



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:37 AM UTC

PDB ID : 2MWG / pdb_00002mwg
BMRB ID : 17643
Title : Full-Length Solution Structure Of YtvA, a LOV-Photoreceptor Protein and Regulator of Bacterial Stress Response
Authors : Jurk, M.; Bardiaux, B.; Schmieder, P.
Deposited on : 2014-11-07

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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 23%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:261, B:1-B:261 (522)	0.27	1

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 7, 9
2	8, 10
3	2, 3

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8372 atoms, of which 4218 are hydrogens and 0 are deuteriums.

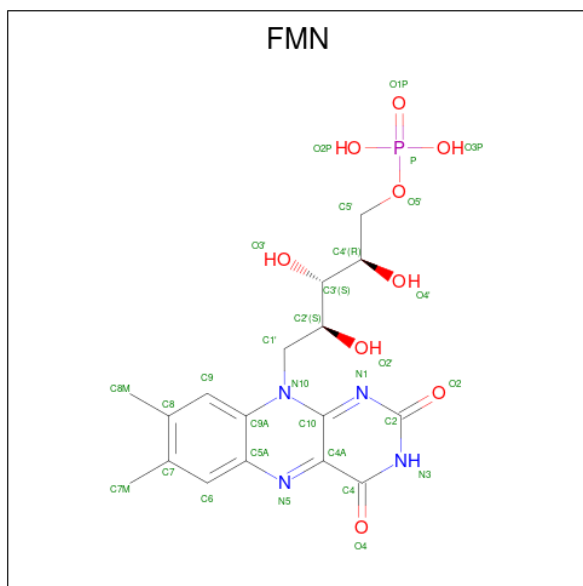
- Molecule 1 is a protein called Blue-light photoreceptor.

Mol	Chain	Residues	Atoms						Trace
1	A	261	Total	C	H	N	O	S	0
			4136	1302	2090	333	403	8	
1	B	261	Total	C	H	N	O	S	0
			4136	1302	2090	333	403	8	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O34627
B	1	GLY	-	expression tag	UNP O34627

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



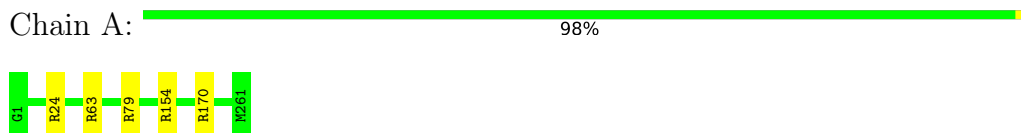
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			50	17	19	4	9	1
2	B	1	Total	C	H	N	O	P
			50	17	19	4	9	1

4 Residue-property plots [i](#)

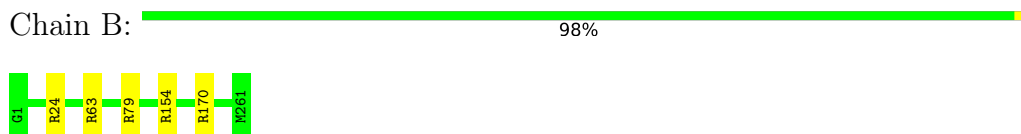
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Blue-light photoreceptor



- Molecule 1: Blue-light photoreceptor

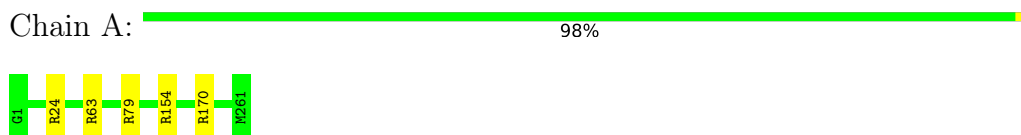


4.2 Scores per residue for each member of the ensemble

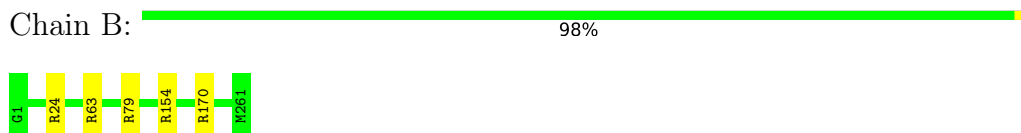
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Blue-light photoreceptor

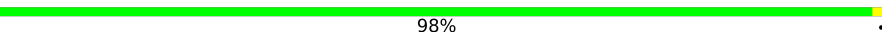


- Molecule 1: Blue-light photoreceptor



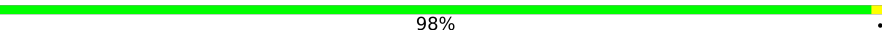
4.2.2 Score per residue for model 2

- Molecule 1: Blue-light photoreceptor

Chain A:  98% .



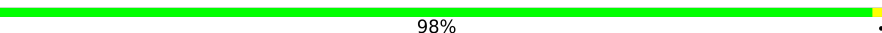
- Molecule 1: Blue-light photoreceptor

Chain B:  98% .



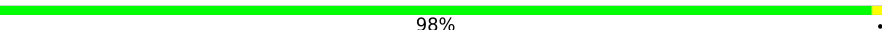
4.2.3 Score per residue for model 3

- Molecule 1: Blue-light photoreceptor

Chain A:  98% .



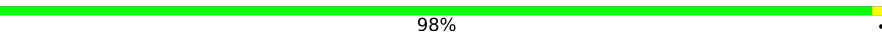
- Molecule 1: Blue-light photoreceptor

Chain B:  98% .



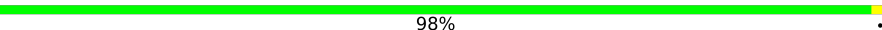
4.2.4 Score per residue for model 4

- Molecule 1: Blue-light photoreceptor

Chain A:  98% .



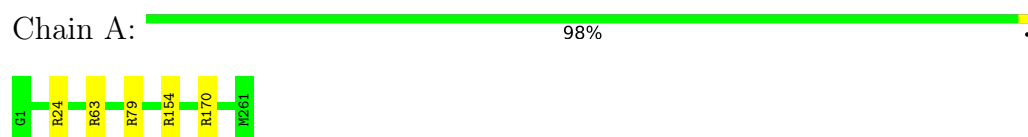
- Molecule 1: Blue-light photoreceptor

Chain B:  98% .

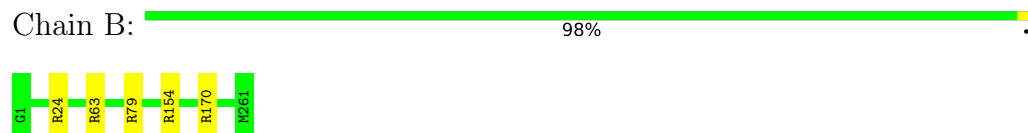


4.2.5 Score per residue for model 5

- Molecule 1: Blue-light photoreceptor

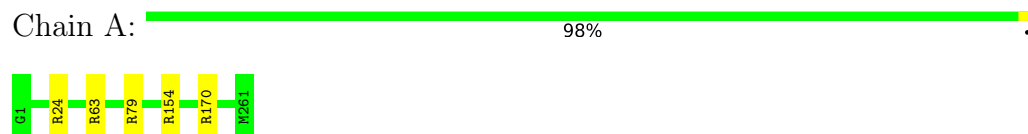


- Molecule 1: Blue-light photoreceptor

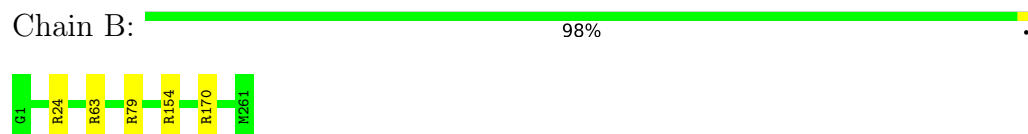


4.2.6 Score per residue for model 6

- Molecule 1: Blue-light photoreceptor

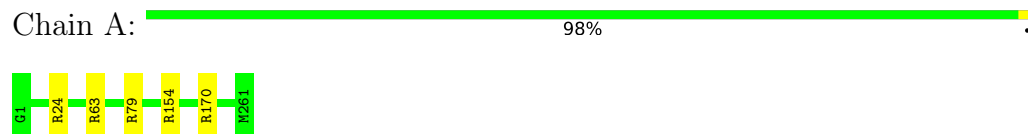


- Molecule 1: Blue-light photoreceptor

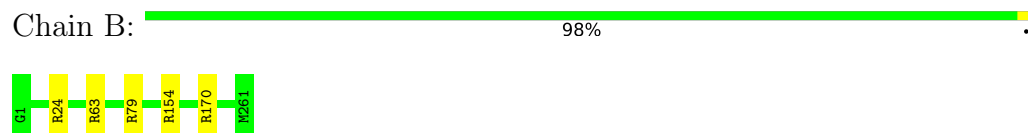


4.2.7 Score per residue for model 7

- Molecule 1: Blue-light photoreceptor

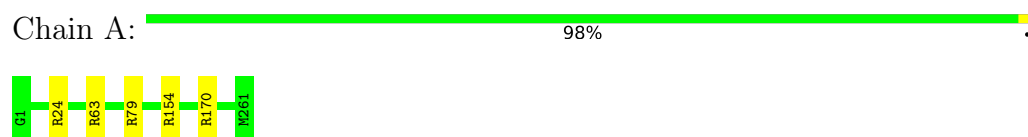


- Molecule 1: Blue-light photoreceptor

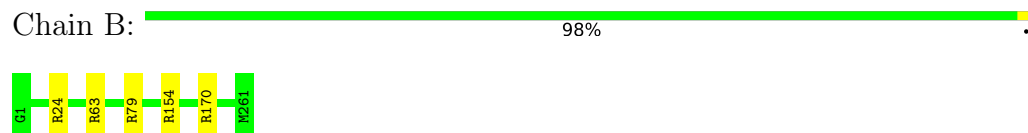


4.2.8 Score per residue for model 8

- Molecule 1: Blue-light photoreceptor

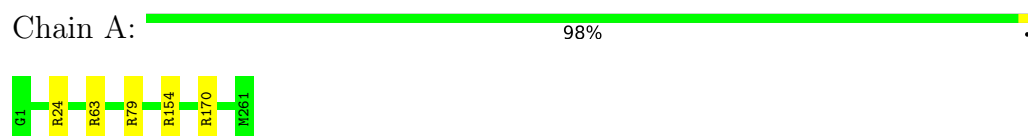


- Molecule 1: Blue-light photoreceptor

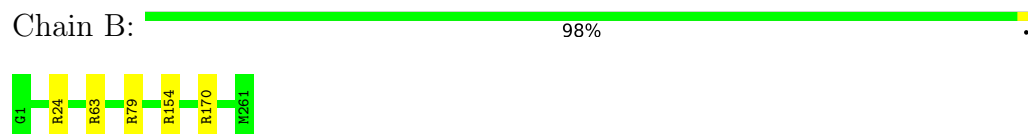


4.2.9 Score per residue for model 9

- Molecule 1: Blue-light photoreceptor

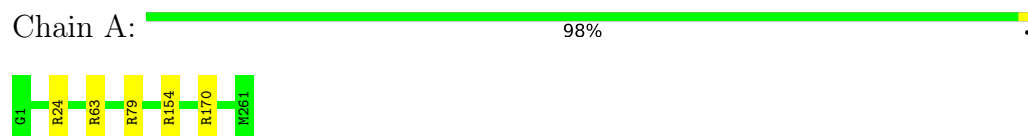


- Molecule 1: Blue-light photoreceptor

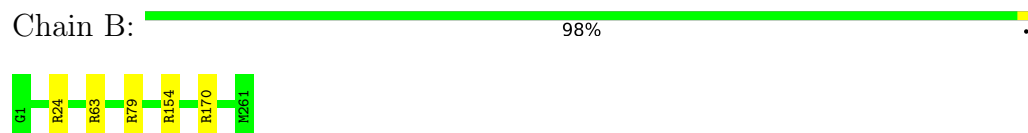


4.2.10 Score per residue for model 10

- Molecule 1: Blue-light photoreceptor



- Molecule 1: Blue-light photoreceptor



5 Refinement protocol and experimental data overview

The models were refined using the following method: *monte-carlo simulated annealing using torsion angle dynamics, simulated annealing..*

Of the 100 calculated structures, 10 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
CS-ROSETTA	structure solution	v3.2
X-PLOR NIH	structure solution	v2.30
X-PLOR NIH	refinement	v2.30
X-PLOR NIH	geometry optimization	v2.30

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	1643
Number of shifts mapped to atoms	1643
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	23%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 23% for the well-defined parts and 23% 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	1643
Number of shifts mapped to atoms	1643
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	255	0.22 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	239	0.90 ± 0.09	Should be checked
$^{13}\text{C}'$	255	-0.17 ± 0.11	None needed (< 0.5 ppm)
^{15}N	242	-0.45 ± 0.12	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 23%, i.e. 1632 atoms were assigned a chemical shift out of a possible 7174. 0 out of 94 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	994/2596 (38%)	242/1052 (23%)	510/1044 (49%)	242/500 (48%)
Sidechain	636/4200 (15%)	306/2736 (11%)	330/1334 (25%)	0/130 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/378 (1%)	1/182 (1%)	0/182 (0%)	1/14 (7%)
Overall	1632/7174 (23%)	549/3970 (14%)	840/2560 (33%)	243/644 (38%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 23%, i.e. 1632 atoms were assigned a chemical shift out of a possible 7174. 0 out of 94 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	994/2596 (38%)	242/1052 (23%)	510/1044 (49%)	242/500 (48%)
Sidechain	636/4200 (15%)	306/2736 (11%)	330/1334 (25%)	0/130 (0%)
Aromatic	2/378 (1%)	1/182 (1%)	0/182 (0%)	1/14 (7%)
Overall	1632/7174 (23%)	549/3970 (14%)	840/2560 (33%)	243/644 (38%)

7.1.4 Statistically unusual chemical shifts [i](#)

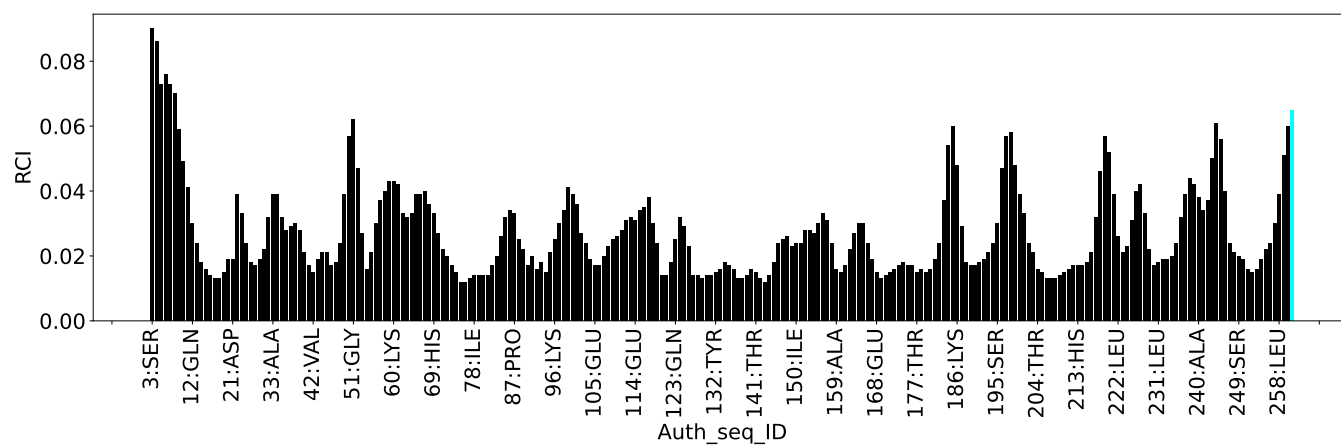
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	204	THR	HG1	5.87	0.08 – 2.19	22.4
1	A	247	THR	HG1	5.59	0.08 – 2.19	21.1
1	A	225	THR	HG1	5.38	0.08 – 2.19	20.1
1	A	179	THR	HG1	5.07	0.08 – 2.19	18.6
1	A	70	THR	HG1	4.93	0.08 – 2.19	18.0
1	A	30	THR	HG1	4.89	0.08 – 2.19	17.8
1	A	148	THR	HG1	4.74	0.08 – 2.19	17.1
1	A	220	THR	HG1	4.36	0.08 – 2.19	15.3

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1192
Intra-residue ($ i-j =0$)	58
Sequential ($ i-j =1$)	452
Medium range ($ i-j >1$ and $ i-j <5$)	380
Long range ($ i-j \geq 5$)	294
Inter-chain	0
Hydrogen bond restraints	8
Disulfide bond restraints	0
Total dihedral-angle restraints	814
Number of unmapped restraints	0
Number of restraints per residue	3.8
Number of long range restraints per residue ¹	0.6

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)	56.5	0.2
0.2-0.5 (Medium)	24.6	0.5
>0.5 (Large)	2.4	0.88

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)	46.2	9.98
10.0-20.0 (Medium)	7.1	19.89
>20.0 (Large)	1.5	22.97

9 Distance violation analysis ⓘ

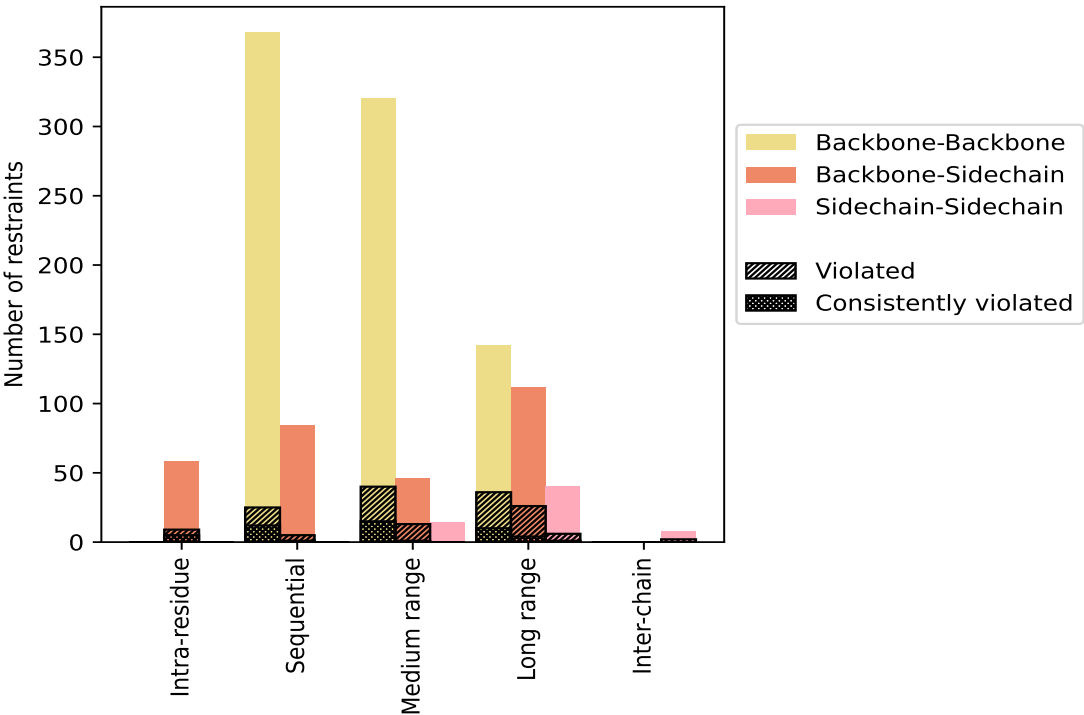
9.1 Summary of distance violations ⓘ

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)	58	4.9	9	15.5	0.8	5	8.6	0.4
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	58	4.9	9	15.5	0.8	5	8.6	0.4
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	452	37.9	30	6.6	2.5	13	2.9	1.1
Backbone-Backbone	368	30.9	25	6.8	2.1	12	3.3	1.0
Backbone-Sidechain	84	7.0	5	6.0	0.4	1	1.2	0.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	380	31.9	53	13.9	4.4	16	4.2	1.3
Backbone-Backbone	320	26.8	40	12.5	3.4	15	4.7	1.3
Backbone-Sidechain	46	3.9	13	28.3	1.1	1	2.2	0.1
Sidechain-Sidechain	14	1.2	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	294	24.7	68	23.1	5.7	15	5.1	1.3
Backbone-Backbone	142	11.9	36	25.4	3.0	10	7.0	0.8
Backbone-Sidechain	112	9.4	26	23.2	2.2	4	3.6	0.3
Sidechain-Sidechain	40	3.4	6	15.0	0.5	1	2.5	0.1
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	8	0.7	2	25.0	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1192	100.0	162	13.6	13.6	49	4.1	4.1
Backbone-Backbone	830	69.6	101	12.2	8.5	37	4.5	3.1
Backbone-Sidechain	300	25.2	53	17.7	4.4	11	3.7	0.9
Sidechain-Sidechain	62	5.2	8	12.9	0.7	1	1.6	0.1

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

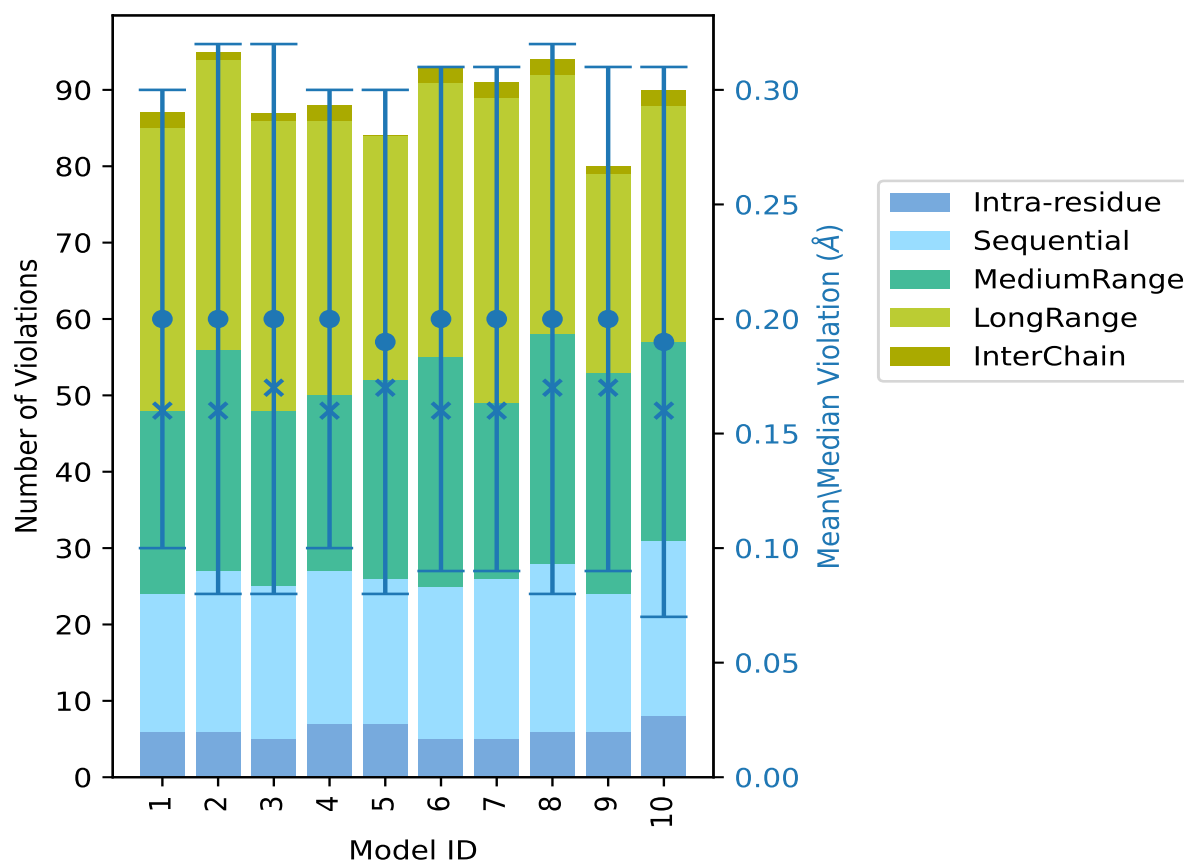
9.2 Distance violation statistics for each model [i](#)

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	6	18	24	37	2	87	0.2	0.67	0.1	0.16
2	6	21	29	38	1	95	0.2	0.88	0.12	0.16
3	5	20	23	38	1	87	0.2	0.8	0.12	0.17
4	7	20	23	36	2	88	0.2	0.6	0.1	0.16
5	7	19	26	32	0	84	0.19	0.74	0.11	0.17
6	5	20	30	36	2	93	0.2	0.79	0.11	0.16
7	5	21	23	40	2	91	0.2	0.71	0.11	0.16
8	6	22	30	34	2	94	0.2	0.84	0.12	0.17
9	6	18	29	26	1	80	0.2	0.66	0.11	0.17
10	8	23	26	31	2	90	0.19	0.82	0.12	0.16

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1024(IR:49, SQ:422, MR:327, LR:226, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	14	15	0	30	1	10.0
1	6	9	7	0	23	2	20.0
3	2	4	8	0	17	3	30.0

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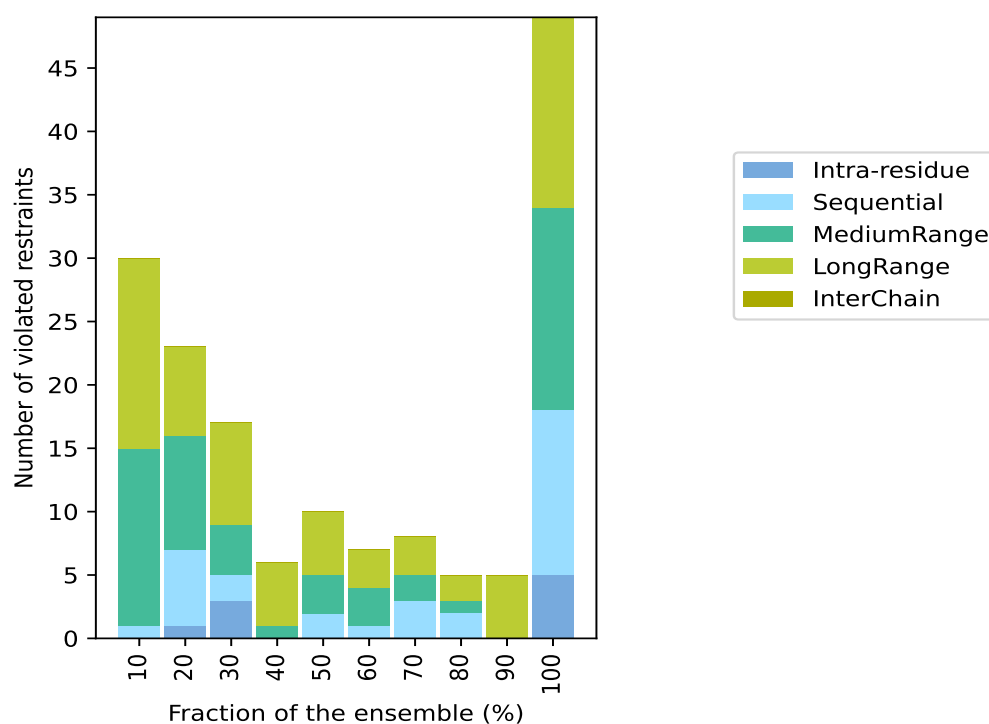
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	5	0	6	4	40.0
0	2	3	5	0	10	5	50.0
0	1	3	3	0	7	6	60.0
0	3	2	3	0	8	7	70.0
0	2	1	2	0	5	8	80.0
0	0	0	5	0	5	9	90.0
5	13	16	15	0	49	10	100.0

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

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

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

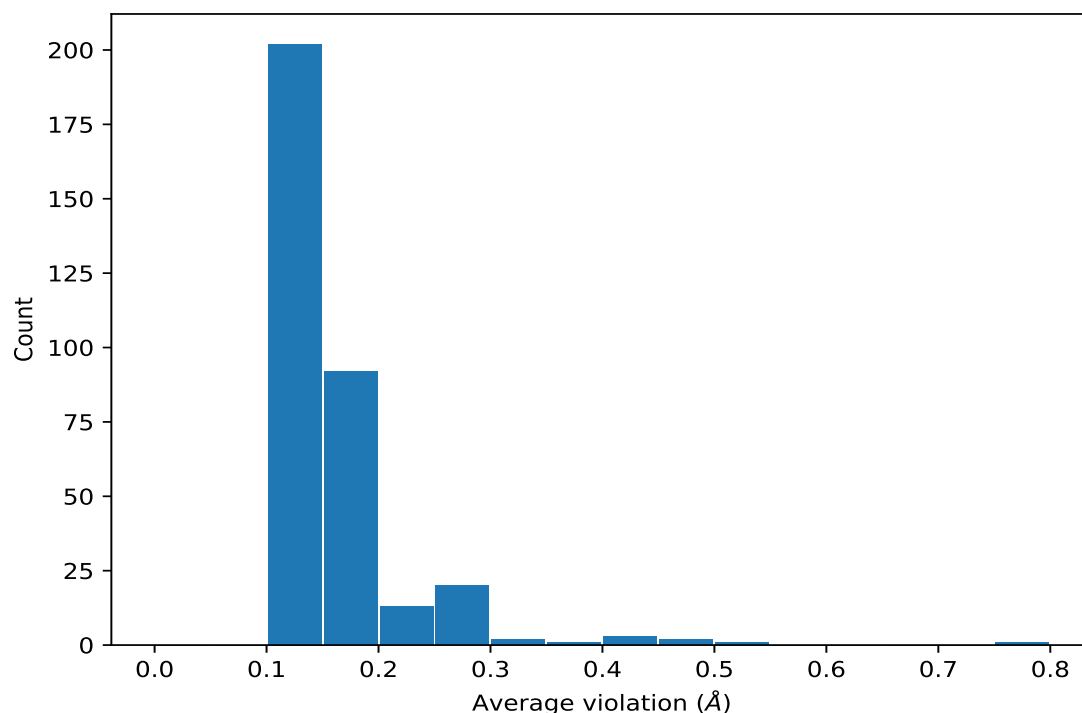


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	10	0.75	0.09	0.76
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	10	0.53	0.02	0.54
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	10	0.45	0.04	0.44
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	10	0.45	0.03	0.44
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	10	0.42	0.03	0.44
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	10	0.42	0.09	0.4
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	10	0.42	0.06	0.4
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	10	0.37	0.04	0.37
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	10	0.31	0.02	0.3
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	10	0.31	0.02	0.3
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	10	0.29	0.04	0.3
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	10	0.29	0.02	0.3
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	10	0.28	0.03	0.27
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	10	0.28	0.01	0.29
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	10	0.28	0.06	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	10	0.28	0.06	0.28
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	10	0.28	0.06	0.28
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	10	0.28	0.06	0.28
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	10	0.28	0.06	0.28
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	10	0.28	0.06	0.28
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	10	0.26	0.01	0.26
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	10	0.26	0.01	0.26
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	10	0.26	0.01	0.26
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	10	0.26	0.01	0.26
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	10	0.26	0.01	0.26
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	10	0.26	0.01	0.26
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	10	0.25	0.1	0.24
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	10	0.25	0.05	0.26
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	10	0.25	0.05	0.26
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	10	0.25	0.05	0.26
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	10	0.24	0.04	0.24
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	10	0.23	0.04	0.24
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	10	0.23	0.04	0.24
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	10	0.23	0.04	0.24
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	10	0.22	0.04	0.2
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	10	0.22	0.01	0.22
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	10	0.22	0.01	0.22
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	10	0.19	0.04	0.18
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	10	0.19	0.04	0.18
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	10	0.19	0.04	0.18
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	10	0.19	0.01	0.19
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	10	0.18	0.02	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	10	0.18	0.02	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	10	0.18	0.02	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	10	0.18	0.02	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	10	0.18	0.02	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	10	0.18	0.02	0.18
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	10	0.18	0.04	0.18
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	10	0.18	0.04	0.18
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	10	0.18	0.04	0.18
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	10	0.18	0.04	0.18
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	10	0.18	0.04	0.18
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	10	0.18	0.04	0.18
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	10	0.18	0.01	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	10	0.18	0.0	0.18
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	10	0.18	0.02	0.18
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	10	0.17	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	10	0.17	0.03	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	10	0.17	0.03	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	10	0.17	0.03	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	10	0.17	0.03	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	10	0.17	0.03	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	10	0.17	0.03	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	10	0.17	0.03	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	10	0.17	0.03	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	10	0.17	0.03	0.18
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	10	0.17	0.02	0.17
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	10	0.16	0.02	0.17
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	10	0.16	0.01	0.16
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	10	0.16	0.01	0.16
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	10	0.16	0.05	0.15
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	10	0.16	0.01	0.16
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	10	0.16	0.01	0.16
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	10	0.16	0.02	0.16
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	10	0.15	0.03	0.16
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	10	0.15	0.03	0.16
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	10	0.15	0.03	0.16
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	10	0.15	0.03	0.16
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	10	0.15	0.03	0.16
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	10	0.15	0.03	0.16
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	10	0.14	0.01	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	10	0.14	0.01	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	10	0.14	0.01	0.15
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	10	0.14	0.03	0.14
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	10	0.14	0.01	0.14
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	10	0.14	0.01	0.14
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	10	0.14	0.01	0.14
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	10	0.14	0.01	0.14
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	10	0.14	0.01	0.14
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	10	0.13	0.01	0.14
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	10	0.13	0.01	0.12
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	10	0.13	0.01	0.12
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	10	0.13	0.01	0.12
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	10	0.13	0.01	0.12
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	10	0.13	0.01	0.12
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	10	0.13	0.01	0.12
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	10	0.12	0.01	0.12
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	9	0.23	0.05	0.25
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	9	0.23	0.05	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	9	0.2	0.03	0.2
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	9	0.19	0.05	0.19
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	9	0.19	0.05	0.19
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	9	0.19	0.05	0.19
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	9	0.19	0.05	0.17
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	9	0.18	0.03	0.18
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	9	0.18	0.03	0.18
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	9	0.18	0.03	0.18
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	9	0.14	0.03	0.14
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	8	0.23	0.02	0.24
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	8	0.17	0.05	0.16
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	8	0.15	0.03	0.15
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	8	0.12	0.01	0.12
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	8	0.11	0.01	0.11
(2,383)	1:166:A:LEU:H	1:199:A:GLN:H	7	0.2	0.05	0.21
(2,223)	1:93:A:GLN:HE21	1:103:A:TRP:HE1	7	0.18	0.02	0.18
(2,223)	1:93:A:GLN:HE22	1:103:A:TRP:HE1	7	0.18	0.02	0.18
(2,793)	1:88:B:VAL:HG11	1:89:B:THR:H	7	0.15	0.03	0.15
(2,793)	1:88:B:VAL:HG12	1:89:B:THR:H	7	0.15	0.03	0.15
(2,793)	1:88:B:VAL:HG13	1:89:B:THR:H	7	0.15	0.03	0.15
(2,793)	1:88:B:VAL:HG21	1:89:B:THR:H	7	0.15	0.03	0.15
(2,793)	1:88:B:VAL:HG22	1:89:B:THR:H	7	0.15	0.03	0.15
(2,793)	1:88:B:VAL:HG23	1:89:B:THR:H	7	0.15	0.03	0.15
(2,261)	1:112:A:GLU:H	1:113:A:ILE:H	7	0.15	0.02	0.15
(2,445)	1:191:A:ILE:HD11	1:223:A:ILE:H	7	0.15	0.03	0.14
(2,445)	1:191:A:ILE:HD12	1:223:A:ILE:H	7	0.15	0.03	0.14
(2,445)	1:191:A:ILE:HD13	1:223:A:ILE:H	7	0.15	0.03	0.14
(2,234)	1:97:A:LYS:H	1:100:A:THR:H	7	0.13	0.02	0.13
(2,10)	1:25:A:VAL:HG11	1:26:A:GLY:H	7	0.13	0.01	0.13
(2,10)	1:25:A:VAL:HG12	1:26:A:GLY:H	7	0.13	0.01	0.13
(2,10)	1:25:A:VAL:HG13	1:26:A:GLY:H	7	0.13	0.01	0.13
(2,10)	1:25:A:VAL:HG21	1:26:A:GLY:H	7	0.13	0.01	0.13
(2,10)	1:25:A:VAL:HG22	1:26:A:GLY:H	7	0.13	0.01	0.13
(2,10)	1:25:A:VAL:HG23	1:26:A:GLY:H	7	0.13	0.01	0.13
(2,1127)	1:230:B:GLU:H	1:232:B:ALA:H	7	0.12	0.01	0.12
(1,8)	2:900:B:FMN:O4'	1:66:B:GLN:NE2	6	0.19	0.07	0.17
(2,521)	1:224:A:ILE:H	1:248:A:TYR:H	6	0.17	0.02	0.18
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG11	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG12	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG13	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG21	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG22	6	0.16	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG23	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG11	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG12	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG13	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG21	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG22	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG23	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG11	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG12	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG13	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG21	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG22	6	0.16	0.02	0.15
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG23	6	0.16	0.02	0.15
(2,881)	1:126:B:ILE:HD11	1:130:B:LYS:H	6	0.14	0.02	0.14
(2,881)	1:126:B:ILE:HD12	1:130:B:LYS:H	6	0.14	0.02	0.14
(2,881)	1:126:B:ILE:HD13	1:130:B:LYS:H	6	0.14	0.02	0.14
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG11	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG12	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG13	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG21	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG22	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG23	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG11	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG12	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG13	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG21	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG22	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG23	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG11	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG12	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG13	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG21	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG22	6	0.13	0.02	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG23	6	0.13	0.02	0.12
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD11	6	0.13	0.01	0.12
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD12	6	0.13	0.01	0.12
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD13	6	0.13	0.01	0.12
(2,232)	1:97:A:LYS:H	1:98:A:ASP:H	6	0.11	0.01	0.11
(2,576)	1:251:A:VAL:HG11	1:255:A:VAL:H	6	0.11	0.0	0.11
(2,576)	1:251:A:VAL:HG12	1:255:A:VAL:H	6	0.11	0.0	0.11
(2,576)	1:251:A:VAL:HG13	1:255:A:VAL:H	6	0.11	0.0	0.11
(2,576)	1:251:A:VAL:HG21	1:255:A:VAL:H	6	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,576)	1:251:A:VAL:HG22	1:255:A:VAL:H	6	0.11	0.0	0.11
(2,576)	1:251:A:VAL:HG23	1:255:A:VAL:H	6	0.11	0.0	0.11
(2,695)	1:56:B:GLU:H	1:58:B:LEU:H	5	0.2	0.04	0.22
(2,384)	1:166:A:LEU:H	1:201:A:ASN:H	5	0.18	0.06	0.2
(2,203)	1:88:A:VAL:HG11	1:108:A:ILE:H	5	0.17	0.02	0.17
(2,203)	1:88:A:VAL:HG12	1:108:A:ILE:H	5	0.17	0.02	0.17
(2,203)	1:88:A:VAL:HG13	1:108:A:ILE:H	5	0.17	0.02	0.17
(2,203)	1:88:A:VAL:HG21	1:108:A:ILE:H	5	0.17	0.02	0.17
(2,203)	1:88:A:VAL:HG22	1:108:A:ILE:H	5	0.17	0.02	0.17
(2,203)	1:88:A:VAL:HG23	1:108:A:ILE:H	5	0.17	0.02	0.17
(2,692)	1:55:B:GLU:H	1:58:B:LEU:H	5	0.17	0.04	0.18
(2,381)	1:165:A:ASN:H	1:198:A:ALA:H	5	0.15	0.03	0.14
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD11	5	0.14	0.02	0.15
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD12	5	0.14	0.02	0.15
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD13	5	0.14	0.02	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD11	5	0.14	0.02	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD12	5	0.14	0.02	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD13	5	0.14	0.02	0.15
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD11	5	0.14	0.02	0.15
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD12	5	0.14	0.02	0.15
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD13	5	0.14	0.02	0.15
(2,973)	1:165:B:ASN:H	1:198:B:ALA:H	5	0.14	0.03	0.12
(2,109)	1:59:A:GLY:H	1:60:A:LYS:H	5	0.12	0.02	0.11
(2,907)	1:138:B:ASP:H	1:141:B:THR:H	5	0.11	0.01	0.11
(2,1137)	1:236:B:ASN:H	1:237:B:LYS:H	5	0.11	0.01	0.11
(2,186)	1:82:A:LEU:HD11	1:86:A:GLU:H	4	0.18	0.05	0.16
(2,186)	1:82:A:LEU:HD12	1:86:A:GLU:H	4	0.18	0.05	0.16
(2,186)	1:82:A:LEU:HD13	1:86:A:GLU:H	4	0.18	0.05	0.16
(2,186)	1:82:A:LEU:HD21	1:86:A:GLU:H	4	0.18	0.05	0.16
(2,186)	1:82:A:LEU:HD22	1:86:A:GLU:H	4	0.18	0.05	0.16
(2,186)	1:82:A:LEU:HD23	1:86:A:GLU:H	4	0.18	0.05	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD11	4	0.17	0.02	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD12	4	0.17	0.02	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD13	4	0.17	0.02	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD21	4	0.17	0.02	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD22	4	0.17	0.02	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD23	4	0.17	0.02	0.16
(2,130)	1:67:A:GLY:H	1:95:A:TYR:H	4	0.16	0.03	0.16
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD11	4	0.12	0.01	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD12	4	0.12	0.01	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD13	4	0.12	0.01	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD21	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD22	4	0.12	0.01	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD23	4	0.12	0.01	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD11	4	0.12	0.01	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD12	4	0.12	0.01	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD13	4	0.12	0.01	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD21	4	0.12	0.01	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD22	4	0.12	0.01	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD23	4	0.12	0.01	0.12
(2,1060)	1:200:B:VAL:HG11	1:205:B:ALA:H	4	0.11	0.02	0.11
(2,1060)	1:200:B:VAL:HG12	1:205:B:ALA:H	4	0.11	0.02	0.11
(2,1060)	1:200:B:VAL:HG13	1:205:B:ALA:H	4	0.11	0.02	0.11
(2,1060)	1:200:B:VAL:HG21	1:205:B:ALA:H	4	0.11	0.02	0.11
(2,1060)	1:200:B:VAL:HG22	1:205:B:ALA:H	4	0.11	0.02	0.11
(2,1060)	1:200:B:VAL:HG23	1:205:B:ALA:H	4	0.11	0.02	0.11
(2,1111)	1:224:B:ILE:H	1:246:B:LYS:H	3	0.18	0.04	0.18
(2,1064)	1:201:B:ASN:H	1:205:B:ALA:H	3	0.17	0.05	0.19
(2,962)	1:162:B:LEU:H	1:193:B:ASP:H	3	0.15	0.03	0.16
(2,778)	1:82:B:LEU:HD11	1:86:B:GLU:H	3	0.14	0.04	0.13
(2,778)	1:82:B:LEU:HD12	1:86:B:GLU:H	3	0.14	0.04	0.13
(2,778)	1:82:B:LEU:HD13	1:86:B:GLU:H	3	0.14	0.04	0.13
(2,778)	1:82:B:LEU:HD21	1:86:B:GLU:H	3	0.14	0.04	0.13
(2,778)	1:82:B:LEU:HD22	1:86:B:GLU:H	3	0.14	0.04	0.13
(2,778)	1:82:B:LEU:HD23	1:86:B:GLU:H	3	0.14	0.04	0.13
(2,341)	1:150:A:ILE:HD11	1:159:A:ALA:H	3	0.14	0.03	0.15
(2,341)	1:150:A:ILE:HD12	1:159:A:ALA:H	3	0.14	0.03	0.15
(2,341)	1:150:A:ILE:HD13	1:159:A:ALA:H	3	0.14	0.03	0.15
(2,4)	1:4:A:PHE:H	1:5:A:GLN:H	3	0.13	0.02	0.13
(2,975)	1:166:B:LEU:H	1:199:B:GLN:H	3	0.13	0.03	0.12
(2,1118)	1:226:B:GLY:H	1:248:B:TYR:H	3	0.13	0.01	0.13
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD11	3	0.13	0.02	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD12	3	0.13	0.02	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD13	3	0.13	0.02	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD21	3	0.13	0.02	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD22	3	0.13	0.02	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD23	3	0.13	0.02	0.14
(2,191)	1:83:A:GLN:H	1:85:A:LYS:H	3	0.12	0.01	0.12
(2,379)	1:165:A:ASN:H	1:167:A:THR:H	3	0.12	0.01	0.11
(2,54)	1:39:A:ILE:HD11	1:60:A:LYS:H	3	0.12	0.0	0.12
(2,54)	1:39:A:ILE:HD12	1:60:A:LYS:H	3	0.12	0.0	0.12
(2,54)	1:39:A:ILE:HD13	1:60:A:LYS:H	3	0.12	0.0	0.12
(2,209)	1:90:A:VAL:HG11	1:90:A:VAL:H	3	0.12	0.01	0.11
(2,209)	1:90:A:VAL:HG12	1:90:A:VAL:H	3	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,209)	1:90:A:VAL:HG13	1:90:A:VAL:H	3	0.12	0.01	0.11
(2,209)	1:90:A:VAL:HG21	1:90:A:VAL:H	3	0.12	0.01	0.11
(2,209)	1:90:A:VAL:HG22	1:90:A:VAL:H	3	0.12	0.01	0.11
(2,209)	1:90:A:VAL:HG23	1:90:A:VAL:H	3	0.12	0.01	0.11
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD11	3	0.11	0.01	0.11
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD12	3	0.11	0.01	0.11
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD13	3	0.11	0.01	0.11
(2,200)	1:88:A:VAL:HG11	1:88:A:VAL:H	3	0.11	0.01	0.12
(2,200)	1:88:A:VAL:HG12	1:88:A:VAL:H	3	0.11	0.01	0.12
(2,200)	1:88:A:VAL:HG13	1:88:A:VAL:H	3	0.11	0.01	0.12
(2,200)	1:88:A:VAL:HG21	1:88:A:VAL:H	3	0.11	0.01	0.12
(2,200)	1:88:A:VAL:HG22	1:88:A:VAL:H	3	0.11	0.01	0.12
(2,200)	1:88:A:VAL:HG23	1:88:A:VAL:H	3	0.11	0.01	0.12
(2,1150)	1:242:B:PHE:H	1:243:B:SER:H	3	0.11	0.0	0.11
(2,801)	1:90:B:VAL:HG11	1:90:B:VAL:H	3	0.1	0.0	0.1
(2,801)	1:90:B:VAL:HG12	1:90:B:VAL:H	3	0.1	0.0	0.1
(2,801)	1:90:B:VAL:HG13	1:90:B:VAL:H	3	0.1	0.0	0.1
(2,801)	1:90:B:VAL:HG21	1:90:B:VAL:H	3	0.1	0.0	0.1
(2,801)	1:90:B:VAL:HG22	1:90:B:VAL:H	3	0.1	0.0	0.1
(2,801)	1:90:B:VAL:HG23	1:90:B:VAL:H	3	0.1	0.0	0.1
(2,248)	1:105:A:GLU:H	1:126:A:ILE:H	2	0.16	0.02	0.16
(2,697)	1:57:B:ILE:H	1:58:B:LEU:H	2	0.16	0.02	0.16
(2,246)	1:105:A:GLU:H	1:124:A:ASN:H	2	0.15	0.01	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD11	2	0.15	0.0	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD12	2	0.15	0.0	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD13	2	0.15	0.0	0.15
(2,596)	1:4:B:PHE:H	1:5:B:GLN:H	2	0.14	0.0	0.14
(2,615)	1:28:B:VAL:HG11	1:30:B:THR:H	2	0.14	0.03	0.14
(2,615)	1:28:B:VAL:HG12	1:30:B:THR:H	2	0.14	0.03	0.14
(2,615)	1:28:B:VAL:HG13	1:30:B:THR:H	2	0.14	0.03	0.14
(2,615)	1:28:B:VAL:HG21	1:30:B:THR:H	2	0.14	0.03	0.14
(2,615)	1:28:B:VAL:HG22	1:30:B:THR:H	2	0.14	0.03	0.14
(2,615)	1:28:B:VAL:HG23	1:30:B:THR:H	2	0.14	0.03	0.14
(2,50)	1:39:A:ILE:H	1:59:A:GLY:H	2	0.14	0.02	0.14
(2,212)	1:90:A:VAL:HG11	1:106:A:LEU:H	2	0.14	0.04	0.14
(2,212)	1:90:A:VAL:HG12	1:106:A:LEU:H	2	0.14	0.04	0.14
(2,212)	1:90:A:VAL:HG13	1:106:A:LEU:H	2	0.14	0.04	0.14
(2,212)	1:90:A:VAL:HG21	1:106:A:LEU:H	2	0.14	0.04	0.14
(2,212)	1:90:A:VAL:HG22	1:106:A:LEU:H	2	0.14	0.04	0.14
(2,212)	1:90:A:VAL:HG23	1:106:A:LEU:H	2	0.14	0.04	0.14
(2,925)	1:147:B:SER:HG	1:148:B:THR:H	2	0.14	0.02	0.14
(2,259)	1:111:A:MET:H	1:119:A:PHE:H	2	0.12	0.01	0.12

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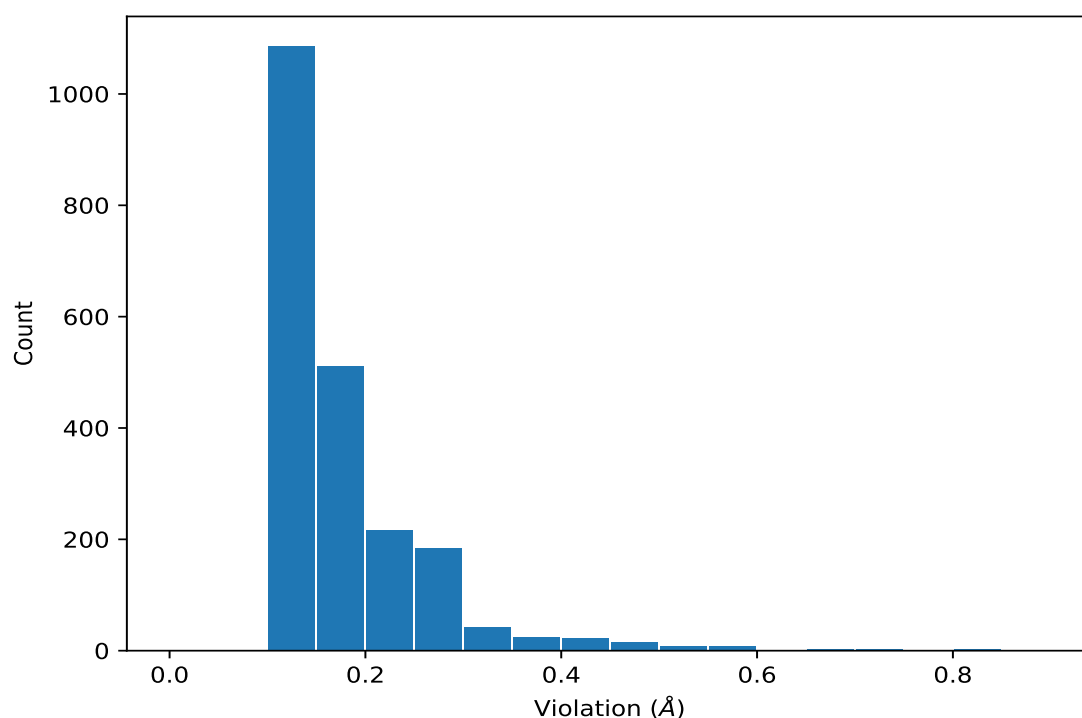
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,820)	1:96:B:LYS:H	1:98:B:ASP:H	2	0.12	0.02	0.12
(2,1070)	1:203:B:GLN:H	1:206:B:ASP:H	2	0.12	0.0	0.12
(2,225)	1:94:A:ASN:H	1:102:A:PHE:H	2	0.11	0.01	0.11
(2,236)	1:98:A:ASP:H	1:100:A:THR:H	2	0.11	0.01	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD11	2	0.11	0.0	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD12	2	0.11	0.0	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD13	2	0.11	0.0	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD21	2	0.11	0.0	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD22	2	0.11	0.0	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD23	2	0.11	0.0	0.11
(2,1155)	1:244:B:SER:H	1:245:B:LEU:H	2	0.11	0.0	0.11
(2,1168)	1:251:B:VAL:HG11	1:255:B:VAL:H	2	0.11	0.01	0.11
(2,1168)	1:251:B:VAL:HG12	1:255:B:VAL:H	2	0.11	0.01	0.11
(2,1168)	1:251:B:VAL:HG13	1:255:B:VAL:H	2	0.11	0.01	0.11
(2,1168)	1:251:B:VAL:HG21	1:255:B:VAL:H	2	0.11	0.01	0.11
(2,1168)	1:251:B:VAL:HG22	1:255:B:VAL:H	2	0.11	0.01	0.11
(2,1168)	1:251:B:VAL:HG23	1:255:B:VAL:H	2	0.11	0.01	0.11
(2,875)	1:124:B:ASN:H	1:126:B:ILE:H	2	0.11	0.0	0.11
(2,1100)	1:215:B:LEU:H	1:217:B:LEU:H	2	0.11	0.0	0.11
(2,98)	1:55:A:GLU:H	1:56:A:GLU:H	2	0.1	0.0	0.1
(2,157)	1:76:A:ASP:H	1:79:A:ARG:H	2	0.1	0.0	0.1
(2,330)	1:146:A:LEU:HD11	1:146:A:LEU:H	2	0.1	0.0	0.1
(2,330)	1:146:A:LEU:HD12	1:146:A:LEU:H	2	0.1	0.0	0.1
(2,330)	1:146:A:LEU:HD13	1:146:A:LEU:H	2	0.1	0.0	0.1
(2,330)	1:146:A:LEU:HD21	1:146:A:LEU:H	2	0.1	0.0	0.1
(2,330)	1:146:A:LEU:HD22	1:146:A:LEU:H	2	0.1	0.0	0.1
(2,330)	1:146:A:LEU:HD23	1:146:A:LEU:H	2	0.1	0.0	0.1
(2,627)	1:30:B:THR:H	1:41:B:TYR:H	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	2	0.88
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	8	0.84
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	10	0.82
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	3	0.8
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	6	0.79
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	5	0.74
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	7	0.71
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	1	0.67
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	9	0.66
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	4	0.6
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	7	0.56
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	8	0.56
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	9	0.56
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	4	0.55
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	3	0.55
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	4	0.55
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	10	0.54
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	3	0.54
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	1	0.53
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	5	0.53
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	2	0.53
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	3	0.51
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	9	0.51
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	2	0.5
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	6	0.49
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	7	0.49
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	6	0.48
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	10	0.47
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	6	0.47
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	6	0.47
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	7	0.47
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	10	0.46
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	2	0.46
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	8	0.46
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	3	0.46
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	1	0.46
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	6	0.45
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	7	0.45
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	8	0.45
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	4	0.44
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	6	0.44
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	2	0.44
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	8	0.44
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	10	0.44
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	6	0.43
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	7	0.43
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	9	0.43
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	2	0.42
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	9	0.42
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	3	0.42
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	5	0.42
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	3	0.42
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	1	0.41
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	5	0.41
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	1	0.41
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	1	0.41
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	5	0.4
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	2	0.4
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	5	0.4
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	9	0.4
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	7	0.39
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	8	0.39
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	4	0.39
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	1	0.39
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	10	0.39
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	7	0.38
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	9	0.37
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	2	0.37
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	8	0.37
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	4	0.37
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	10	0.37
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	10	0.37
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	10	0.37
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	10	0.37
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	10	0.37
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	10	0.37
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	10	0.36
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	2	0.36
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	8	0.36
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	8	0.36
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	8	0.36
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	8	0.36
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	8	0.36
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	8	0.36
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	10	0.35
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	5	0.35
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	1	0.35
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	5	0.35
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	4	0.34
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	7	0.34
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	2	0.34
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	4	0.34
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	7	0.34
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	7	0.34
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	7	0.34
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	7	0.34
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	7	0.34
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	7	0.34
(1,8)	2:900:B:FMN:O4'	1:66:B:GLN:NE2	4	0.34
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	2	0.33
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	6	0.33
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	4	0.33
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	8	0.33
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	9	0.32
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	9	0.32
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	10	0.32
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	1	0.32
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	4	0.32
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	4	0.32
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	4	0.32
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	4	0.32
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	4	0.32
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	4	0.32
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	4	0.31
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	3	0.31
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	10	0.31
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	1	0.31
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	5	0.31
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	10	0.31
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	10	0.31
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	10	0.31
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	10	0.31
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	5	0.31
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	6	0.31
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	9	0.31
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	10	0.31
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	3	0.3
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	5	0.3
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	2	0.3
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	9	0.3
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	8	0.3
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	8	0.3
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	8	0.3
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	7	0.3
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	8	0.3
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	5	0.3
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	9	0.3
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	9	0.3
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	4	0.3
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	7	0.29
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	4	0.29
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	1	0.29
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	1	0.29
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	1	0.29
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	1	0.29
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	2	0.29
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	8	0.29
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	1	0.29
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	2	0.29
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	3	0.29
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	6	0.29
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	10	0.29
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	2	0.29
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	2	0.29
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	1	0.28
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	8	0.28
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	7	0.28
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	8	0.28
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	2	0.28
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	2	0.28
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	2	0.28
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	7	0.28
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	7	0.28
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	7	0.28
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	4	0.28
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	3	0.28
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	4	0.28
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	4	0.28
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	6	0.28
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	4	0.28
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	7	0.28
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	1	0.28
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	1	0.28
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	1	0.28
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	1	0.28
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	1	0.28
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	1	0.28
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	7	0.28
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	7	0.28
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	7	0.28
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	7	0.28
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	7	0.28
(2,383)	1:166:A:LEU:H	1:199:A:GLN:H	4	0.28
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	3	0.27
(2,1076)	1:206:B:ASP:H	1:208:B:ILE:H	6	0.27
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	9	0.27
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	9	0.27
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	9	0.27
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	8	0.27
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	8	0.27
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	8	0.27
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	9	0.27
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	9	0.27
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	9	0.27
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	1	0.27
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	3	0.27
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	7	0.27
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	2	0.27
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	5	0.27
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	6	0.27
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	1	0.27
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	3	0.27
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	5	0.27
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	4	0.27
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	4	0.27
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	7	0.27
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	7	0.27
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	9	0.27
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	9	0.27
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	9	0.27
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	9	0.27
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	9	0.27
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	9	0.27
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	4	0.27
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	4	0.27
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	4	0.27
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	4	0.27
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	4	0.27
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	4	0.27
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	10	0.27
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	10	0.27
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	10	0.27
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	10	0.27
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	10	0.27
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	2	0.26
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	2	0.26
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	2	0.26
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	3	0.26
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	3	0.26
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	3	0.26
(2,930)	1:150:B:ILE:H	1:151:B:VAL:H	10	0.26
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	3	0.26
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	10	0.26
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	3	0.26
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	5	0.26
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	8	0.26
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	2	0.26
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	2	0.26
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	2	0.26
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	1	0.26
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	1	0.26
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	1	0.26
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	1	0.26
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	1	0.26
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	1	0.26
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	6	0.26
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	6	0.26
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	6	0.26
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	6	0.26
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	6	0.26
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	6	0.26
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	8	0.26
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	8	0.26
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	8	0.26
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	8	0.26
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	8	0.26
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	8	0.26
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	4	0.26
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	4	0.26
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	4	0.26
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	7	0.26
(2,384)	1:166:A:LEU:H	1:201:A:ASN:H	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	2	0.25
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	5	0.25
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	3	0.25
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	3	0.25
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	3	0.25
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	1	0.25
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	8	0.25
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	6	0.25
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	6	0.25
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	10	0.25
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	10	0.25
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	2	0.25
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	2	0.25
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	2	0.25
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	2	0.25
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	2	0.25
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	2	0.25
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	5	0.25
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	5	0.25
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	5	0.25
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	5	0.25
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	5	0.25
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	5	0.25
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	1	0.25
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	1	0.25
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	1	0.25
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	2	0.25
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	2	0.25
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	2	0.25
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	2	0.25
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	2	0.25
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	2	0.25
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	9	0.25
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	9	0.25
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	9	0.25
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	9	0.25
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	9	0.25
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	9	0.25
(2,186)	1:82:A:LEU:HD11	1:86:A:GLU:H	8	0.25
(2,186)	1:82:A:LEU:HD12	1:86:A:GLU:H	8	0.25
(2,186)	1:82:A:LEU:HD13	1:86:A:GLU:H	8	0.25
(2,186)	1:82:A:LEU:HD21	1:86:A:GLU:H	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,186)	1:82:A:LEU:HD22	1:86:A:GLU:H	8	0.25
(2,186)	1:82:A:LEU:HD23	1:86:A:GLU:H	8	0.25
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	7	0.25
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	7	0.24
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	3	0.24
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	8	0.24
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	5	0.24
(2,856)	1:113:B:ILE:H	1:115:B:ASP:H	8	0.24
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	7	0.24
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	10	0.24
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	9	0.24
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	8	0.24
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	8	0.24
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	8	0.24
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	3	0.24
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	3	0.24
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	3	0.24
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	3	0.24
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	3	0.24
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	3	0.24
(2,715)	1:65:B:LEU:HD11	1:66:B:GLN:H	5	0.24
(2,715)	1:65:B:LEU:HD12	1:66:B:GLN:H	5	0.24
(2,715)	1:65:B:LEU:HD13	1:66:B:GLN:H	5	0.24
(2,715)	1:65:B:LEU:HD21	1:66:B:GLN:H	5	0.24
(2,715)	1:65:B:LEU:HD22	1:66:B:GLN:H	5	0.24
(2,715)	1:65:B:LEU:HD23	1:66:B:GLN:H	5	0.24
(2,695)	1:56:B:GLU:H	1:58:B:LEU:H	8	0.24
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	3	0.24
(2,1111)	1:224:B:ILE:H	1:246:B:LYS:H	8	0.23
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	9	0.23
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	10	0.23
(2,1064)	1:201:B:ASN:H	1:205:B:ALA:H	8	0.23
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	7	0.23
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	7	0.23
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	7	0.23
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	4	0.23
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	1	0.23
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	6	0.23
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	2	0.23
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	1	0.23
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	1	0.23
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	8	0.23
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	2	0.23
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	4	0.23
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	6	0.23
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	6	0.23
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	6	0.23
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	6	0.23
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	6	0.23
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	6	0.23
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	6	0.23
(2,695)	1:56:B:GLU:H	1:58:B:LEU:H	5	0.23
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	6	0.23
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	6	0.23
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	6	0.23
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	1	0.23
(2,383)	1:166:A:LEU:H	1:199:A:GLN:H	7	0.23
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	8	0.22
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	2	0.22
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	4	0.22
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	8	0.22
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	9	0.22
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	5	0.22
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	5	0.22
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	5	0.22
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	4	0.22
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	4	0.22
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	4	0.22
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	3	0.22
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	7	0.22
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	9	0.22
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	2	0.22
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	2	0.22
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	2	0.22
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	2	0.22
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	2	0.22
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	2	0.22
(2,793)	1:88:B:VAL:HG11	1:89:B:THR:H	3	0.22
(2,793)	1:88:B:VAL:HG12	1:89:B:THR:H	3	0.22
(2,793)	1:88:B:VAL:HG13	1:89:B:THR:H	3	0.22
(2,793)	1:88:B:VAL:HG21	1:89:B:THR:H	3	0.22
(2,793)	1:88:B:VAL:HG22	1:89:B:THR:H	3	0.22
(2,793)	1:88:B:VAL:HG23	1:89:B:THR:H	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	6	0.22
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	6	0.22
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	6	0.22
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	6	0.22
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	6	0.22
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	6	0.22
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	6	0.22
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	6	0.22
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	6	0.22
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	7	0.22
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	7	0.22
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	7	0.22
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	7	0.22
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	7	0.22
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	7	0.22
(2,695)	1:56:B:GLU:H	1:58:B:LEU:H	9	0.22
(2,692)	1:55:B:GLU:H	1:58:B:LEU:H	9	0.22
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	5	0.22
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	5	0.22
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	5	0.22
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	2	0.22
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	10	0.22
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	10	0.22
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	10	0.22
(2,384)	1:166:A:LEU:H	1:201:A:ASN:H	2	0.22
(2,383)	1:166:A:LEU:H	1:199:A:GLN:H	3	0.22
(1,8)	2:900:B:FMN:O4'	1:66:B:GLN:NE2	7	0.22
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	1	0.21
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	3	0.21
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	6	0.21
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	10	0.21
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	6	0.21
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	6	0.21
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	6	0.21
(2,969)	1:164:B:GLY:H	1:197:B:LEU:H	9	0.21
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	3	0.21
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	2	0.21
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	4	0.21
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	5	0.21
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	8	0.21
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	9	0.21
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	6	0.21
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	3	0.21
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	3	0.21
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	3	0.21
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	3	0.21
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	3	0.21
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	3	0.21
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	4	0.21
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	4	0.21
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	4	0.21
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	4	0.21
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	4	0.21
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	4	0.21
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	9	0.21
(2,383)	1:166:A:LEU:H	1:199:A:GLN:H	1	0.21
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	7	0.21
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD11	5	0.21
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD12	5	0.21
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD13	5	0.21
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD21	5	0.21
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD22	5	0.21
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD23	5	0.21
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	6	0.21
(2,1161)	1:249:B:SER:H	1:250:B:ASN:H	5	0.2
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	6	0.2
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	6	0.2
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	6	0.2
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	6	0.2
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	9	0.2
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	10	0.2
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	1	0.2
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	1	0.2
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	5	0.2
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	1	0.2
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	1	0.2
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	1	0.2
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	1	0.2
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	1	0.2
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	1	0.2
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	10	0.2
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	10	0.2
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	10	0.2
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	10	0.2
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	10	0.2
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	4	0.2
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	4	0.2
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	4	0.2
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	4	0.2
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	4	0.2
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	4	0.2
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	10	0.2
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	10	0.2
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	10	0.2
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	10	0.2
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	10	0.2
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	10	0.2
(2,778)	1:82:B:LEU:HD11	1:86:B:GLU:H	8	0.2
(2,778)	1:82:B:LEU:HD12	1:86:B:GLU:H	8	0.2
(2,778)	1:82:B:LEU:HD13	1:86:B:GLU:H	8	0.2
(2,778)	1:82:B:LEU:HD21	1:86:B:GLU:H	8	0.2
(2,778)	1:82:B:LEU:HD22	1:86:B:GLU:H	8	0.2
(2,778)	1:82:B:LEU:HD23	1:86:B:GLU:H	8	0.2
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	4	0.2
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	4	0.2
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	4	0.2
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	4	0.2
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	4	0.2
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	4	0.2
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	4	0.2
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	4	0.2
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	4	0.2
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	8	0.2
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	4	0.2
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	8	0.2
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	8	0.2
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	8	0.2
(2,384)	1:166:A:LEU:H	1:201:A:ASN:H	8	0.2
(2,381)	1:165:A:ASN:H	1:198:A:ALA:H	4	0.2
(2,242)	1:103:A:TRP:H	1:127:A:THR:H	6	0.2
(2,223)	1:93:A:GLN:HE21	1:103:A:TRP:HE1	2	0.2
(2,223)	1:93:A:GLN:HE22	1:103:A:TRP:HE1	2	0.2
(2,223)	1:93:A:GLN:HE21	1:103:A:TRP:HE1	4	0.2
(2,223)	1:93:A:GLN:HE22	1:103:A:TRP:HE1	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,203)	1:88:A:VAL:HG11	1:108:A:ILE:H	10	0.2
(2,203)	1:88:A:VAL:HG12	1:108:A:ILE:H	10	0.2
(2,203)	1:88:A:VAL:HG13	1:108:A:ILE:H	10	0.2
(2,203)	1:88:A:VAL:HG21	1:108:A:ILE:H	10	0.2
(2,203)	1:88:A:VAL:HG22	1:108:A:ILE:H	10	0.2
(2,203)	1:88:A:VAL:HG23	1:108:A:ILE:H	10	0.2
(2,130)	1:67:A:GLY:H	1:95:A:TYR:H	2	0.2
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	4	0.2
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	8	0.2
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	2	0.19
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	8	0.19
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	4	0.19
(2,1083)	1:208:B:ILE:H	1:209:B:PHE:H	7	0.19
(2,1064)	1:201:B:ASN:H	1:205:B:ALA:H	2	0.19
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	5	0.19
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	5	0.19
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	5	0.19
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	8	0.19
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	7	0.19
(2,890)	1:130:B:LYS:H	1:131:B:GLU:H	10	0.19
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	3	0.19
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	8	0.19
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	2	0.19
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	4	0.19
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	6	0.19
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	1	0.19
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	3	0.19
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	4	0.19
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	9	0.19
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	9	0.19
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	9	0.19
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	9	0.19
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	9	0.19
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	9	0.19
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	9	0.19
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	9	0.19
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	9	0.19
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	9	0.19
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	9	0.19
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	9	0.19
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	9	0.19
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	3	0.19
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	3	0.19
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	4	0.19
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	4	0.19
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	4	0.19
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	4	0.19
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	5	0.19
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	7	0.19
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	1	0.19
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	1	0.19
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	1	0.19
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	9	0.19
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	9	0.19
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	9	0.19
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG11	7	0.19
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG12	7	0.19
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG13	7	0.19
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG21	7	0.19
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG22	7	0.19
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG23	7	0.19
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG11	7	0.19
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG12	7	0.19
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG13	7	0.19
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG21	7	0.19
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG22	7	0.19
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG23	7	0.19
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG11	7	0.19
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG12	7	0.19
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG13	7	0.19
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG21	7	0.19
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG22	7	0.19
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG23	7	0.19
(2,521)	1:224:A:ILE:H	1:248:A:TYR:H	2	0.19
(2,521)	1:224:A:ILE:H	1:248:A:TYR:H	6	0.19
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	2	0.19
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	2	0.19
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	2	0.19
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	9	0.19
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	9	0.19
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	9	0.19
(2,383)	1:166:A:LEU:H	1:199:A:GLN:H	6	0.19
(2,186)	1:82:A:LEU:HD11	1:86:A:GLU:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,186)	1:82:A:LEU:HD12	1:86:A:GLU:H	6	0.19
(2,186)	1:82:A:LEU:HD13	1:86:A:GLU:H	6	0.19
(2,186)	1:82:A:LEU:HD21	1:86:A:GLU:H	6	0.19
(2,186)	1:82:A:LEU:HD22	1:86:A:GLU:H	6	0.19
(2,186)	1:82:A:LEU:HD23	1:86:A:GLU:H	6	0.19
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	9	0.18
(2,1111)	1:224:B:ILE:H	1:246:B:LYS:H	2	0.18
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	3	0.18
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	6	0.18
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	1	0.18
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	1	0.18
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	1	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	1	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	3	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	4	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	5	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	6	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	7	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	9	0.18
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	10	0.18
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	2	0.18
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	3	0.18
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	9	0.18
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	5	0.18
(2,973)	1:165:B:ASN:H	1:198:B:ALA:H	4	0.18
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	3	0.18
(2,881)	1:126:B:ILE:HD11	1:130:B:LYS:H	5	0.18
(2,881)	1:126:B:ILE:HD12	1:130:B:LYS:H	5	0.18
(2,881)	1:126:B:ILE:HD13	1:130:B:LYS:H	5	0.18
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	6	0.18
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	1	0.18
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	8	0.18
(2,810)	1:92:B:ILE:H	1:104:B:ASN:H	7	0.18
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	8	0.18
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	10	0.18
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	5	0.18
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	5	0.18
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	5	0.18
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	5	0.18
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	5	0.18
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	5	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	1	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	1	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	1	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	1	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	1	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	1	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	1	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	1	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	2	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	2	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	2	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	2	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	2	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	2	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	2	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	2	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	2	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	3	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	3	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	3	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	3	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	3	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	3	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	3	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	3	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	3	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	7	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	7	0.18
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	7	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	7	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	7	0.18
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	7	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	7	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	7	0.18
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	7	0.18
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	6	0.18
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	7	0.18
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	7	0.18
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	7	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	3	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	3	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	3	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	3	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	3	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	6	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	6	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	6	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	6	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	6	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	6	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	8	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	8	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	8	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	8	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	8	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	8	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	9	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	9	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	9	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	9	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	9	0.18
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	9	0.18
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	2	0.18
(2,697)	1:57:B:ILE:H	1:58:B:LEU:H	2	0.18
(2,692)	1:55:B:GLU:H	1:58:B:LEU:H	5	0.18
(2,692)	1:55:B:GLU:H	1:58:B:LEU:H	8	0.18
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	2	0.18
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	2	0.18
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	2	0.18
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	3	0.18
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	3	0.18
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	3	0.18
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	6	0.18
(2,521)	1:224:A:ILE:H	1:248:A:TYR:H	1	0.18
(2,521)	1:224:A:ILE:H	1:248:A:TYR:H	7	0.18
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	1	0.18
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	1	0.18
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	1	0.18
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	3	0.18
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	3	0.18
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	3	0.18
(2,445)	1:191:A:ILE:HD11	1:223:A:ILE:H	7	0.18
(2,445)	1:191:A:ILE:HD12	1:223:A:ILE:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,445)	1:191:A:ILE:HD13	1:223:A:ILE:H	7	0.18
(2,445)	1:191:A:ILE:HD11	1:223:A:ILE:H	9	0.18
(2,445)	1:191:A:ILE:HD12	1:223:A:ILE:H	9	0.18
(2,445)	1:191:A:ILE:HD13	1:223:A:ILE:H	9	0.18
(2,248)	1:105:A:GLU:H	1:126:A:ILE:H	4	0.18
(2,223)	1:93:A:GLN:HE21	1:103:A:TRP:HE1	6	0.18
(2,223)	1:93:A:GLN:HE22	1:103:A:TRP:HE1	6	0.18
(2,223)	1:93:A:GLN:HE21	1:103:A:TRP:HE1	7	0.18
(2,223)	1:93:A:GLN:HE22	1:103:A:TRP:HE1	7	0.18
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	5	0.18
(2,203)	1:88:A:VAL:HG11	1:108:A:ILE:H	7	0.18
(2,203)	1:88:A:VAL:HG12	1:108:A:ILE:H	7	0.18
(2,203)	1:88:A:VAL:HG13	1:108:A:ILE:H	7	0.18
(2,203)	1:88:A:VAL:HG21	1:108:A:ILE:H	7	0.18
(2,203)	1:88:A:VAL:HG22	1:108:A:ILE:H	7	0.18
(2,203)	1:88:A:VAL:HG23	1:108:A:ILE:H	7	0.18
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	3	0.17
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	5	0.17
(2,1037)	1:191:B:ILE:HD11	1:223:B:ILE:H	10	0.17
(2,1037)	1:191:B:ILE:HD12	1:223:B:ILE:H	10	0.17
(2,1037)	1:191:B:ILE:HD13	1:223:B:ILE:H	10	0.17
(2,1011)	1:177:B:THR:H	1:178:B:LEU:H	2	0.17
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	5	0.17
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	10	0.17
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	1	0.17
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	6	0.17
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	8	0.17
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	9	0.17
(2,975)	1:166:B:LEU:H	1:199:B:GLN:H	4	0.17
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	10	0.17
(2,962)	1:162:B:LEU:H	1:193:B:ASP:H	5	0.17
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	3	0.17
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	8	0.17
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	10	0.17
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	5	0.17
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	8	0.17
(2,881)	1:126:B:ILE:HD11	1:130:B:LYS:H	3	0.17
(2,881)	1:126:B:ILE:HD12	1:130:B:LYS:H	3	0.17
(2,881)	1:126:B:ILE:HD13	1:130:B:LYS:H	3	0.17
(2,857)	1:113:B:ILE:H	1:116:B:LYS:H	10	0.17
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	5	0.17
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	10	0.17
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	5	0.17
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	2	0.17
(2,809)	1:92:B:ILE:H	1:93:B:GLN:H	7	0.17
(2,795)	1:88:B:VAL:HG11	1:108:B:ILE:H	6	0.17
(2,795)	1:88:B:VAL:HG12	1:108:B:ILE:H	6	0.17
(2,795)	1:88:B:VAL:HG13	1:108:B:ILE:H	6	0.17
(2,795)	1:88:B:VAL:HG21	1:108:B:ILE:H	6	0.17
(2,795)	1:88:B:VAL:HG22	1:108:B:ILE:H	6	0.17
(2,795)	1:88:B:VAL:HG23	1:108:B:ILE:H	6	0.17
(2,793)	1:88:B:VAL:HG11	1:89:B:THR:H	1	0.17
(2,793)	1:88:B:VAL:HG12	1:89:B:THR:H	1	0.17
(2,793)	1:88:B:VAL:HG13	1:89:B:THR:H	1	0.17
(2,793)	1:88:B:VAL:HG21	1:89:B:THR:H	1	0.17
(2,793)	1:88:B:VAL:HG22	1:89:B:THR:H	1	0.17
(2,793)	1:88:B:VAL:HG23	1:89:B:THR:H	1	0.17
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	7	0.17
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	5	0.17
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	5	0.17
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	5	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	1	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	1	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	1	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	1	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	1	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	1	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	2	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	2	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	2	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	2	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	2	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	2	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	5	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	5	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	5	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	5	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	5	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	5	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD11	10	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD12	10	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD13	10	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD21	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD22	10	0.17
(2,713)	1:65:B:LEU:H	1:65:B:LEU:HD23	10	0.17
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	1	0.17
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	5	0.17
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	10	0.17
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	8	0.17
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	9	0.17
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG11	3	0.17
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG12	3	0.17
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG13	3	0.17
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG21	3	0.17
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG22	3	0.17
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG23	3	0.17
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG11	3	0.17
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG12	3	0.17
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG13	3	0.17
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG21	3	0.17
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG22	3	0.17
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG23	3	0.17
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG11	3	0.17
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG12	3	0.17
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG13	3	0.17
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG21	3	0.17
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG22	3	0.17
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG23	3	0.17
(2,615)	1:28:B:VAL:HG11	1:30:B:THR:H	4	0.17
(2,615)	1:28:B:VAL:HG12	1:30:B:THR:H	4	0.17
(2,615)	1:28:B:VAL:HG13	1:30:B:THR:H	4	0.17
(2,615)	1:28:B:VAL:HG21	1:30:B:THR:H	4	0.17
(2,615)	1:28:B:VAL:HG22	1:30:B:THR:H	4	0.17
(2,615)	1:28:B:VAL:HG23	1:30:B:THR:H	4	0.17
(2,261)	1:112:A:GLU:H	1:113:A:ILE:H	9	0.17
(2,261)	1:112:A:GLU:H	1:113:A:ILE:H	10	0.17
(2,234)	1:97:A:LYS:H	1:100:A:THR:H	1	0.17
(2,223)	1:93:A:GLN:HE21	1:103:A:TRP:HE1	1	0.17
(2,223)	1:93:A:GLN:HE22	1:103:A:TRP:HE1	1	0.17
(2,223)	1:93:A:GLN:HE21	1:103:A:TRP:HE1	10	0.17
(2,223)	1:93:A:GLN:HE22	1:103:A:TRP:HE1	10	0.17
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	2	0.17
(2,212)	1:90:A:VAL:HG11	1:106:A:LEU:H	10	0.17
(2,212)	1:90:A:VAL:HG12	1:106:A:LEU:H	10	0.17
(2,212)	1:90:A:VAL:HG13	1:106:A:LEU:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,212)	1:90:A:VAL:HG21	1:106:A:LEU:H	10	0.17
(2,212)	1:90:A:VAL:HG22	1:106:A:LEU:H	10	0.17
(2,212)	1:90:A:VAL:HG23	1:106:A:LEU:H	10	0.17
(2,203)	1:88:A:VAL:HG11	1:108:A:ILE:H	8	0.17
(2,203)	1:88:A:VAL:HG12	1:108:A:ILE:H	8	0.17
(2,203)	1:88:A:VAL:HG13	1:108:A:ILE:H	8	0.17
(2,203)	1:88:A:VAL:HG21	1:108:A:ILE:H	8	0.17
(2,203)	1:88:A:VAL:HG22	1:108:A:ILE:H	8	0.17
(2,203)	1:88:A:VAL:HG23	1:108:A:ILE:H	8	0.17
(2,130)	1:67:A:GLY:H	1:95:A:TYR:H	8	0.17
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	7	0.17
(1,8)	2:900:B:FMN:O4'	1:66:B:GLN:NE2	1	0.17
(1,8)	2:900:B:FMN:O4'	1:66:B:GLN:NE2	6	0.17
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	2	0.17
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	9	0.17
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	1	0.16
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	5	0.16
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	7	0.16
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	10	0.16
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	1	0.16
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	2	0.16
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	7	0.16
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	9	0.16
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	10	0.16
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	7	0.16
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	2	0.16
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	4	0.16
(2,973)	1:165:B:ASN:H	1:198:B:ALA:H	6	0.16
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	7	0.16
(2,962)	1:162:B:LEU:H	1:193:B:ASP:H	4	0.16
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	5	0.16
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	7	0.16
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	9	0.16
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	8	0.16
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	8	0.16
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	8	0.16
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	9	0.16
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	9	0.16
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	9	0.16
(2,925)	1:147:B:SER:HG	1:148:B:THR:H	3	0.16
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	4	0.16
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	4	0.16
(2,855)	1:113:B:ILE:H	1:114:B:GLU:H	3	0.16
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	3	0.16
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	3	0.16
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	3	0.16
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	3	0.16
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	3	0.16
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	3	0.16
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	3	0.16
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	3	0.16
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	7	0.16
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	7	0.16
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	7	0.16
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	7	0.16
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	7	0.16
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	7	0.16
(2,793)	1:88:B:VAL:HG11	1:89:B:THR:H	7	0.16
(2,793)	1:88:B:VAL:HG12	1:89:B:THR:H	7	0.16
(2,793)	1:88:B:VAL:HG13	1:89:B:THR:H	7	0.16
(2,793)	1:88:B:VAL:HG21	1:89:B:THR:H	7	0.16
(2,793)	1:88:B:VAL:HG22	1:89:B:THR:H	7	0.16
(2,793)	1:88:B:VAL:HG23	1:89:B:THR:H	7	0.16
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	1	0.16
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	1	0.16
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	1	0.16
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	1	0.16
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	1	0.16
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	1	0.16
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	6	0.16
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	6	0.16
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	6	0.16
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	6	0.16
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	6	0.16
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	6	0.16
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	7	0.16
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	7	0.16
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	7	0.16
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	7	0.16
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	7	0.16
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	7	0.16
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	5	0.16
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	5	0.16
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	5	0.16
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	5	0.16
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	5	0.16
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	5	0.16
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	5	0.16
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	5	0.16
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	3	0.16
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	4	0.16
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	9	0.16
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	1	0.16
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	6	0.16
(2,695)	1:56:B:GLU:H	1:58:B:LEU:H	6	0.16
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	2	0.16
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	3	0.16
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	6	0.16
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	7	0.16
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	8	0.16
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	9	0.16
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	10	0.16
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	10	0.16
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	10	0.16
(2,642)	1:39:B:ILE:H	1:59:B:GLY:H	5	0.16
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	6	0.16
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG11	2	0.16
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG12	2	0.16
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG13	2	0.16
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG21	2	0.16
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG22	2	0.16
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG23	2	0.16
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG11	2	0.16
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG12	2	0.16
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG13	2	0.16
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG21	2	0.16
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG22	2	0.16
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG23	2	0.16
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG11	2	0.16
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG12	2	0.16
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG13	2	0.16
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG21	2	0.16
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG22	2	0.16
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG23	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	5	0.16
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	5	0.16
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	5	0.16
(2,381)	1:165:A:ASN:H	1:198:A:ALA:H	6	0.16
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	1	0.16
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	6	0.16
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	10	0.16
(2,341)	1:150:A:ILE:HD11	1:159:A:ALA:H	8	0.16
(2,341)	1:150:A:ILE:HD12	1:159:A:ALA:H	8	0.16
(2,341)	1:150:A:ILE:HD13	1:159:A:ALA:H	8	0.16
(2,246)	1:105:A:GLU:H	1:124:A:ASN:H	8	0.16
(2,241)	1:103:A:TRP:H	1:126:A:ILE:H	6	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD11	2	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD12	2	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD13	2	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD21	2	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD22	2	0.16
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD23	2	0.16
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	1	0.16
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	8	0.16
(2,203)	1:88:A:VAL:HG11	1:108:A:ILE:H	4	0.16
(2,203)	1:88:A:VAL:HG12	1:108:A:ILE:H	4	0.16
(2,203)	1:88:A:VAL:HG13	1:108:A:ILE:H	4	0.16
(2,203)	1:88:A:VAL:HG21	1:108:A:ILE:H	4	0.16
(2,203)	1:88:A:VAL:HG22	1:108:A:ILE:H	4	0.16
(2,203)	1:88:A:VAL:HG23	1:108:A:ILE:H	4	0.16
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD11	4	0.16
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD12	4	0.16
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD13	4	0.16
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD11	4	0.16
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD12	4	0.16
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD13	4	0.16
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD11	4	0.16
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD12	4	0.16
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD13	4	0.16
(2,130)	1:67:A:GLY:H	1:95:A:TYR:H	10	0.16
(2,109)	1:59:A:GLY:H	1:60:A:LYS:H	3	0.16
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	6	0.16
(2,50)	1:39:A:ILE:H	1:59:A:GLY:H	7	0.16
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG11	7	0.16
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG12	7	0.16
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG13	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG21	7	0.16
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG22	7	0.16
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG23	7	0.16
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG11	7	0.16
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG12	7	0.16
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG13	7	0.16
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG21	7	0.16
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG22	7	0.16
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG23	7	0.16
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG11	7	0.16
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG12	7	0.16
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG13	7	0.16
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG21	7	0.16
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG22	7	0.16
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG23	7	0.16
(2,4)	1:4:A:PHE:H	1:5:A:GLN:H	6	0.16
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	2	0.15
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	5	0.15
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	4	0.15
(2,1095)	1:212:B:SER:H	1:213:B:HIS:H	8	0.15
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	6	0.15
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	6	0.15
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	6	0.15
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	7	0.15
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	7	0.15
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	7	0.15
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	10	0.15
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	10	0.15
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	10	0.15
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	1	0.15
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	8	0.15
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	10	0.15
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	1	0.15
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	2	0.15
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	6	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	2	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	2	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	2	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	3	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	3	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	3	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	4	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	4	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	7	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	7	0.15
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	7	0.15
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD11	9	0.15
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD12	9	0.15
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD13	9	0.15
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	2	0.15
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	7	0.15
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	2	0.15
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	6	0.15
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	7	0.15
(2,881)	1:126:B:ILE:HD11	1:130:B:LYS:H	8	0.15
(2,881)	1:126:B:ILE:HD12	1:130:B:LYS:H	8	0.15
(2,881)	1:126:B:ILE:HD13	1:130:B:LYS:H	8	0.15
(2,793)	1:88:B:VAL:HG11	1:89:B:THR:H	2	0.15
(2,793)	1:88:B:VAL:HG12	1:89:B:THR:H	2	0.15
(2,793)	1:88:B:VAL:HG13	1:89:B:THR:H	2	0.15
(2,793)	1:88:B:VAL:HG21	1:89:B:THR:H	2	0.15
(2,793)	1:88:B:VAL:HG22	1:89:B:THR:H	2	0.15
(2,793)	1:88:B:VAL:HG23	1:89:B:THR:H	2	0.15
(2,793)	1:88:B:VAL:HG11	1:89:B:THR:H	4	0.15
(2,793)	1:88:B:VAL:HG12	1:89:B:THR:H	4	0.15
(2,793)	1:88:B:VAL:HG13	1:89:B:THR:H	4	0.15
(2,793)	1:88:B:VAL:HG21	1:89:B:THR:H	4	0.15
(2,793)	1:88:B:VAL:HG22	1:89:B:THR:H	4	0.15
(2,793)	1:88:B:VAL:HG23	1:89:B:THR:H	4	0.15
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	8	0.15
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	8	0.15
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	8	0.15
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	8	0.15
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	8	0.15
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	8	0.15
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	8	0.15
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	8	0.15
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	8	0.15
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	2	0.15
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	5	0.15
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	8	0.15
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	10	0.15
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	6	0.15
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	6	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD11	8	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD12	8	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD13	8	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD11	9	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD12	9	0.15
(2,685)	1:53:B:GLU:H	1:57:B:ILE:HD13	9	0.15
(2,661)	1:46:B:PHE:H	1:47:B:VAL:H	4	0.15
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	2	0.15
(2,521)	1:224:A:ILE:H	1:248:A:TYR:H	8	0.15
(2,445)	1:191:A:ILE:HD11	1:223:A:ILE:H	3	0.15
(2,445)	1:191:A:ILE:HD12	1:223:A:ILE:H	3	0.15
(2,445)	1:191:A:ILE:HD13	1:223:A:ILE:H	3	0.15
(2,341)	1:150:A:ILE:HD11	1:159:A:ALA:H	1	0.15
(2,341)	1:150:A:ILE:HD12	1:159:A:ALA:H	1	0.15
(2,341)	1:150:A:ILE:HD13	1:159:A:ALA:H	1	0.15
(2,261)	1:112:A:GLU:H	1:113:A:ILE:H	1	0.15
(2,261)	1:112:A:GLU:H	1:113:A:ILE:H	3	0.15
(2,261)	1:112:A:GLU:H	1:113:A:ILE:H	6	0.15
(2,248)	1:105:A:GLU:H	1:126:A:ILE:H	10	0.15
(2,234)	1:97:A:LYS:H	1:100:A:THR:H	8	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD11	1	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD12	1	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD13	1	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD21	1	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD22	1	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD23	1	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD11	9	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD12	9	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD13	9	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD21	9	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD22	9	0.15
(2,220)	1:92:A:ILE:H	1:106:A:LEU:HD23	9	0.15
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD11	1	0.15
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD12	1	0.15
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD13	1	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD11	1	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD12	1	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD13	1	0.15
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD11	1	0.15
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD12	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD13	1	0.15
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD11	6	0.15
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD12	6	0.15
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD13	6	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD11	6	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD12	6	0.15
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD13	6	0.15
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD11	6	0.15
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD12	6	0.15
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD13	6	0.15
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	9	0.15
(2,10)	1:25:A:VAL:HG11	1:26:A:GLY:H	10	0.15
(2,10)	1:25:A:VAL:HG12	1:26:A:GLY:H	10	0.15
(2,10)	1:25:A:VAL:HG13	1:26:A:GLY:H	10	0.15
(2,10)	1:25:A:VAL:HG21	1:26:A:GLY:H	10	0.15
(2,10)	1:25:A:VAL:HG22	1:26:A:GLY:H	10	0.15
(2,10)	1:25:A:VAL:HG23	1:26:A:GLY:H	10	0.15
(1,8)	2:900:B:FMN:O4'	1:66:B:GLN:NE2	8	0.15
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	1	0.15
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	10	0.15
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	5	0.14
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	7	0.14
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	3	0.14
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	4	0.14
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	4	0.14
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	6	0.14
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	9	0.14
(2,1118)	1:226:B:GLY:H	1:248:B:TYR:H	2	0.14
(2,1060)	1:200:B:VAL:HG11	1:205:B:ALA:H	8	0.14
(2,1060)	1:200:B:VAL:HG12	1:205:B:ALA:H	8	0.14
(2,1060)	1:200:B:VAL:HG13	1:205:B:ALA:H	8	0.14
(2,1060)	1:200:B:VAL:HG21	1:205:B:ALA:H	8	0.14
(2,1060)	1:200:B:VAL:HG22	1:205:B:ALA:H	8	0.14
(2,1060)	1:200:B:VAL:HG23	1:205:B:ALA:H	8	0.14
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	2	0.14
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	2	0.14
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	2	0.14
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	9	0.14
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	9	0.14
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	9	0.14
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD11	1	0.14
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD12	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD13	1	0.14
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD21	1	0.14
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD22	1	0.14
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD23	1	0.14
(2,953)	1:157:B:ILE:H	1:158:B:SER:H	4	0.14
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	6	0.14
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	6	0.14
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	6	0.14
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	10	0.14
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	10	0.14
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	10	0.14
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD11	5	0.14
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD12	5	0.14
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD13	5	0.14
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	7	0.14
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	7	0.14
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	7	0.14
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	7	0.14
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	7	0.14
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	7	0.14
(2,918)	1:145:B:ALA:H	1:147:B:SER:H	1	0.14
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	9	0.14
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	9	0.14
(2,820)	1:96:B:LYS:H	1:98:B:ASP:H	4	0.14
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	8	0.14
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	8	0.14
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	8	0.14
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	8	0.14
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	8	0.14
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	8	0.14
(2,741)	1:75:B:VAL:H	1:78:B:ILE:H	1	0.14
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	3	0.14
(2,695)	1:56:B:GLU:H	1:58:B:LEU:H	10	0.14
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	7	0.14
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	7	0.14
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	7	0.14
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	3	0.14
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	5	0.14
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	7	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG11	1	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG12	1	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG13	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG21	1	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG22	1	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG23	1	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG11	1	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG12	1	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG13	1	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG21	1	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG22	1	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG23	1	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG11	1	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG12	1	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG13	1	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG21	1	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG22	1	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG23	1	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG11	10	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG12	10	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG13	10	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG21	10	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG22	10	0.14
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG23	10	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG11	10	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG12	10	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG13	10	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG21	10	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG22	10	0.14
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG23	10	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG11	10	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG12	10	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG13	10	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG21	10	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG22	10	0.14
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG23	10	0.14
(2,596)	1:4:B:PHE:H	1:5:B:GLN:H	1	0.14
(2,596)	1:4:B:PHE:H	1:5:B:GLN:H	6	0.14
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	2	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD11	2	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD12	2	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD13	2	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD21	2	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD22	2	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD23	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD11	4	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD12	4	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD13	4	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD21	4	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD22	4	0.14
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD23	4	0.14
(2,445)	1:191:A:ILE:HD11	1:223:A:ILE:H	2	0.14
(2,445)	1:191:A:ILE:HD12	1:223:A:ILE:H	2	0.14
(2,445)	1:191:A:ILE:HD13	1:223:A:ILE:H	2	0.14
(2,445)	1:191:A:ILE:HD11	1:223:A:ILE:H	8	0.14
(2,445)	1:191:A:ILE:HD12	1:223:A:ILE:H	8	0.14
(2,445)	1:191:A:ILE:HD13	1:223:A:ILE:H	8	0.14
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD11	1	0.14
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD12	1	0.14
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD13	1	0.14
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD21	1	0.14
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD22	1	0.14
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD23	1	0.14
(2,383)	1:166:A:LEU:H	1:199:A:GLN:H	2	0.14
(2,381)	1:165:A:ASN:H	1:198:A:ALA:H	1	0.14
(2,381)	1:165:A:ASN:H	1:198:A:ALA:H	7	0.14
(2,379)	1:165:A:ASN:H	1:167:A:THR:H	2	0.14
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	4	0.14
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	9	0.14
(2,261)	1:112:A:GLU:H	1:113:A:ILE:H	8	0.14
(2,246)	1:105:A:GLU:H	1:124:A:ASN:H	2	0.14
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	3	0.14
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	7	0.14
(2,191)	1:83:A:GLN:H	1:85:A:LYS:H	4	0.14
(2,186)	1:82:A:LEU:HD11	1:86:A:GLU:H	1	0.14
(2,186)	1:82:A:LEU:HD12	1:86:A:GLU:H	1	0.14
(2,186)	1:82:A:LEU:HD13	1:86:A:GLU:H	1	0.14
(2,186)	1:82:A:LEU:HD21	1:86:A:GLU:H	1	0.14
(2,186)	1:82:A:LEU:HD22	1:86:A:GLU:H	1	0.14
(2,186)	1:82:A:LEU:HD23	1:86:A:GLU:H	1	0.14
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	3	0.14
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG11	3	0.14
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG12	3	0.14
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG13	3	0.14
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG21	3	0.14
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG22	3	0.14
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG23	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG11	3	0.14
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG12	3	0.14
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG13	3	0.14
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG21	3	0.14
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG22	3	0.14
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG23	3	0.14
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG11	3	0.14
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG12	3	0.14
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG13	3	0.14
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG21	3	0.14
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG22	3	0.14
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG23	3	0.14
(2,11)	1:25:A:VAL:HG11	1:123:A:GLN:H	2	0.14
(2,11)	1:25:A:VAL:HG12	1:123:A:GLN:H	2	0.14
(2,11)	1:25:A:VAL:HG13	1:123:A:GLN:H	2	0.14
(2,11)	1:25:A:VAL:HG21	1:123:A:GLN:H	2	0.14
(2,11)	1:25:A:VAL:HG22	1:123:A:GLN:H	2	0.14
(2,11)	1:25:A:VAL:HG23	1:123:A:GLN:H	2	0.14
(2,10)	1:25:A:VAL:HG11	1:26:A:GLY:H	8	0.14
(2,10)	1:25:A:VAL:HG12	1:26:A:GLY:H	8	0.14
(2,10)	1:25:A:VAL:HG13	1:26:A:GLY:H	8	0.14
(2,10)	1:25:A:VAL:HG21	1:26:A:GLY:H	8	0.14
(2,10)	1:25:A:VAL:HG22	1:26:A:GLY:H	8	0.14
(2,10)	1:25:A:VAL:HG23	1:26:A:GLY:H	8	0.14
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	10	0.13
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	10	0.13
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	1	0.13
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	2	0.13
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	3	0.13
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	7	0.13
(2,1127)	1:230:B:GLU:H	1:232:B:ALA:H	1	0.13
(2,1127)	1:230:B:GLU:H	1:232:B:ALA:H	9	0.13
(2,1127)	1:230:B:GLU:H	1:232:B:ALA:H	10	0.13
(2,1118)	1:226:B:GLY:H	1:248:B:TYR:H	5	0.13
(2,1111)	1:224:B:ILE:H	1:246:B:LYS:H	10	0.13
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	1	0.13
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	1	0.13
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	1	0.13
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	3	0.13
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	3	0.13
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	3	0.13
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	5	0.13
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	5	0.13
(2,982)	1:167:B:THR:H	1:171:B:PHE:H	3	0.13
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	2	0.13
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	5	0.13
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	9	0.13
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	5	0.13
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	5	0.13
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	5	0.13
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD11	3	0.13
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD12	3	0.13
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD13	3	0.13
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	2	0.13
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	2	0.13
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	2	0.13
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	2	0.13
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	2	0.13
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	2	0.13
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	4	0.13
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	4	0.13
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	4	0.13
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	4	0.13
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	4	0.13
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	4	0.13
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	8	0.13
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	8	0.13
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	8	0.13
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	8	0.13
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	8	0.13
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	8	0.13
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	9	0.13
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	9	0.13
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	9	0.13
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	9	0.13
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	9	0.13
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	9	0.13
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	1	0.13
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	3	0.13
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	8	0.13
(2,881)	1:126:B:ILE:HD11	1:130:B:LYS:H	9	0.13
(2,881)	1:126:B:ILE:HD12	1:130:B:LYS:H	9	0.13
(2,881)	1:126:B:ILE:HD13	1:130:B:LYS:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	2	0.13
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	4	0.13
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	7	0.13
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD11	3	0.13
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD12	3	0.13
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD13	3	0.13
(2,778)	1:82:B:LEU:HD11	1:86:B:GLU:H	6	0.13
(2,778)	1:82:B:LEU:HD12	1:86:B:GLU:H	6	0.13
(2,778)	1:82:B:LEU:HD13	1:86:B:GLU:H	6	0.13
(2,778)	1:82:B:LEU:HD21	1:86:B:GLU:H	6	0.13
(2,778)	1:82:B:LEU:HD22	1:86:B:GLU:H	6	0.13
(2,778)	1:82:B:LEU:HD23	1:86:B:GLU:H	6	0.13
(2,742)	1:75:B:VAL:H	1:92:B:ILE:HD11	5	0.13
(2,742)	1:75:B:VAL:H	1:92:B:ILE:HD12	5	0.13
(2,742)	1:75:B:VAL:H	1:92:B:ILE:HD13	5	0.13
(2,704)	1:61:B:ASN:H	1:64:B:PHE:H	10	0.13
(2,697)	1:57:B:ILE:H	1:58:B:LEU:H	4	0.13
(2,692)	1:55:B:GLU:H	1:58:B:LEU:H	6	0.13
(2,652)	1:40:B:VAL:HG11	1:59:B:GLY:H	10	0.13
(2,652)	1:40:B:VAL:HG12	1:59:B:GLY:H	10	0.13
(2,652)	1:40:B:VAL:HG13	1:59:B:GLY:H	10	0.13
(2,652)	1:40:B:VAL:HG21	1:59:B:GLY:H	10	0.13
(2,652)	1:40:B:VAL:HG22	1:59:B:GLY:H	10	0.13
(2,652)	1:40:B:VAL:HG23	1:59:B:GLY:H	10	0.13
(2,646)	1:39:B:ILE:HD11	1:60:B:LYS:H	8	0.13
(2,646)	1:39:B:ILE:HD12	1:60:B:LYS:H	8	0.13
(2,646)	1:39:B:ILE:HD13	1:60:B:LYS:H	8	0.13
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	1	0.13
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	9	0.13
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	10	0.13
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG11	5	0.13
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG12	5	0.13
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG13	5	0.13
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG21	5	0.13
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG22	5	0.13
(2,626)	1:29:B:ILE:HD11	1:120:B:VAL:HG23	5	0.13
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG11	5	0.13
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG12	5	0.13
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG13	5	0.13
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG21	5	0.13
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG22	5	0.13
(2,626)	1:29:B:ILE:HD12	1:120:B:VAL:HG23	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG11	5	0.13
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG12	5	0.13
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG13	5	0.13
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG21	5	0.13
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG22	5	0.13
(2,626)	1:29:B:ILE:HD13	1:120:B:VAL:HG23	5	0.13
(2,521)	1:224:A:ILE:H	1:248:A:TYR:H	4	0.13
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	6	0.13
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	6	0.13
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	6	0.13
(2,447)	1:191:A:ILE:HD11	1:255:A:VAL:H	7	0.13
(2,447)	1:191:A:ILE:HD12	1:255:A:VAL:H	7	0.13
(2,447)	1:191:A:ILE:HD13	1:255:A:VAL:H	7	0.13
(2,445)	1:191:A:ILE:HD11	1:223:A:ILE:H	4	0.13
(2,445)	1:191:A:ILE:HD12	1:223:A:ILE:H	4	0.13
(2,445)	1:191:A:ILE:HD13	1:223:A:ILE:H	4	0.13
(2,259)	1:111:A:MET:H	1:119:A:PHE:H	3	0.13
(2,234)	1:97:A:LYS:H	1:100:A:THR:H	5	0.13
(2,234)	1:97:A:LYS:H	1:100:A:THR:H	9	0.13
(2,223)	1:93:A:GLN:HE21	1:103:A:TRP:HE1	8	0.13
(2,223)	1:93:A:GLN:HE22	1:103:A:TRP:HE1	8	0.13
(2,209)	1:90:A:VAL:HG11	1:90:A:VAL:H	10	0.13
(2,209)	1:90:A:VAL:HG12	1:90:A:VAL:H	10	0.13
(2,209)	1:90:A:VAL:HG13	1:90:A:VAL:H	10	0.13
(2,209)	1:90:A:VAL:HG21	1:90:A:VAL:H	10	0.13
(2,209)	1:90:A:VAL:HG22	1:90:A:VAL:H	10	0.13
(2,209)	1:90:A:VAL:HG23	1:90:A:VAL:H	10	0.13
(2,203)	1:88:A:VAL:HG11	1:108:A:ILE:H	1	0.13
(2,203)	1:88:A:VAL:HG12	1:108:A:ILE:H	1	0.13
(2,203)	1:88:A:VAL:HG13	1:108:A:ILE:H	1	0.13
(2,203)	1:88:A:VAL:HG21	1:108:A:ILE:H	1	0.13
(2,203)	1:88:A:VAL:HG22	1:108:A:ILE:H	1	0.13
(2,203)	1:88:A:VAL:HG23	1:108:A:ILE:H	1	0.13
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD11	7	0.13
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD12	7	0.13
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD13	7	0.13
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD11	7	0.13
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD12	7	0.13
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD13	7	0.13
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD11	7	0.13
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD12	7	0.13
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD13	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:71:A:ASP:H	1:92:A:ILE:HD11	1	0.13
(2,137)	1:71:A:ASP:H	1:92:A:ILE:HD12	1	0.13
(2,137)	1:71:A:ASP:H	1:92:A:ILE:HD13	1	0.13
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	8	0.13
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG11	2	0.13
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG12	2	0.13
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG13	2	0.13
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG21	2	0.13
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG22	2	0.13
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG23	2	0.13
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG11	2	0.13
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG12	2	0.13
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG13	2	0.13
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG21	2	0.13
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG22	2	0.13
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG23	2	0.13
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG11	2	0.13
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG12	2	0.13
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG13	2	0.13
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG21	2	0.13
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG22	2	0.13
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG23	2	0.13
(2,10)	1:25:A:VAL:HG11	1:26:A:GLY:H	2	0.13
(2,10)	1:25:A:VAL:HG12	1:26:A:GLY:H	2	0.13
(2,10)	1:25:A:VAL:HG13	1:26:A:GLY:H	2	0.13
(2,10)	1:25:A:VAL:HG21	1:26:A:GLY:H	2	0.13
(2,10)	1:25:A:VAL:HG22	1:26:A:GLY:H	2	0.13
(2,10)	1:25:A:VAL:HG23	1:26:A:GLY:H	2	0.13
(2,10)	1:25:A:VAL:HG11	1:26:A:GLY:H	6	0.13
(2,10)	1:25:A:VAL:HG12	1:26:A:GLY:H	6	0.13
(2,10)	1:25:A:VAL:HG13	1:26:A:GLY:H	6	0.13
(2,10)	1:25:A:VAL:HG21	1:26:A:GLY:H	6	0.13
(2,10)	1:25:A:VAL:HG22	1:26:A:GLY:H	6	0.13
(2,10)	1:25:A:VAL:HG23	1:26:A:GLY:H	6	0.13
(2,4)	1:4:A:PHE:H	1:5:A:GLN:H	1	0.13
(2,1168)	1:251:B:VAL:HG11	1:255:B:VAL:H	1	0.12
(2,1168)	1:251:B:VAL:HG12	1:255:B:VAL:H	1	0.12
(2,1168)	1:251:B:VAL:HG13	1:255:B:VAL:H	1	0.12
(2,1168)	1:251:B:VAL:HG21	1:255:B:VAL:H	1	0.12
(2,1168)	1:251:B:VAL:HG22	1:255:B:VAL:H	1	0.12
(2,1168)	1:251:B:VAL:HG23	1:255:B:VAL:H	1	0.12
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	6	0.12
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	9	0.12
(2,1160)	1:248:B:TYR:H	1:250:B:ASN:H	6	0.12
(2,1143)	1:239:B:ASP:H	1:240:B:ALA:H	8	0.12
(2,1137)	1:236:B:ASN:H	1:237:B:LYS:H	7	0.12
(2,1127)	1:230:B:GLU:H	1:232:B:ALA:H	3	0.12
(2,1118)	1:226:B:GLY:H	1:248:B:TYR:H	6	0.12
(2,1070)	1:203:B:GLN:H	1:206:B:ASP:H	2	0.12
(2,1039)	1:191:B:ILE:HD11	1:255:B:VAL:H	4	0.12
(2,1039)	1:191:B:ILE:HD12	1:255:B:VAL:H	4	0.12
(2,1039)	1:191:B:ILE:HD13	1:255:B:VAL:H	4	0.12
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	8	0.12
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	8	0.12
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	8	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD11	3	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD12	3	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD13	3	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD21	3	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD22	3	0.12
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD23	3	0.12
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	1	0.12
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	2	0.12
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	3	0.12
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	6	0.12
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	7	0.12
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	10	0.12
(2,984)	1:168:B:GLU:H	1:170:B:ARG:H	4	0.12
(2,975)	1:166:B:LEU:H	1:199:B:GLN:H	7	0.12
(2,973)	1:165:B:ASN:H	1:198:B:ALA:H	1	0.12
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	8	0.12
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD11	2	0.12
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD12	2	0.12
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD13	2	0.12
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	1	0.12
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	1	0.12
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	1	0.12
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	1	0.12
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	1	0.12
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	1	0.12
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	3	0.12
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	3	0.12
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	3	0.12
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	3	0.12
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	3	0.12
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	5	0.12
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	5	0.12
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	5	0.12
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	5	0.12
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	5	0.12
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	5	0.12
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	6	0.12
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	6	0.12
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	6	0.12
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	6	0.12
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	6	0.12
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	6	0.12
(2,922)	1:146:B:LEU:HD11	1:146:B:LEU:H	10	0.12
(2,922)	1:146:B:LEU:HD12	1:146:B:LEU:H	10	0.12
(2,922)	1:146:B:LEU:HD13	1:146:B:LEU:H	10	0.12
(2,922)	1:146:B:LEU:HD21	1:146:B:LEU:H	10	0.12
(2,922)	1:146:B:LEU:HD22	1:146:B:LEU:H	10	0.12
(2,922)	1:146:B:LEU:HD23	1:146:B:LEU:H	10	0.12
(2,907)	1:138:B:ASP:H	1:141:B:THR:H	2	0.12
(2,907)	1:138:B:ASP:H	1:141:B:THR:H	6	0.12
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	5	0.12
(2,884)	1:127:B:THR:H	1:129:B:GLN:H	10	0.12
(2,881)	1:126:B:ILE:HD11	1:130:B:LYS:H	1	0.12
(2,881)	1:126:B:ILE:HD12	1:130:B:LYS:H	1	0.12
(2,881)	1:126:B:ILE:HD13	1:130:B:LYS:H	1	0.12
(2,881)	1:126:B:ILE:HD11	1:130:B:LYS:H	10	0.12
(2,881)	1:126:B:ILE:HD12	1:130:B:LYS:H	10	0.12
(2,881)	1:126:B:ILE:HD13	1:130:B:LYS:H	10	0.12
(2,878)	1:125:B:ASP:H	1:127:B:THR:H	4	0.12
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	8	0.12
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	9	0.12
(2,834)	1:103:B:TRP:H	1:127:B:THR:H	4	0.12
(2,818)	1:94:B:ASN:H	1:104:B:ASN:H	9	0.12
(2,815)	1:93:B:GLN:HE21	1:103:B:TRP:HE1	9	0.12
(2,815)	1:93:B:GLN:HE22	1:103:B:TRP:HE1	9	0.12
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	4	0.12
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	4	0.12
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	4	0.12
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	4	0.12
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	4	0.12
(2,803)	1:90:B:VAL:HG11	1:92:B:ILE:H	8	0.12
(2,803)	1:90:B:VAL:HG12	1:92:B:ILE:H	8	0.12
(2,803)	1:90:B:VAL:HG13	1:92:B:ILE:H	8	0.12
(2,803)	1:90:B:VAL:HG21	1:92:B:ILE:H	8	0.12
(2,803)	1:90:B:VAL:HG22	1:92:B:ILE:H	8	0.12
(2,803)	1:90:B:VAL:HG23	1:92:B:ILE:H	8	0.12
(2,793)	1:88:B:VAL:HG11	1:89:B:THR:H	10	0.12
(2,793)	1:88:B:VAL:HG12	1:89:B:THR:H	10	0.12
(2,793)	1:88:B:VAL:HG13	1:89:B:THR:H	10	0.12
(2,793)	1:88:B:VAL:HG21	1:89:B:THR:H	10	0.12
(2,793)	1:88:B:VAL:HG22	1:89:B:THR:H	10	0.12
(2,793)	1:88:B:VAL:HG23	1:89:B:THR:H	10	0.12
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	10	0.12
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	10	0.12
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	10	0.12
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	10	0.12
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	10	0.12
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	10	0.12
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	10	0.12
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	10	0.12
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	10	0.12
(2,692)	1:55:B:GLU:H	1:58:B:LEU:H	10	0.12
(2,670)	1:47:B:VAL:HG11	1:54:B:THR:H	8	0.12
(2,670)	1:47:B:VAL:HG12	1:54:B:THR:H	8	0.12
(2,670)	1:47:B:VAL:HG13	1:54:B:THR:H	8	0.12
(2,670)	1:47:B:VAL:HG21	1:54:B:THR:H	8	0.12
(2,670)	1:47:B:VAL:HG22	1:54:B:THR:H	8	0.12
(2,670)	1:47:B:VAL:HG23	1:54:B:THR:H	8	0.12
(2,667)	1:47:B:VAL:HG11	1:51:B:GLY:H	8	0.12
(2,667)	1:47:B:VAL:HG12	1:51:B:GLY:H	8	0.12
(2,667)	1:47:B:VAL:HG13	1:51:B:GLY:H	8	0.12
(2,667)	1:47:B:VAL:HG21	1:51:B:GLY:H	8	0.12
(2,667)	1:47:B:VAL:HG22	1:51:B:GLY:H	8	0.12
(2,667)	1:47:B:VAL:HG23	1:51:B:GLY:H	8	0.12
(2,603)	1:25:B:VAL:HG11	1:123:B:GLN:H	2	0.12
(2,603)	1:25:B:VAL:HG12	1:123:B:GLN:H	2	0.12
(2,603)	1:25:B:VAL:HG13	1:123:B:GLN:H	2	0.12
(2,603)	1:25:B:VAL:HG21	1:123:B:GLN:H	2	0.12
(2,603)	1:25:B:VAL:HG22	1:123:B:GLN:H	2	0.12
(2,603)	1:25:B:VAL:HG23	1:123:B:GLN:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,595)	1:3:B:SER:H	1:7:B:PHE:H	2	0.12
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	6	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD11	3	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD12	3	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD13	3	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD21	3	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD22	3	0.12
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD23	3	0.12
(2,384)	1:166:A:LEU:H	1:201:A:ASN:H	6	0.12
(2,383)	1:166:A:LEU:H	1:199:A:GLN:H	5	0.12
(2,357)	1:154:A:ARG:H	1:157:A:ILE:HD11	2	0.12
(2,357)	1:154:A:ARG:H	1:157:A:ILE:HD12	2	0.12
(2,357)	1:154:A:ARG:H	1:157:A:ILE:HD13	2	0.12
(2,343)	1:151:A:VAL:H	1:159:A:ALA:H	8	0.12
(2,290)	1:126:A:ILE:HD11	1:128:A:LYS:H	8	0.12
(2,290)	1:126:A:ILE:HD12	1:128:A:LYS:H	8	0.12
(2,290)	1:126:A:ILE:HD13	1:128:A:LYS:H	8	0.12
(2,261)	1:112:A:GLU:H	1:113:A:ILE:H	2	0.12
(2,259)	1:111:A:MET:H	1:119:A:PHE:H	5	0.12
(2,236)	1:98:A:ASP:H	1:100:A:THR:H	4	0.12
(2,234)	1:97:A:LYS:H	1:100:A:THR:H	6	0.12
(2,232)	1:97:A:LYS:H	1:98:A:ASP:H	3	0.12
(2,232)	1:97:A:LYS:H	1:98:A:ASP:H	5	0.12
(2,225)	1:94:A:ASN:H	1:102:A:PHE:H	6	0.12
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	9	0.12
(2,200)	1:88:A:VAL:HG11	1:88:A:VAL:H	4	0.12
(2,200)	1:88:A:VAL:HG12	1:88:A:VAL:H	4	0.12
(2,200)	1:88:A:VAL:HG13	1:88:A:VAL:H	4	0.12
(2,200)	1:88:A:VAL:HG21	1:88:A:VAL:H	4	0.12
(2,200)	1:88:A:VAL:HG22	1:88:A:VAL:H	4	0.12
(2,200)	1:88:A:VAL:HG23	1:88:A:VAL:H	4	0.12
(2,200)	1:88:A:VAL:HG11	1:88:A:VAL:H	10	0.12
(2,200)	1:88:A:VAL:HG12	1:88:A:VAL:H	10	0.12
(2,200)	1:88:A:VAL:HG13	1:88:A:VAL:H	10	0.12
(2,200)	1:88:A:VAL:HG21	1:88:A:VAL:H	10	0.12
(2,200)	1:88:A:VAL:HG22	1:88:A:VAL:H	10	0.12
(2,200)	1:88:A:VAL:HG23	1:88:A:VAL:H	10	0.12
(2,191)	1:83:A:GLN:H	1:85:A:LYS:H	6	0.12
(2,186)	1:82:A:LEU:HD11	1:86:A:GLU:H	3	0.12
(2,186)	1:82:A:LEU:HD12	1:86:A:GLU:H	3	0.12
(2,186)	1:82:A:LEU:HD13	1:86:A:GLU:H	3	0.12
(2,186)	1:82:A:LEU:HD21	1:86:A:GLU:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,186)	1:82:A:LEU:HD22	1:86:A:GLU:H	3	0.12
(2,186)	1:82:A:LEU:HD23	1:86:A:GLU:H	3	0.12
(2,165)	1:78:A:ILE:H	1:90:A:VAL:HG11	7	0.12
(2,165)	1:78:A:ILE:H	1:90:A:VAL:HG12	7	0.12
(2,165)	1:78:A:ILE:H	1:90:A:VAL:HG13	7	0.12
(2,165)	1:78:A:ILE:H	1:90:A:VAL:HG21	7	0.12
(2,165)	1:78:A:ILE:H	1:90:A:VAL:HG22	7	0.12
(2,165)	1:78:A:ILE:H	1:90:A:VAL:HG23	7	0.12
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	10	0.12
(2,54)	1:39:A:ILE:HD11	1:60:A:LYS:H	5	0.12
(2,54)	1:39:A:ILE:HD12	1:60:A:LYS:H	5	0.12
(2,54)	1:39:A:ILE:HD13	1:60:A:LYS:H	5	0.12
(2,54)	1:39:A:ILE:HD11	1:60:A:LYS:H	6	0.12
(2,54)	1:39:A:ILE:HD12	1:60:A:LYS:H	6	0.12
(2,54)	1:39:A:ILE:HD13	1:60:A:LYS:H	6	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG11	1	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG12	1	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG13	1	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG21	1	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG22	1	0.12
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG23	1	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG11	1	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG12	1	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG13	1	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG21	1	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG22	1	0.12
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG23	1	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG11	1	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG12	1	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG13	1	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG21	1	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG22	1	0.12
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG23	1	0.12
(1,8)	2:900:B:FMN:O4'	1:66:B:GLN:NE2	10	0.12
(2,1163)	1:250:B:ASN:H	1:253:B:ASP:H	1	0.11
(2,1155)	1:244:B:SER:H	1:245:B:LEU:H	8	0.11
(2,1155)	1:244:B:SER:H	1:245:B:LEU:H	10	0.11
(2,1150)	1:242:B:PHE:H	1:243:B:SER:H	7	0.11
(2,1150)	1:242:B:PHE:H	1:243:B:SER:H	8	0.11
(2,1137)	1:236:B:ASN:H	1:237:B:LYS:H	5	0.11
(2,1137)	1:236:B:ASN:H	1:237:B:LYS:H	9	0.11
(2,1137)	1:236:B:ASN:H	1:237:B:LYS:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1127)	1:230:B:GLU:H	1:232:B:ALA:H	2	0.11
(2,1100)	1:215:B:LEU:H	1:217:B:LEU:H	2	0.11
(2,1073)	1:205:B:ALA:H	1:231:B:LEU:HD11	4	0.11
(2,1073)	1:205:B:ALA:H	1:231:B:LEU:HD12	4	0.11
(2,1073)	1:205:B:ALA:H	1:231:B:LEU:HD13	4	0.11
(2,1073)	1:205:B:ALA:H	1:231:B:LEU:HD21	4	0.11
(2,1073)	1:205:B:ALA:H	1:231:B:LEU:HD22	4	0.11
(2,1073)	1:205:B:ALA:H	1:231:B:LEU:HD23	4	0.11
(2,1070)	1:203:B:GLN:H	1:206:B:ASP:H	5	0.11
(2,1060)	1:200:B:VAL:HG11	1:205:B:ALA:H	1	0.11
(2,1060)	1:200:B:VAL:HG12	1:205:B:ALA:H	1	0.11
(2,1060)	1:200:B:VAL:HG13	1:205:B:ALA:H	1	0.11
(2,1060)	1:200:B:VAL:HG21	1:205:B:ALA:H	1	0.11
(2,1060)	1:200:B:VAL:HG22	1:205:B:ALA:H	1	0.11
(2,1060)	1:200:B:VAL:HG23	1:205:B:ALA:H	1	0.11
(2,1036)	1:191:B:ILE:HD11	1:191:B:ILE:H	4	0.11
(2,1036)	1:191:B:ILE:HD12	1:191:B:ILE:H	4	0.11
(2,1036)	1:191:B:ILE:HD13	1:191:B:ILE:H	4	0.11
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD11	7	0.11
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD12	7	0.11
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD13	7	0.11
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD21	7	0.11
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD22	7	0.11
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD23	7	0.11
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	5	0.11
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	8	0.11
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	9	0.11
(2,973)	1:165:B:ASN:H	1:198:B:ALA:H	2	0.11
(2,973)	1:165:B:ASN:H	1:198:B:ALA:H	7	0.11
(2,971)	1:165:B:ASN:H	1:167:B:THR:H	10	0.11
(2,967)	1:163:B:VAL:H	1:197:B:LEU:H	3	0.11
(2,964)	1:162:B:LEU:H	1:196:B:GLY:H	6	0.11
(2,962)	1:162:B:LEU:H	1:193:B:ASP:H	7	0.11
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD11	1	0.11
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD12	1	0.11
(2,952)	1:157:B:ILE:H	1:157:B:ILE:HD13	1	0.11
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD11	1	0.11
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD12	1	0.11
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD13	1	0.11
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD11	10	0.11
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD12	10	0.11
(2,934)	1:151:B:VAL:H	1:153:B:ILE:HD13	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,925)	1:147:B:SER:HG	1:148:B:THR:H	10	0.11
(2,907)	1:138:B:ASP:H	1:141:B:THR:H	4	0.11
(2,907)	1:138:B:ASP:H	1:141:B:THR:H	7	0.11
(2,882)	1:126:B:ILE:HD11	1:128:B:LYS:H	8	0.11
(2,882)	1:126:B:ILE:HD12	1:128:B:LYS:H	8	0.11
(2,882)	1:126:B:ILE:HD13	1:128:B:LYS:H	8	0.11
(2,875)	1:124:B:ASN:H	1:126:B:ILE:H	3	0.11
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	3	0.11
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	5	0.11
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD11	6	0.11
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD12	6	0.11
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD13	6	0.11
(2,820)	1:96:B:LYS:H	1:98:B:ASP:H	7	0.11
(2,801)	1:90:B:VAL:HG11	1:90:B:VAL:H	10	0.11
(2,801)	1:90:B:VAL:HG12	1:90:B:VAL:H	10	0.11
(2,801)	1:90:B:VAL:HG13	1:90:B:VAL:H	10	0.11
(2,801)	1:90:B:VAL:HG21	1:90:B:VAL:H	10	0.11
(2,801)	1:90:B:VAL:HG22	1:90:B:VAL:H	10	0.11
(2,801)	1:90:B:VAL:HG23	1:90:B:VAL:H	10	0.11
(2,793)	1:88:B:VAL:HG11	1:89:B:THR:H	8	0.11
(2,793)	1:88:B:VAL:HG12	1:89:B:THR:H	8	0.11
(2,793)	1:88:B:VAL:HG13	1:89:B:THR:H	8	0.11
(2,793)	1:88:B:VAL:HG21	1:89:B:THR:H	8	0.11
(2,793)	1:88:B:VAL:HG22	1:89:B:THR:H	8	0.11
(2,793)	1:88:B:VAL:HG23	1:89:B:THR:H	8	0.11
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	2	0.11
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	2	0.11
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	2	0.11
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	2	0.11
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	2	0.11
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	2	0.11
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	3	0.11
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	3	0.11
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	3	0.11
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	3	0.11
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	3	0.11
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	3	0.11
(2,792)	1:88:B:VAL:HG11	1:88:B:VAL:H	5	0.11
(2,792)	1:88:B:VAL:HG12	1:88:B:VAL:H	5	0.11
(2,792)	1:88:B:VAL:HG13	1:88:B:VAL:H	5	0.11
(2,792)	1:88:B:VAL:HG21	1:88:B:VAL:H	5	0.11
(2,792)	1:88:B:VAL:HG22	1:88:B:VAL:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,792)	1:88:B:VAL:HG23	1:88:B:VAL:H	5	0.11
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD11	9	0.11
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD12	9	0.11
(2,764)	1:78:B:ILE:HD11	1:92:B:ILE:HD13	9	0.11
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD11	9	0.11
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD12	9	0.11
(2,764)	1:78:B:ILE:HD12	1:92:B:ILE:HD13	9	0.11
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD11	9	0.11
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD12	9	0.11
(2,764)	1:78:B:ILE:HD13	1:92:B:ILE:HD13	9	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD11	4	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD12	4	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD13	4	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD21	4	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD22	4	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD23	4	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD11	7	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD12	7	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD13	7	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD21	7	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD22	7	0.11
(2,711)	1:64:B:PHE:H	1:65:B:LEU:HD23	7	0.11
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	4	0.11
(2,640)	1:36:B:ASP:H	1:37:B:ASN:H	8	0.11
(2,615)	1:28:B:VAL:HG11	1:30:B:THR:H	6	0.11
(2,615)	1:28:B:VAL:HG12	1:30:B:THR:H	6	0.11
(2,615)	1:28:B:VAL:HG13	1:30:B:THR:H	6	0.11
(2,615)	1:28:B:VAL:HG21	1:30:B:THR:H	6	0.11
(2,615)	1:28:B:VAL:HG22	1:30:B:THR:H	6	0.11
(2,615)	1:28:B:VAL:HG23	1:30:B:THR:H	6	0.11
(2,576)	1:251:A:VAL:HG11	1:255:A:VAL:H	1	0.11
(2,576)	1:251:A:VAL:HG12	1:255:A:VAL:H	1	0.11
(2,576)	1:251:A:VAL:HG13	1:255:A:VAL:H	1	0.11
(2,576)	1:251:A:VAL:HG21	1:255:A:VAL:H	1	0.11
(2,576)	1:251:A:VAL:HG22	1:255:A:VAL:H	1	0.11
(2,576)	1:251:A:VAL:HG23	1:255:A:VAL:H	1	0.11
(2,576)	1:251:A:VAL:HG11	1:255:A:VAL:H	2	0.11
(2,576)	1:251:A:VAL:HG12	1:255:A:VAL:H	2	0.11
(2,576)	1:251:A:VAL:HG13	1:255:A:VAL:H	2	0.11
(2,576)	1:251:A:VAL:HG21	1:255:A:VAL:H	2	0.11
(2,576)	1:251:A:VAL:HG22	1:255:A:VAL:H	2	0.11
(2,576)	1:251:A:VAL:HG23	1:255:A:VAL:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,576)	1:251:A:VAL:HG11	1:255:A:VAL:H	5	0.11
(2,576)	1:251:A:VAL:HG12	1:255:A:VAL:H	5	0.11
(2,576)	1:251:A:VAL:HG13	1:255:A:VAL:H	5	0.11
(2,576)	1:251:A:VAL:HG21	1:255:A:VAL:H	5	0.11
(2,576)	1:251:A:VAL:HG22	1:255:A:VAL:H	5	0.11
(2,576)	1:251:A:VAL:HG23	1:255:A:VAL:H	5	0.11
(2,576)	1:251:A:VAL:HG11	1:255:A:VAL:H	10	0.11
(2,576)	1:251:A:VAL:HG12	1:255:A:VAL:H	10	0.11
(2,576)	1:251:A:VAL:HG13	1:255:A:VAL:H	10	0.11
(2,576)	1:251:A:VAL:HG21	1:255:A:VAL:H	10	0.11
(2,576)	1:251:A:VAL:HG22	1:255:A:VAL:H	10	0.11
(2,576)	1:251:A:VAL:HG23	1:255:A:VAL:H	10	0.11
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	3	0.11
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	5	0.11
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	9	0.11
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	10	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD11	5	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD12	5	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD13	5	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD21	5	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD22	5	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD23	5	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD11	7	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD12	7	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD13	7	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD21	7	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD22	7	0.11
(2,441)	1:190:A:LEU:H	1:258:A:LEU:HD23	7	0.11
(2,384)	1:166:A:LEU:H	1:201:A:ASN:H	5	0.11
(2,379)	1:165:A:ASN:H	1:167:A:THR:H	6	0.11
(2,379)	1:165:A:ASN:H	1:167:A:THR:H	10	0.11
(2,372)	1:162:A:LEU:H	1:196:A:GLY:H	1	0.11
(2,365)	1:158:A:SER:H	1:190:A:LEU:H	3	0.11
(2,232)	1:97:A:LYS:H	1:98:A:ASP:H	4	0.11
(2,232)	1:97:A:LYS:H	1:98:A:ASP:H	10	0.11
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	6	0.11
(2,209)	1:90:A:VAL:HG11	1:90:A:VAL:H	1	0.11
(2,209)	1:90:A:VAL:HG12	1:90:A:VAL:H	1	0.11
(2,209)	1:90:A:VAL:HG13	1:90:A:VAL:H	1	0.11
(2,209)	1:90:A:VAL:HG21	1:90:A:VAL:H	1	0.11
(2,209)	1:90:A:VAL:HG22	1:90:A:VAL:H	1	0.11
(2,209)	1:90:A:VAL:HG23	1:90:A:VAL:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,209)	1:90:A:VAL:HG11	1:90:A:VAL:H	5	0.11
(2,209)	1:90:A:VAL:HG12	1:90:A:VAL:H	5	0.11
(2,209)	1:90:A:VAL:HG13	1:90:A:VAL:H	5	0.11
(2,209)	1:90:A:VAL:HG21	1:90:A:VAL:H	5	0.11
(2,209)	1:90:A:VAL:HG22	1:90:A:VAL:H	5	0.11
(2,209)	1:90:A:VAL:HG23	1:90:A:VAL:H	5	0.11
(2,194)	1:85:A:LYS:H	1:86:A:GLU:H	7	0.11
(2,191)	1:83:A:GLN:H	1:85:A:LYS:H	7	0.11
(2,160)	1:77:A:ASN:H	1:80:A:THR:H	9	0.11
(2,130)	1:67:A:GLY:H	1:95:A:TYR:H	3	0.11
(2,109)	1:59:A:GLY:H	1:60:A:LYS:H	4	0.11
(2,109)	1:59:A:GLY:H	1:60:A:LYS:H	5	0.11
(2,109)	1:59:A:GLY:H	1:60:A:LYS:H	6	0.11
(2,90)	1:52:A:TYR:H	1:97:A:LYS:H	2	0.11
(2,54)	1:39:A:ILE:HD11	1:60:A:LYS:H	4	0.11
(2,54)	1:39:A:ILE:HD12	1:60:A:LYS:H	4	0.11
(2,54)	1:39:A:ILE:HD13	1:60:A:LYS:H	4	0.11
(2,50)	1:39:A:ILE:H	1:59:A:GLY:H	3	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG11	5	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG12	5	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG13	5	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG21	5	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG22	5	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG23	5	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG11	5	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG12	5	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG13	5	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG21	5	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG22	5	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG23	5	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG11	5	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG12	5	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG13	5	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG21	5	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG22	5	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG23	5	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG11	10	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG12	10	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG13	10	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG21	10	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG22	10	0.11
(2,34)	1:29:A:ILE:HD11	1:120:A:VAL:HG23	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG11	10	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG12	10	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG13	10	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG21	10	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG22	10	0.11
(2,34)	1:29:A:ILE:HD12	1:120:A:VAL:HG23	10	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG11	10	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG12	10	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG13	10	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG21	10	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG22	10	0.11
(2,34)	1:29:A:ILE:HD13	1:120:A:VAL:HG23	10	0.11
(2,10)	1:25:A:VAL:HG11	1:26:A:GLY:H	1	0.11
(2,10)	1:25:A:VAL:HG12	1:26:A:GLY:H	1	0.11
(2,10)	1:25:A:VAL:HG13	1:26:A:GLY:H	1	0.11
(2,10)	1:25:A:VAL:HG21	1:26:A:GLY:H	1	0.11
(2,10)	1:25:A:VAL:HG22	1:26:A:GLY:H	1	0.11
(2,10)	1:25:A:VAL:HG23	1:26:A:GLY:H	1	0.11
(2,10)	1:25:A:VAL:HG11	1:26:A:GLY:H	4	0.11
(2,10)	1:25:A:VAL:HG12	1:26:A:GLY:H	4	0.11
(2,10)	1:25:A:VAL:HG13	1:26:A:GLY:H	4	0.11
(2,10)	1:25:A:VAL:HG21	1:26:A:GLY:H	4	0.11
(2,10)	1:25:A:VAL:HG22	1:26:A:GLY:H	4	0.11
(2,10)	1:25:A:VAL:HG23	1:26:A:GLY:H	4	0.11
(2,10)	1:25:A:VAL:HG11	1:26:A:GLY:H	5	0.11
(2,10)	1:25:A:VAL:HG12	1:26:A:GLY:H	5	0.11
(2,10)	1:25:A:VAL:HG13	1:26:A:GLY:H	5	0.11
(2,10)	1:25:A:VAL:HG21	1:26:A:GLY:H	5	0.11
(2,10)	1:25:A:VAL:HG22	1:26:A:GLY:H	5	0.11
(2,10)	1:25:A:VAL:HG23	1:26:A:GLY:H	5	0.11
(2,4)	1:4:A:PHE:H	1:5:A:GLN:H	8	0.11
(1,4)	2:900:A:FMN:O4'	1:66:A:GLN:NE2	3	0.11
(2,1168)	1:251:B:VAL:HG11	1:255:B:VAL:H	2	0.1
(2,1168)	1:251:B:VAL:HG12	1:255:B:VAL:H	2	0.1
(2,1168)	1:251:B:VAL:HG13	1:255:B:VAL:H	2	0.1
(2,1168)	1:251:B:VAL:HG21	1:255:B:VAL:H	2	0.1
(2,1168)	1:251:B:VAL:HG22	1:255:B:VAL:H	2	0.1
(2,1168)	1:251:B:VAL:HG23	1:255:B:VAL:H	2	0.1
(2,1150)	1:242:B:PHE:H	1:243:B:SER:H	9	0.1
(2,1137)	1:236:B:ASN:H	1:237:B:LYS:H	8	0.1
(2,1127)	1:230:B:GLU:H	1:232:B:ALA:H	6	0.1
(2,1127)	1:230:B:GLU:H	1:232:B:ALA:H	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1100)	1:215:B:LEU:H	1:217:B:LEU:H	6	0.1
(2,1064)	1:201:B:ASN:H	1:205:B:ALA:H	3	0.1
(2,1060)	1:200:B:VAL:HG11	1:205:B:ALA:H	3	0.1
(2,1060)	1:200:B:VAL:HG12	1:205:B:ALA:H	3	0.1
(2,1060)	1:200:B:VAL:HG13	1:205:B:ALA:H	3	0.1
(2,1060)	1:200:B:VAL:HG21	1:205:B:ALA:H	3	0.1
(2,1060)	1:200:B:VAL:HG22	1:205:B:ALA:H	3	0.1
(2,1060)	1:200:B:VAL:HG23	1:205:B:ALA:H	3	0.1
(2,1060)	1:200:B:VAL:HG11	1:205:B:ALA:H	10	0.1
(2,1060)	1:200:B:VAL:HG12	1:205:B:ALA:H	10	0.1
(2,1060)	1:200:B:VAL:HG13	1:205:B:ALA:H	10	0.1
(2,1060)	1:200:B:VAL:HG21	1:205:B:ALA:H	10	0.1
(2,1060)	1:200:B:VAL:HG22	1:205:B:ALA:H	10	0.1
(2,1060)	1:200:B:VAL:HG23	1:205:B:ALA:H	10	0.1
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD11	5	0.1
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD12	5	0.1
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD13	5	0.1
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD21	5	0.1
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD22	5	0.1
(2,1033)	1:190:B:LEU:H	1:258:B:LEU:HD23	5	0.1
(2,1019)	1:180:B:ASN:H	1:182:B:LEU:H	6	0.1
(2,1015)	1:178:B:LEU:H	1:180:B:ASN:H	6	0.1
(2,993)	1:172:B:ASN:H	1:173:B:SER:H	4	0.1
(2,975)	1:166:B:LEU:H	1:199:B:GLN:H	3	0.1
(2,907)	1:138:B:ASP:H	1:141:B:THR:H	9	0.1
(2,875)	1:124:B:ASN:H	1:126:B:ILE:H	8	0.1
(2,863)	1:114:B:GLU:H	1:116:B:LYS:H	10	0.1
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD11	4	0.1
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD12	4	0.1
(2,848)	1:107:B:ASN:H	1:122:B:ILE:HD13	4	0.1
(2,801)	1:90:B:VAL:HG11	1:90:B:VAL:H	2	0.1
(2,801)	1:90:B:VAL:HG12	1:90:B:VAL:H	2	0.1
(2,801)	1:90:B:VAL:HG13	1:90:B:VAL:H	2	0.1
(2,801)	1:90:B:VAL:HG21	1:90:B:VAL:H	2	0.1
(2,801)	1:90:B:VAL:HG22	1:90:B:VAL:H	2	0.1
(2,801)	1:90:B:VAL:HG23	1:90:B:VAL:H	2	0.1
(2,801)	1:90:B:VAL:HG11	1:90:B:VAL:H	5	0.1
(2,801)	1:90:B:VAL:HG12	1:90:B:VAL:H	5	0.1
(2,801)	1:90:B:VAL:HG13	1:90:B:VAL:H	5	0.1
(2,801)	1:90:B:VAL:HG21	1:90:B:VAL:H	5	0.1
(2,801)	1:90:B:VAL:HG22	1:90:B:VAL:H	5	0.1
(2,801)	1:90:B:VAL:HG23	1:90:B:VAL:H	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,778)	1:82:B:LEU:HD11	1:86:B:GLU:H	1	0.1
(2,778)	1:82:B:LEU:HD12	1:86:B:GLU:H	1	0.1
(2,778)	1:82:B:LEU:HD13	1:86:B:GLU:H	1	0.1
(2,778)	1:82:B:LEU:HD21	1:86:B:GLU:H	1	0.1
(2,778)	1:82:B:LEU:HD22	1:86:B:GLU:H	1	0.1
(2,778)	1:82:B:LEU:HD23	1:86:B:GLU:H	1	0.1
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD11	9	0.1
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD12	9	0.1
(2,729)	1:71:B:ASP:H	1:92:B:ILE:HD13	9	0.1
(2,627)	1:30:B:THR:H	1:41:B:TYR:H	5	0.1
(2,627)	1:30:B:THR:H	1:41:B:TYR:H	10	0.1
(2,576)	1:251:A:VAL:HG11	1:255:A:VAL:H	7	0.1
(2,576)	1:251:A:VAL:HG12	1:255:A:VAL:H	7	0.1
(2,576)	1:251:A:VAL:HG13	1:255:A:VAL:H	7	0.1
(2,576)	1:251:A:VAL:HG21	1:255:A:VAL:H	7	0.1
(2,576)	1:251:A:VAL:HG22	1:255:A:VAL:H	7	0.1
(2,576)	1:251:A:VAL:HG23	1:255:A:VAL:H	7	0.1
(2,576)	1:251:A:VAL:HG11	1:255:A:VAL:H	9	0.1
(2,576)	1:251:A:VAL:HG12	1:255:A:VAL:H	9	0.1
(2,576)	1:251:A:VAL:HG13	1:255:A:VAL:H	9	0.1
(2,576)	1:251:A:VAL:HG21	1:255:A:VAL:H	9	0.1
(2,576)	1:251:A:VAL:HG22	1:255:A:VAL:H	9	0.1
(2,576)	1:251:A:VAL:HG23	1:255:A:VAL:H	9	0.1
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	7	0.1
(2,538)	1:232:A:ALA:H	1:233:A:MET:H	8	0.1
(2,533)	1:228:A:LYS:H	1:232:A:ALA:H	9	0.1
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD11	7	0.1
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD12	7	0.1
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD13	7	0.1
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD21	7	0.1
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD22	7	0.1
(2,481)	1:205:A:ALA:H	1:231:A:LEU:HD23	7	0.1
(2,445)	1:191:A:ILE:HD11	1:223:A:ILE:H	6	0.1
(2,445)	1:191:A:ILE:HD12	1:223:A:ILE:H	6	0.1
(2,445)	1:191:A:ILE:HD13	1:223:A:ILE:H	6	0.1
(2,381)	1:165:A:ASN:H	1:198:A:ALA:H	2	0.1
(2,341)	1:150:A:ILE:HD11	1:159:A:ALA:H	7	0.1
(2,341)	1:150:A:ILE:HD12	1:159:A:ALA:H	7	0.1
(2,341)	1:150:A:ILE:HD13	1:159:A:ALA:H	7	0.1
(2,330)	1:146:A:LEU:HD11	1:146:A:LEU:H	4	0.1
(2,330)	1:146:A:LEU:HD12	1:146:A:LEU:H	4	0.1
(2,330)	1:146:A:LEU:HD13	1:146:A:LEU:H	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:146:A:LEU:HD21	1:146:A:LEU:H	4	0.1
(2,330)	1:146:A:LEU:HD22	1:146:A:LEU:H	4	0.1
(2,330)	1:146:A:LEU:HD23	1:146:A:LEU:H	4	0.1
(2,330)	1:146:A:LEU:HD11	1:146:A:LEU:H	8	0.1
(2,330)	1:146:A:LEU:HD12	1:146:A:LEU:H	8	0.1
(2,330)	1:146:A:LEU:HD13	1:146:A:LEU:H	8	0.1
(2,330)	1:146:A:LEU:HD21	1:146:A:LEU:H	8	0.1
(2,330)	1:146:A:LEU:HD22	1:146:A:LEU:H	8	0.1
(2,330)	1:146:A:LEU:HD23	1:146:A:LEU:H	8	0.1
(2,311)	1:136:A:LEU:H	1:138:A:ASP:H	9	0.1
(2,236)	1:98:A:ASP:H	1:100:A:THR:H	7	0.1
(2,234)	1:97:A:LYS:H	1:100:A:THR:H	2	0.1
(2,234)	1:97:A:LYS:H	1:100:A:THR:H	10	0.1
(2,232)	1:97:A:LYS:H	1:98:A:ASP:H	2	0.1
(2,232)	1:97:A:LYS:H	1:98:A:ASP:H	7	0.1
(2,225)	1:94:A:ASN:H	1:102:A:PHE:H	9	0.1
(2,219)	1:92:A:ILE:H	1:106:A:LEU:H	10	0.1
(2,212)	1:90:A:VAL:HG11	1:106:A:LEU:H	8	0.1
(2,212)	1:90:A:VAL:HG12	1:106:A:LEU:H	8	0.1
(2,212)	1:90:A:VAL:HG13	1:106:A:LEU:H	8	0.1
(2,212)	1:90:A:VAL:HG21	1:106:A:LEU:H	8	0.1
(2,212)	1:90:A:VAL:HG22	1:106:A:LEU:H	8	0.1
(2,212)	1:90:A:VAL:HG23	1:106:A:LEU:H	8	0.1
(2,200)	1:88:A:VAL:HG11	1:88:A:VAL:H	9	0.1
(2,200)	1:88:A:VAL:HG12	1:88:A:VAL:H	9	0.1
(2,200)	1:88:A:VAL:HG13	1:88:A:VAL:H	9	0.1
(2,200)	1:88:A:VAL:HG21	1:88:A:VAL:H	9	0.1
(2,200)	1:88:A:VAL:HG22	1:88:A:VAL:H	9	0.1
(2,200)	1:88:A:VAL:HG23	1:88:A:VAL:H	9	0.1
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD11	3	0.1
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD12	3	0.1
(2,172)	1:78:A:ILE:HD11	1:92:A:ILE:HD13	3	0.1
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD11	3	0.1
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD12	3	0.1
(2,172)	1:78:A:ILE:HD12	1:92:A:ILE:HD13	3	0.1
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD11	3	0.1
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD12	3	0.1
(2,172)	1:78:A:ILE:HD13	1:92:A:ILE:HD13	3	0.1
(2,157)	1:76:A:ASP:H	1:79:A:ARG:H	5	0.1
(2,157)	1:76:A:ASP:H	1:79:A:ARG:H	7	0.1
(2,149)	1:75:A:VAL:H	1:78:A:ILE:H	6	0.1
(2,112)	1:61:A:ASN:H	1:64:A:PHE:H	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:59:A:GLY:H	1:60:A:LYS:H	10	0.1
(2,98)	1:55:A:GLU:H	1:56:A:GLU:H	2	0.1
(2,98)	1:55:A:GLU:H	1:56:A:GLU:H	6	0.1
(2,77)	1:47:A:VAL:HG11	1:53:A:GLU:H	4	0.1
(2,77)	1:47:A:VAL:HG12	1:53:A:GLU:H	4	0.1
(2,77)	1:47:A:VAL:HG13	1:53:A:GLU:H	4	0.1
(2,77)	1:47:A:VAL:HG21	1:53:A:GLU:H	4	0.1
(2,77)	1:47:A:VAL:HG22	1:53:A:GLU:H	4	0.1
(2,77)	1:47:A:VAL:HG23	1:53:A:GLU:H	4	0.1

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

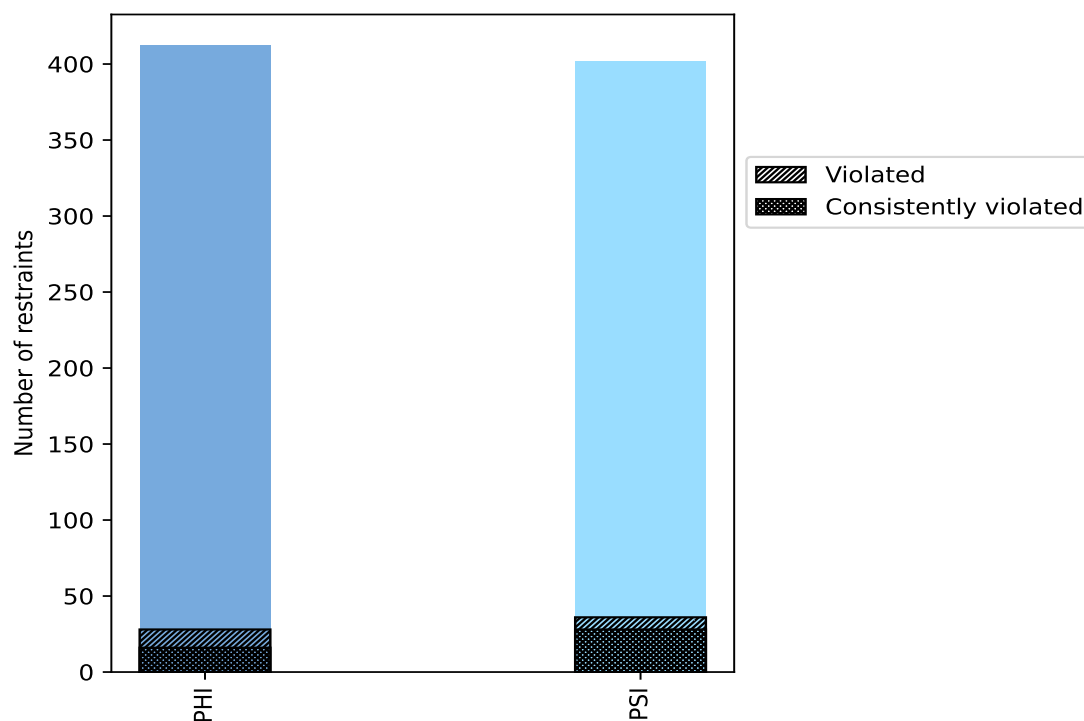
10.1 Summary of dihedral-angle violations [i](#)

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	412	50.6	28	6.8	3.4	16	3.9	2.0
PSI	402	49.4	36	9.0	4.4	28	7.0	3.4
Total	814	100.0	64	7.9	7.9	44	5.4	5.4

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](#)



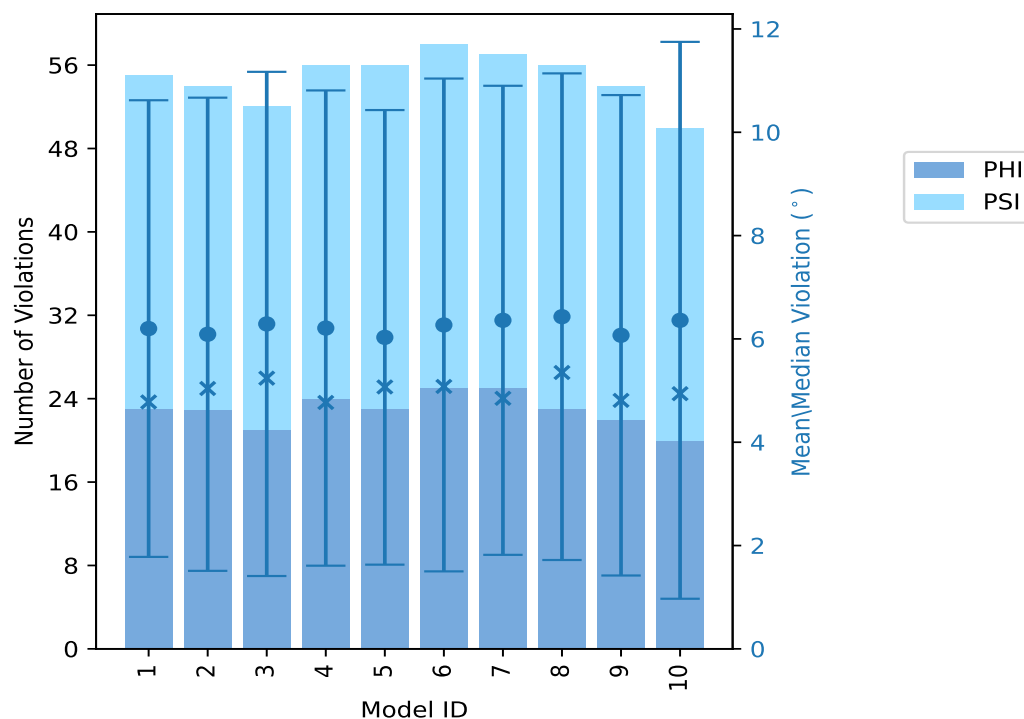
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	23	32	55	6.2	19.8	4.42	4.78
2	23	31	54	6.09	21.26	4.58	5.04
3	21	31	52	6.29	20.81	4.88	5.24
4	24	32	56	6.21	20.14	4.6	4.77
5	23	33	56	6.03	20.41	4.4	5.07
6	25	33	58	6.27	22.14	4.77	5.08
7	25	32	57	6.36	19.82	4.54	4.85
8	23	33	56	6.43	21.09	4.71	5.35
9	22	32	54	6.07	19.56	4.65	4.81
10	20	30	50	6.36	22.97	5.39	4.94

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



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

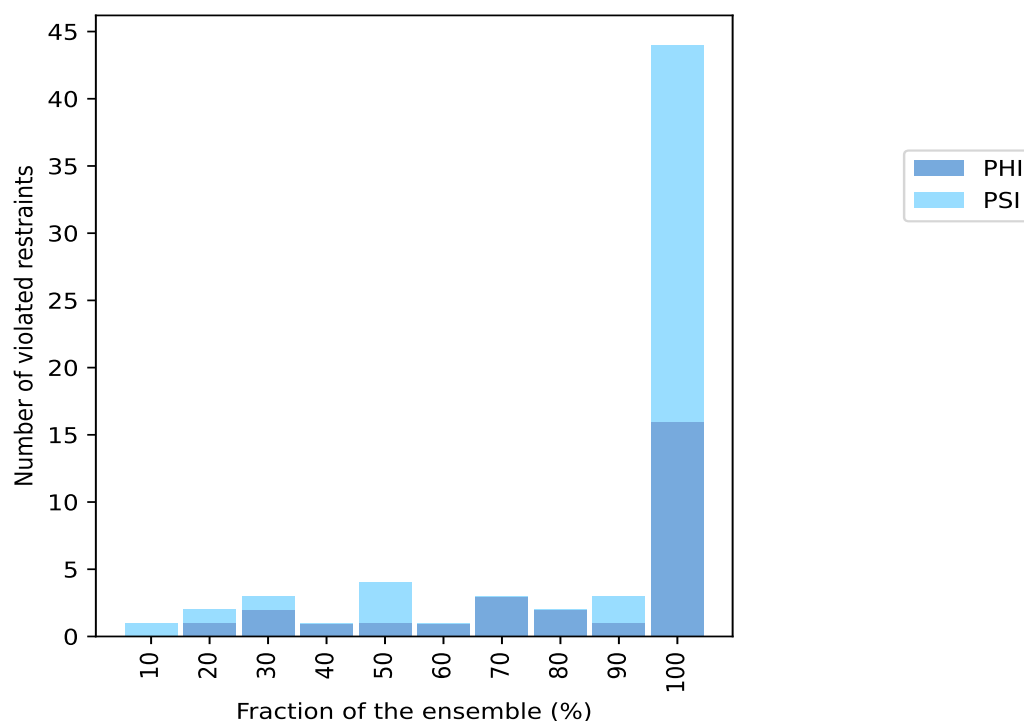
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	1	10.0
1	1	2	2	20.0
2	1	3	3	30.0
1	0	1	4	40.0
1	3	4	5	50.0
1	0	1	6	60.0
3	0	3	7	70.0
2	0	2	8	80.0
1	2	3	9	90.0
16	28	44	10	100.0

¹ Number of models with violations

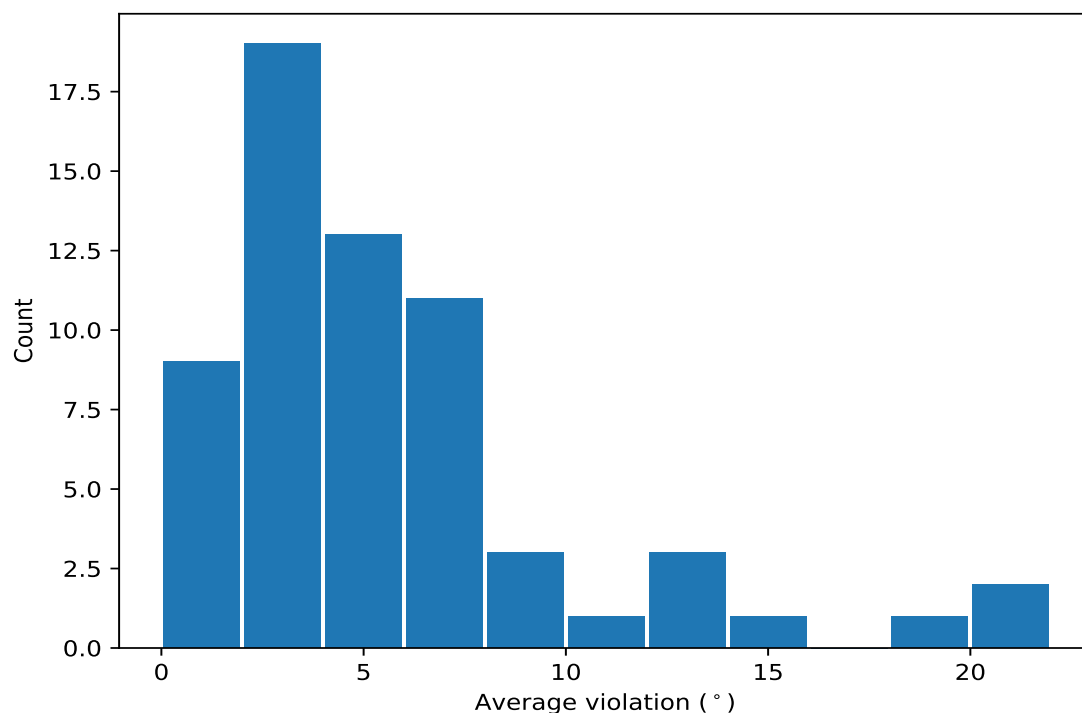
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	10	20.51	1.22	20.27
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	10	20.25	1.14	19.96
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	10	18.16	3.88	18.86
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	10	14.74	0.7	14.99
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	10	13.57	0.48	13.66
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	10	13.22	0.36	13.26
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	10	13.15	0.47	13.25
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	10	11.75	1.0	12.2
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	10	8.42	0.39	8.42
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	10	8.27	1.05	8.35
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	10	8.11	1.46	8.2
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	10	7.9	2.14	8.38
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	10	7.32	0.86	7.22

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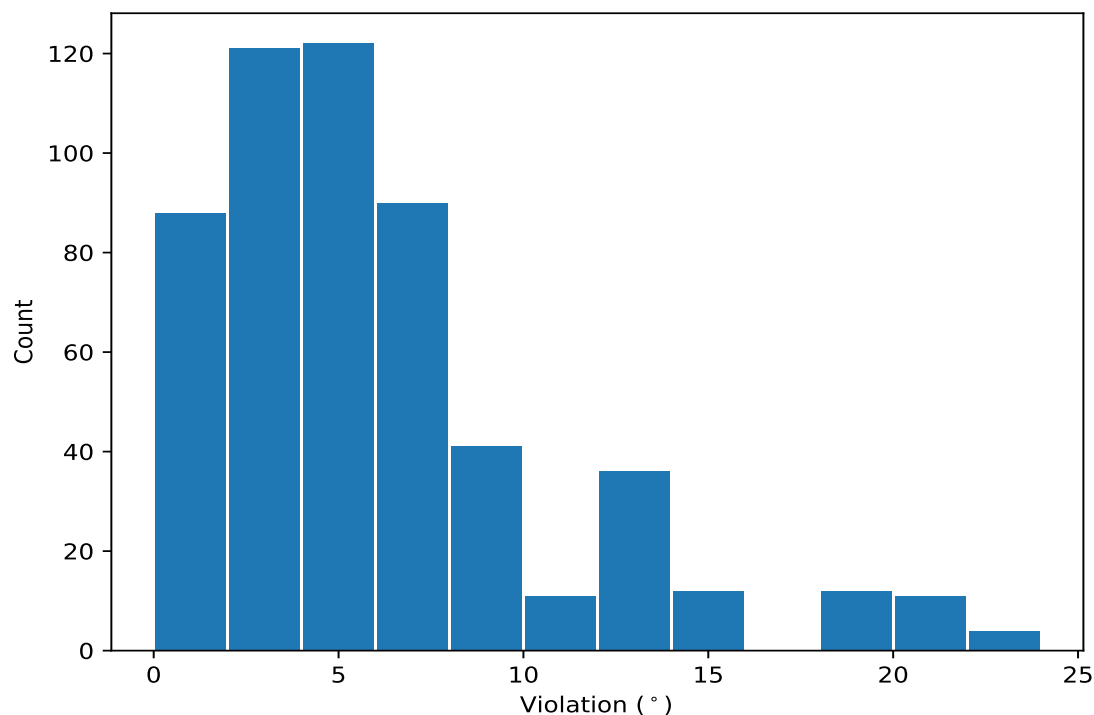
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	10	7.14	1.51	7.0
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	10	6.9	1.92	6.39
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	10	6.77	0.54	6.94
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	10	6.66	1.56	7.44
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	10	6.46	1.68	6.32
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	10	6.39	1.91	6.62
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	10	6.24	1.31	6.68
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	10	6.16	0.63	6.43
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	10	5.88	0.41	5.84
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	10	5.86	2.49	5.66
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	10	5.79	0.43	5.88
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	10	5.78	2.18	4.94
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	10	5.59	0.32	5.56
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	10	5.45	0.91	5.46
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	10	5.42	1.42	5.06
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	10	4.5	0.49	4.53
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	10	4.46	1.14	4.59
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	10	3.99	1.11	4.51
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	10	3.99	1.45	4.4
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	10	3.89	0.45	3.92
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	10	3.7	0.45	3.88
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	10	3.34	0.41	3.35
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	10	3.06	0.86	3.08
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	10	2.98	0.41	3.16
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	10	2.58	0.68	2.73
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	10	2.55	0.81	2.41
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	10	2.44	0.73	2.12
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	10	2.33	0.75	2.18
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	10	1.57	0.44	1.48
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	10	1.48	0.16	1.44
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	10	1.33	0.11	1.33
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	9	5.55	1.49	5.07
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	9	2.76	0.54	2.74
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	9	2.25	0.63	2.32
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	8	5.96	3.21	5.53
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	8	1.61	0.25	1.64
(1,603)	1:245:B:LEU:C	1:246:B:LYS:N	1:246:B:LYS:CA	1:246:B:LYS:C	7	5.33	1.24	5.5
(1,115)	1:152:A:PRO:C	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	7	4.25	0.6	4.36
(1,522)	1:152:B:PRO:C	1:153:B:ILE:N	1:153:B:ILE:CA	1:153:B:ILE:C	7	3.75	0.54	3.78
(1,174)	1:220:A:THR:C	1:221:A:GLU:N	1:221:A:GLU:CA	1:221:A:GLU:C	6	2.96	1.64	2.84
(1,275)	1:103:A:TRP:N	1:103:A:TRP:CA	1:103:A:TRP:C	1:104:A:ASN:N	5	2.13	0.44	1.98
(1,340)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:LEU:N	5	2.1	0.29	1.99
(1,599)	1:240:B:ALA:C	1:241:B:ASN:N	1:241:B:ASN:CA	1:241:B:ASN:C	5	1.8	0.58	1.77
(1,779)	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	1:219:B:GLY:N	5	1.5	0.45	1.26
(1,518)	1:148:B:THR:C	1:149:B:PRO:N	1:149:B:PRO:CA	1:149:B:PRO:C	4	1.56	0.27	1.6
(1,259)	1:84:A:ASN:N	1:84:A:ASN:CA	1:84:A:ASN:C	1:85:A:LYS:N	3	7.6	1.21	7.35
(1,58)	1:83:A:GLN:C	1:84:A:ASN:N	1:84:A:ASN:CA	1:84:A:ASN:C	3	3.09	0.84	3.45
(1,451)	1:68:B:LYS:C	1:69:B:HIS:N	1:69:B:HIS:CA	1:69:B:HIS:C	3	1.12	0.08	1.07
(1,65)	1:92:A:ILE:C	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	2	2.21	0.92	2.21
(1,700)	1:129:B:GLN:N	1:129:B:GLN:CA	1:129:B:GLN:C	1:130:B:LYS:N	2	1.38	0.36	1.38

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	10	22.97
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	10	22.67
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	10	22.44
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	6	22.14
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	6	21.77
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	6	21.54
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	2	21.26
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	8	21.09
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	2	21.06
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	3	20.81
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	3	20.57
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	3	20.44
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	5	20.41
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	4	20.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	4	20.03
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	5	19.89
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	7	19.82
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	1	19.8
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	8	19.59
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	9	19.56
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	7	19.43
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	1	19.31
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	8	19.12
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	9	18.78
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	9	18.61
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	7	18.16
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	4	18.09
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	5	15.82
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	3	15.63
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	5	15.44
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	7	15.21
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	8	15.15
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	2	15.08
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	1	15.0
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	9	14.9
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	1	14.57
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	8	14.37
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	10	14.19
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	4	14.02
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	10	13.94
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	4	13.88
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	5	13.79
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	9	13.77
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	10	13.75
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	10	13.72
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	1	13.57
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	1	13.55
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	3	13.55
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	7	13.54
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	7	13.51
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	3	13.5
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	3	13.45
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	7	13.4
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	1	13.38
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	4	13.32
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	2	13.28
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	6	13.26
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	8	13.25
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	2	13.18
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	8	13.17
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	4	13.15
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	9	13.14
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	6	12.97
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	2	12.89
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	8	12.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	9	12.72
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	6	12.64
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	5	12.6
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	6	12.59
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	6	12.59
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	2	12.41
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	1	12.24
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	3	12.23
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	5	12.18
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	9	12.18
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	5	11.2
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	7	11.17
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	7	10.73
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	8	10.7
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	7	10.57
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	10	10.56
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	4	10.44
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	4	10.41
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	8	10.3
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	2	10.27
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	1	10.16
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	4	9.98
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	10	9.79
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	9	9.75
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	4	9.62
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	7	9.56
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	1	9.55
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	9	9.5
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	6	9.44
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	10	9.37
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	3	9.33
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	1	9.28
(1,259)	1:84:A:ASN:N	1:84:A:ASN:CA	1:84:A:ASN:C	1:85:A:LYS:N	7	9.19
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	8	9.18
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	2	9.02
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	7	8.99
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	5	8.93
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	2	8.9
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	2	8.9
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	2	8.9
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	9	8.86
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	9	8.85
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	6	8.67
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	6	8.67
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	10	8.56
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1	8.5
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	1	8.49
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	4	8.47
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	6	8.45
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	9	8.42
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	3	8.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	7	8.37
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	2	8.36
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	4	8.27
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	5	8.27
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	8	8.25
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	10	8.23
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	2	8.23
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	5	8.16
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	8	8.13
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	3	8.1
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	4	8.04
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	6	7.98
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	2	7.91
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	8	7.91
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	7	7.89
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	4	7.88
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	1	7.86
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	8	7.85
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	2	7.85
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	5	7.84
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	8	7.82
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	8	7.78
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	6	7.78
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	7	7.77
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	5	7.76
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	9	7.74
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	6	7.65
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	10	7.64
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	1	7.62
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	4	7.54
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	3	7.53
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	1	7.53
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	2	7.5
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	7	7.38
(1,259)	1:84:A:ASN:N	1:84:A:ASN:CA	1:84:A:ASN:C	1:85:A:LYS:N	4	7.35
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	9	7.27
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	7	7.25
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	5	7.25
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	6	7.23
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	8	7.14
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	9	7.14
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	4	7.13
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	6	7.13
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	7	7.11
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	6	7.09
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	7	7.07
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	4	7.05
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	10	7.05
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	6	7.03
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	3	7.01
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	2	6.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	7	6.99
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	3	6.96
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	1	6.95
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	3	6.94
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	10	6.88
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1	6.84
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	7	6.83
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	6	6.78
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	1	6.74
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	2	6.7
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	4	6.68
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	10	6.65
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	8	6.62
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	3	6.61
(1,603)	1:245:B:LEU:C	1:246:B:LYS:N	1:246:B:LYS:CA	1:246:B:LYS:C	7	6.6
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	3	6.58
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	10	6.58
(1,603)	1:245:B:LEU:C	1:246:B:LYS:N	1:246:B:LYS:CA	1:246:B:LYS:C	5	6.56
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	5	6.54
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	5	6.53
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	9	6.52
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	8	6.52
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	4	6.52
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	6	6.52
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	5	6.52
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	5	6.48
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	10	6.47
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	9	6.45
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	8	6.45
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	8	6.36
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	3	6.34
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	2	6.31
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	3	6.31
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	5	6.31
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	10	6.28
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	3	6.28
(1,259)	1:84:A:ASN:N	1:84:A:ASN:CA	1:84:A:ASN:C	1:85:A:LYS:N	6	6.26
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	9	6.25
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	5	6.23
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	2	6.2
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	6	6.18
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	9	6.17
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	4	6.16
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	4	6.14
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	8	6.13
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	9	6.12
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	5	6.1
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	10	6.1
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	4	6.08
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	2	6.03
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	7	5.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	6	5.94
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	7	5.92
(1,603)	1:245:B:LEU:C	1:246:B:LYS:N	1:246:B:LYS:CA	1:246:B:LYS:C	1	5.91
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	1	5.9
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	10	5.88
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	4	5.86
(1,805)	1:247:B:THR:N	1:247:B:THR:CA	1:247:B:THR:C	1:248:B:TYR:N	5	5.85
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	9	5.83
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	8	5.83
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	8	5.79
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	2	5.76
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	8	5.76
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	3	5.74
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	7	5.7
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	5	5.67
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	1	5.67
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	8	5.65
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	2	5.63
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	7	5.61
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	1	5.6
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	9	5.6
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	4	5.57
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	9	5.53
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	3	5.52
(1,603)	1:245:B:LEU:C	1:246:B:LYS:N	1:246:B:LYS:CA	1:246:B:LYS:C	6	5.5
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	9	5.48
(1,205)	1:256:A:LYS:C	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	8	5.48
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	2	5.47
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	5	5.47
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	5	5.4
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	3	5.39
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	3	5.38
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	9	5.37
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	5	5.35
(1,603)	1:245:B:LEU:C	1:246:B:LYS:N	1:246:B:LYS:CA	1:246:B:LYS:C	3	5.34
(1,724)	1:154:B:ARG:N	1:154:B:ARG:CA	1:154:B:ARG:C	1:155:B:ASN:N	10	5.33
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	3	5.3
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	6	5.29
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	6	5.29
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	2	5.28
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	6	5.23
(1,174)	1:220:A:THR:C	1:221:A:GLU:N	1:221:A:GLU:CA	1:221:A:GLU:C	2	5.23
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	1	5.22
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	8	5.22
(1,737)	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1:172:B:ASN:N	10	5.22
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	1	5.19
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	3	5.18
(1,406)	1:257:A:VAL:N	1:257:A:VAL:CA	1:257:A:VAL:C	1:258:A:LEU:N	6	5.18
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	4	5.17
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	5	5.14
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	7	5.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	1	5.09
(1,813)	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	1:258:B:LEU:N	10	5.07
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	1	5.07
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	5	5.0
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	5	4.99
(1,399)	1:248:A:TYR:N	1:248:A:TYR:CA	1:248:A:TYR:C	1:249:A:SER:N	6	4.99
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	9	4.99
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	8	4.94
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	10	4.94
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	10	4.94
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	8	4.87
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	3	4.87
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	2	4.85
(1,115)	1:152:A:PRO:C	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	7	4.85
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	4	4.8
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	1	4.78
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	5	4.75
(1,115)	1:152:A:PRO:C	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	4	4.74
(1,603)	1:245:B:LEU:C	1:246:B:LYS:N	1:246:B:LYS:CA	1:246:B:LYS:C	4	4.72
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	5	4.72
(1,115)	1:152:A:PRO:C	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1	4.72
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	1	4.71
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	7	4.71
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	1	4.67
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	1	4.65
(1,283)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:TYR:N	4	4.65
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	6	4.64
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	9	4.63
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	10	4.62
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	8	4.62
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	10	4.61
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	9	4.6
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	9	4.59
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	6	4.59
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	5	4.57
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	5	4.56
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	3	4.55
(1,174)	1:220:A:THR:C	1:221:A:GLU:N	1:221:A:GLU:CA	1:221:A:GLU:C	1	4.55
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	1	4.53
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	8	4.53
(1,522)	1:152:B:PRO:C	1:153:B:ILE:N	1:153:B:ILE:CA	1:153:B:ILE:C	1	4.53
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	8	4.52
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	3	4.51
(1,522)	1:152:B:PRO:C	1:153:B:ILE:N	1:153:B:ILE:CA	1:153:B:ILE:C	6	4.45
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	3	4.45
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	4	4.44
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1	4.44
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	5	4.4
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	9	4.37
(1,115)	1:152:A:PRO:C	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	6	4.36
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	4	4.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	6	4.31
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	4	4.29
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	10	4.27
(1,113)	1:150:A:ILE:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	6	4.26
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	3	4.23
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	3	4.22
(1,115)	1:152:A:PRO:C	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	5	4.19
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	8	4.17
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	6	4.14
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	2	4.13
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	4	4.13
(1,727)	1:160:B:LEU:N	1:160:B:LEU:CA	1:160:B:LEU:C	1:161:B:PRO:N	7	4.12
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	5	4.09
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	7	4.08
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	3	4.08
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	2	4.08
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	3	4.02
(1,314)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	2	4.0
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	7	4.0
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	9	3.99
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	2	3.98
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	10	3.95
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	2	3.94
(1,115)	1:152:A:PRO:C	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	8	3.91
(1,58)	1:83:A:GLN:C	1:84:A:ASN:N	1:84:A:ASN:CA	1:84:A:ASN:C	7	3.89
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	10	3.88
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	5	3.87
(1,395)	1:244:A:SER:N	1:244:A:SER:CA	1:244:A:SER:C	1:245:A:LEU:N	7	3.86
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	7	3.85
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	3	3.83
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	9	3.83
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	8	3.82
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	7	3.8
(1,522)	1:152:B:PRO:C	1:153:B:ILE:N	1:153:B:ILE:CA	1:153:B:ILE:C	4	3.79
(1,174)	1:220:A:THR:C	1:221:A:GLU:N	1:221:A:GLU:CA	1:221:A:GLU:C	6	3.79
(1,522)	1:152:B:PRO:C	1:153:B:ILE:N	1:153:B:ILE:CA	1:153:B:ILE:C	8	3.78
(1,721)	1:151:B:VAL:N	1:151:B:VAL:CA	1:151:B:VAL:C	1:152:B:PRO:N	2	3.77
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	7	3.76
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	10	3.74
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	1	3.72
(1,615)	1:6:B:SER:N	1:6:B:SER:CA	1:6:B:SER:C	1:7:B:PHE:N	6	3.7
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	6	3.7
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	7	3.7
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	9	3.69
(1,747)	1:181:B:ILE:N	1:181:B:ILE:CA	1:181:B:ILE:C	1:182:B:LEU:N	2	3.68
(1,320)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:PRO:N	7	3.66
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	9	3.66
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	8	3.64
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	1	3.63
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	3	3.61
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	6	3.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	5	3.53
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	5	3.51
(1,522)	1:152:B:PRO:C	1:153:B:ILE:N	1:153:B:ILE:CA	1:153:B:ILE:C	7	3.49
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	4	3.46
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	5	3.45
(1,58)	1:83:A:GLN:C	1:84:A:ASN:N	1:84:A:ASN:CA	1:84:A:ASN:C	4	3.45
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	9	3.42
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	7	3.4
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	10	3.37
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	8	3.32
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	6	3.31
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	10	3.3
(1,581)	1:220:B:THR:C	1:221:B:GLU:N	1:221:B:GLU:CA	1:221:B:GLU:C	2	3.29
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	7	3.27
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	7	3.27
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	3	3.23
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	4	3.22
(1,522)	1:152:B:PRO:C	1:153:B:ILE:N	1:153:B:ILE:CA	1:153:B:ILE:C	2	3.22
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	6	3.22
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	6	3.2
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	4	3.19
(1,112)	1:149:A:PRO:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	7	3.19
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	3	3.19
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	2	3.17
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	8	3.17
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	8	3.15
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	7	3.13
(1,65)	1:92:A:ILE:C	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	2	3.13
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	8	3.1
(1,208)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:PHE:N	6	3.09
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	9	3.08
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	3	3.06
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	10	3.03
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	1	3.03
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	4	3.01
(1,537)	1:170:B:ARG:C	1:171:B:PHE:N	1:171:B:PHE:CA	1:171:B:PHE:C	1	3.0
(1,115)	1:152:A:PRO:C	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	2	3.0
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	9	2.98
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	5	2.97
(1,522)	1:152:B:PRO:C	1:153:B:ILE:N	1:153:B:ILE:CA	1:153:B:ILE:C	5	2.97
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	2	2.97
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	4	2.93
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	2	2.9
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	1	2.9
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	8	2.9
(1,801)	1:243:B:SER:N	1:243:B:SER:CA	1:243:B:SER:C	1:244:B:SER:N	4	2.88
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	8	2.88
(1,275)	1:103:A:TRP:N	1:103:A:TRP:CA	1:103:A:TRP:C	1:104:A:ASN:N	7	2.87
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	5	2.86
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	10	2.83
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	2	2.83

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,599)	1:240:B:ALA:C	1:241:B:ASN:N	1:241:B:ASN:CA	1:241:B:ASN:C	9	2.81
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	1	2.8
(1,130)	1:170:A:ARG:C	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1	2.8
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	7	2.77
(1,317)	1:154:A:ARG:N	1:154:A:ARG:CA	1:154:A:ARG:C	1:155:A:ASN:N	10	2.76
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	2	2.75
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	5	2.75
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	10	2.74
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	6	2.71
(1,603)	1:245:B:LEU:C	1:246:B:LYS:N	1:246:B:LYS:CA	1:246:B:LYS:C	9	2.71
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	6	2.71
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	1	2.7
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	6	2.66
(1,802)	1:244:B:SER:N	1:244:B:SER:CA	1:244:B:SER:C	1:245:B:LEU:N	4	2.62
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	9	2.61
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	10	2.58
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	3	2.51
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	10	2.49
(1,340)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:LEU:N	8	2.45
(1,340)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:LEU:N	9	2.44
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	1	2.44
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	1	2.39
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	3	2.38
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	6	2.32
(1,275)	1:103:A:TRP:N	1:103:A:TRP:CA	1:103:A:TRP:C	1:104:A:ASN:N	1	2.29
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	4	2.24
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	4	2.24
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	2	2.24
(1,779)	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	1:219:B:GLY:N	9	2.21
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	5	2.19
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	8	2.18
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	7	2.15
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	7	2.12
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	10	2.12
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	4	2.11
(1,330)	1:171:A:PHE:N	1:171:A:PHE:CA	1:171:A:PHE:C	1:172:A:ASN:N	1	2.09
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	4	2.02
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	5	2.0
(1,340)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:LEU:N	5	1.99
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	10	1.98
(1,275)	1:103:A:TRP:N	1:103:A:TRP:CA	1:103:A:TRP:C	1:104:A:ASN:N	8	1.98
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	8	1.97
(1,275)	1:103:A:TRP:N	1:103:A:TRP:CA	1:103:A:TRP:C	1:104:A:ASN:N	4	1.97
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	2	1.97
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	6	1.97
(1,599)	1:240:B:ALA:C	1:241:B:ASN:N	1:241:B:ASN:CA	1:241:B:ASN:C	8	1.94
(1,58)	1:83:A:GLN:C	1:84:A:ASN:N	1:84:A:ASN:CA	1:84:A:ASN:C	6	1.94
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	7	1.91
(1,340)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:LEU:N	1	1.91
(1,518)	1:148:B:THR:C	1:149:B:PRO:N	1:149:B:PRO:CA	1:149:B:PRO:C	10	1.9
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	3	1.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	1	1.89
(1,174)	1:220:A:THR:C	1:221:A:GLU:N	1:221:A:GLU:CA	1:221:A:GLU:C	3	1.88
(1,766)	1:205:B:ALA:N	1:205:B:ALA:CA	1:205:B:ALA:C	1:206:B:ASP:N	3	1.86
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	6	1.86
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	9	1.85
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	4	1.85
(1,779)	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	1:219:B:GLY:N	8	1.84
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	6	1.81
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	9	1.78
(1,599)	1:240:B:ALA:C	1:241:B:ASN:N	1:241:B:ASN:CA	1:241:B:ASN:C	7	1.77
(1,524)	1:154:B:ARG:C	1:155:B:ASN:N	1:155:B:ASN:CA	1:155:B:ASN:C	9	1.76
(1,700)	1:129:B:GLN:N	1:129:B:GLN:CA	1:129:B:GLN:C	1:130:B:LYS:N	3	1.74
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	5	1.74
(1,340)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:LEU:N	6	1.72
(1,343)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:SER:N	5	1.71
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	3	1.7
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	2	1.69
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	1	1.67
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	3	1.66
(1,518)	1:148:B:THR:C	1:149:B:PRO:N	1:149:B:PRO:CA	1:149:B:PRO:C	9	1.62
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	1	1.61
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	10	1.59
(1,518)	1:148:B:THR:C	1:149:B:PRO:N	1:149:B:PRO:CA	1:149:B:PRO:C	8	1.59
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	9	1.58
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	8	1.57
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	9	1.54
(1,275)	1:103:A:TRP:N	1:103:A:TRP:CA	1:103:A:TRP:C	1:104:A:ASN:N	6	1.54
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	5	1.54
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	9	1.51
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	3	1.5
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	3	1.44
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	7	1.44
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	3	1.44
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	4	1.44
(1,620)	1:14:B:GLU:N	1:14:B:GLU:CA	1:14:B:GLU:C	1:15:B:VAL:N	6	1.41
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	6	1.41
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	9	1.41
(1,75)	1:103:A:TRP:C	1:104:A:ASN:N	1:104:A:ASN:CA	1:104:A:ASN:C	10	1.41
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	2	1.36
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	4	1.36
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	7	1.36
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	8	1.34
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	2	1.33
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	1	1.32
(1,553)	1:187:B:ASP:C	1:188:B:ASP:N	1:188:B:ASP:CA	1:188:B:ASP:C	5	1.3
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	9	1.29
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	10	1.29
(1,65)	1:92:A:ILE:C	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	6	1.29
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1	1.29
(1,779)	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	1:219:B:GLY:N	5	1.26
(1,599)	1:240:B:ALA:C	1:241:B:ASN:N	1:241:B:ASN:CA	1:241:B:ASN:C	2	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,37)	1:56:A:GLU:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	4	1.24
(1,599)	1:240:B:ALA:C	1:241:B:ASN:N	1:241:B:ASN:CA	1:241:B:ASN:C	4	1.23
(1,451)	1:68:B:LYS:C	1:69:B:HIS:N	1:69:B:HIS:CA	1:69:B:HIS:C	4	1.23
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	1	1.23
(1,806)	1:248:B:TYR:N	1:248:B:TYR:CA	1:248:B:TYR:C	1:249:B:SER:N	9	1.21
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	8	1.21
(1,398)	1:247:A:THR:N	1:247:A:THR:CA	1:247:A:THR:C	1:248:A:TYR:N	9	1.21
(1,174)	1:220:A:THR:C	1:221:A:GLU:N	1:221:A:GLU:CA	1:221:A:GLU:C	7	1.21
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	5	1.21
(1,34)	1:53:A:GLU:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	7	1.2
(1,580)	1:219:B:GLY:C	1:220:B:THR:N	1:220:B:THR:CA	1:220:B:THR:C	10	1.18
(1,779)	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	1:219:B:GLY:N	2	1.17
(1,518)	1:148:B:THR:C	1:149:B:PRO:N	1:149:B:PRO:CA	1:149:B:PRO:C	2	1.15
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	2	1.15
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	4	1.14
(1,117)	1:154:A:ARG:C	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	10	1.12
(1,323)	1:163:A:VAL:N	1:163:A:VAL:CA	1:163:A:VAL:C	1:164:A:GLY:N	7	1.11
(1,146)	1:187:A:ASP:C	1:188:A:ASP:N	1:188:A:ASP:CA	1:188:A:ASP:C	8	1.11
(1,812)	1:256:B:LYS:N	1:256:B:LYS:CA	1:256:B:LYS:C	1:257:B:VAL:N	2	1.08
(1,174)	1:220:A:THR:C	1:221:A:GLU:N	1:221:A:GLU:CA	1:221:A:GLU:C	5	1.08
(1,451)	1:68:B:LYS:C	1:69:B:HIS:N	1:69:B:HIS:CA	1:69:B:HIS:C	10	1.07
(1,451)	1:68:B:LYS:C	1:69:B:HIS:N	1:69:B:HIS:CA	1:69:B:HIS:C	3	1.06
(1,779)	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	1:219:B:GLY:N	10	1.04
(1,700)	1:129:B:GLN:N	1:129:B:GLN:CA	1:129:B:GLN:C	1:130:B:LYS:N	5	1.01