CA	1:27:X:GLU:C	1:28:X:PHE:N	2	1.26
(1,213)	1:120:X:VAL:C	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	19	1.24
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	12	1.24
(1,113)	1:65:X:GLU:C	1:66:X:ASP:N	1:66:X:ASP:CA	1:66:X:ASP:C	8	1.24
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	2	1.24
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	18	1.23
(1,166)	1:95:X:VAL:N	1:95:X:VAL:CA	1:95:X:VAL:C	1:96:X:GLY:N	19	1.22
(1,38)	1:25:X:GLY:N	1:25:X:GLY:CA	1:25:X:GLY:C	1:26:X:ILE:N	10	1.21
(1,250)	1:141:X:ILE:N	1:141:X:ILE:CA	1:141:X:ILE:C	1:142:X:GLN:N	8	1.2
(1,247)	1:139:X:SER:C	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	15	1.2
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	15	1.2
(1,177)	1:100:X:THR:C	1:101:X:LEU:N	1:101:X:LEU:CA	1:101:X:LEU:C	6	1.19
(1,230)	1:131:X:GLY:N	1:131:X:GLY:CA	1:131:X:GLY:C	1:132:X:LYS:N	12	1.18
(1,28)	1:18:X:ALA:N	1:18:X:ALA:CA	1:18:X:ALA:C	1:19:X:LEU:N	20	1.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,215)	1:123:X:GLU:C	1:124:X:MET:N	1:124:X:MET:CA	1:124:X:MET:C	15	1.17
(1,189)	1:108:X:GLN:C	1:109:X:ASN:N	1:109:X:ASN:CA	1:109:X:ASN:C	13	1.16
(1,86)	1:52:X:ALA:N	1:52:X:ALA:CA	1:52:X:ALA:C	1:53:X:ASP:N	3	1.16
(1,66)	1:41:X:ASP:N	1:41:X:ASP:CA	1:41:X:ASP:C	1:42:X:SER:N	20	1.16
(1,92)	1:55:X:SER:N	1:55:X:SER:CA	1:55:X:SER:C	1:56:X:HIS:N	1	1.15
(1,14)	1:11:X:MET:N	1:11:X:MET:CA	1:11:X:MET:C	1:12:X:ILE:N	17	1.15
(1,248)	1:140:X:ASN:N	1:140:X:ASN:CA	1:140:X:ASN:C	1:141:X:ILE:N	18	1.14
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	4	1.14
(1,35)	1:22:X:GLU:C	1:23:X:LEU:N	1:23:X:LEU:CA	1:23:X:LEU:C	19	1.14
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	20	1.11
(1,56)	1:36:X:LEU:N	1:36:X:LEU:CA	1:36:X:LEU:C	1:37:X:ARG:N	2	1.11
(1,55)	1:35:X:THR:C	1:36:X:LEU:N	1:36:X:LEU:CA	1:36:X:LEU:C	17	1.11
(1,51)	1:33:X:THR:C	1:34:X:SER:N	1:34:X:SER:CA	1:34:X:SER:C	9	1.11
(1,123)	1:71:X:ALA:C	1:72:X:TYR:N	1:72:X:TYR:CA	1:72:X:TYR:C	16	1.1
(1,241)	1:136:X:PHE:C	1:137:X:ALA:N	1:137:X:ALA:CA	1:137:X:ALA:C	7	1.09
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	6	1.09
(1,213)	1:120:X:VAL:C	1:121:X:ASP:N	1:121:X:ASP:CA	1:121:X:ASP:C	15	1.08
(1,126)	1:73:X:ASN:N	1:73:X:ASN:CA	1:73:X:ASN:C	1:74:X:LEU:N	8	1.07
(1,211)	1:119:X:ALA:C	1:120:X:VAL:N	1:120:X:VAL:CA	1:120:X:VAL:C	9	1.06
(1,185)	1:106:X:ALA:C	1:107:X:VAL:N	1:107:X:VAL:CA	1:107:X:VAL:C	20	1.06
(1,182)	1:103:X:LEU:N	1:103:X:LEU:CA	1:103:X:LEU:C	1:104:X:ARG:N	16	1.06
(1,153)	1:88:X:ALA:C	1:89:X:GLU:N	1:89:X:GLU:CA	1:89:X:GLU:C	14	1.05
(1,193)	1:110:X:ARG:C	1:111:X:ARG:N	1:111:X:ARG:CA	1:111:X:ARG:C	20	1.02
(1,67)	1:41:X:ASP:C	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	15	1.02
(1,59)	1:37:X:ARG:C	1:38:X:ILE:N	1:38:X:ILE:CA	1:38:X:ILE:C	10	1.02
(1,42)	1:27:X:GLU:N	1:27:X:GLU:CA	1:27:X:GLU:C	1:28:X:PHE:N	1	1.02
(1,39)	1:25:X:GLY:C	1:26:X:ILE:N	1:26:X:ILE:CA	1:26:X:ILE:C	17	1.02
(1,244)	1:138:X:LEU:N	1:138:X:LEU:CA	1:138:X:LEU:C	1:139:X:SER:N	6	1.01
(1,224)	1:128:X:THR:N	1:128:X:THR:CA	1:128:X:THR:C	1:129:X:VAL:N	12	1.01
(1,222)	1:127:X:VAL:N	1:127:X:VAL:CA	1:127:X:VAL:C	1:128:X:THR:N	14	1.01
(1,207)	1:117:X:ILE:C	1:118:X:LYS:N	1:118:X:LYS:CA	1:118:X:LYS:C	20	1.01
(1,196)	1:112:X:LYS:N	1:112:X:LYS:CA	1:112:X:LYS:C	1:113:X:TRP:N	13	1.01
(1,64)	1:40:X:ILE:N	1:40:X:ILE:CA	1:40:X:ILE:C	1:41:X:ASP:N	13	1.01