



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:10 PM UTC

PDB ID : 2N1F / pdb_00002n1f
EMDB ID : EMD-2971
BMRB ID : 26550
Title : Structure and assembly of the mouse ASC filament by combined NMR spectroscopy and cryo-electron microscopy
Authors : Sborgi, L.; Ravotti, F.; Dandey, V.; Dick, M.; Mazur, A.; Reckel, S.; Chami, M.; Scherer, S.; Bockmann, A.; Egelman, E.; Stahlberg, H.; Broz, P.; Meier, B.; Hiller, S.
Deposited on : 2015-04-01

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:

EMDB validation analysis : **NOT EXECUTED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **NOT EXECUTED**
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

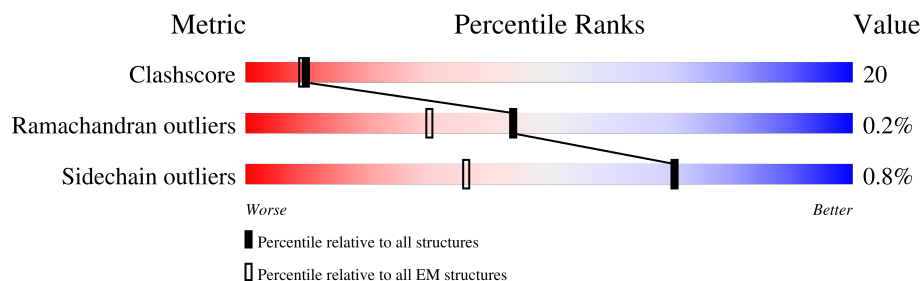
The following experimental techniques were used to determine the structure:

SOLID-STATE NMR, ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

The overall completeness of chemical shifts assignment is 3%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	89	71% 27% .
1	B	89	72% 28%
1	C	89	70% 30%
1	D	89	69% 31%
1	E	89	71% 29%
1	F	89	73% 27%
1	G	89	72% 28%
1	H	89	73% 27%

Continued on next page...

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Mol	Chain	Length	Quality of chain	
1	I	89		
1	J	89		
1	K	89		
1	L	89		
1	M	89		
1	N	89		
1	O	89		

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:4-A:90, B:2-B:90, C:2-C:90, D:2-D:90, E:2-E:90, F:2-F:90, G:2-G:90, H:2-H:90, I:2-I:90, J:2-J:90, K:2-K:90, L:2-L:90, M:2-M:90, N:2-N:90, O:2-O:90 (1333)	0.14	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 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 4, 6, 8
2	1, 5, 9
Single-model clusters	3; 7; 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10590 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Apoptosis-associated speck-like protein.

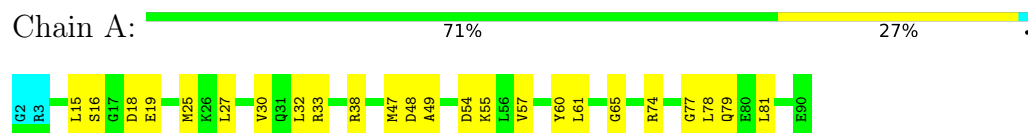
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	B	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	C	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	D	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	E	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	F	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	G	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	H	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	I	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	J	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	K	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	L	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	M	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	N	89	Total	C	N	O	S	0	
			706	445	119	138	4		
1	O	89	Total	C	N	O	S	0	
			706	445	119	138	4		

4 Residue-property plots [i](#)

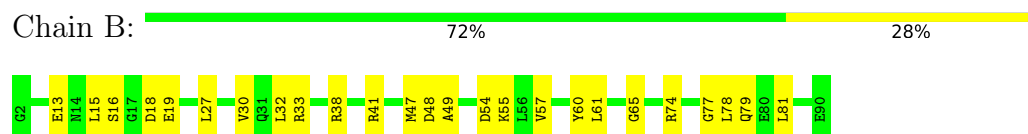
4.1 Average score per residue in the NMR ensemble

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.

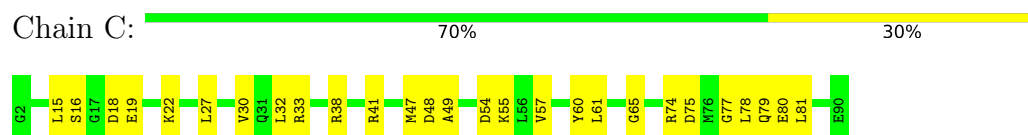
- Molecule 1: Apoptosis-associated speck-like protein



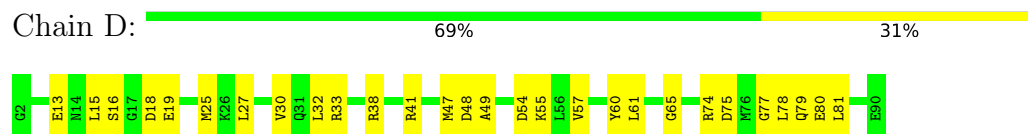
- Molecule 1: Apoptosis-associated speck-like protein



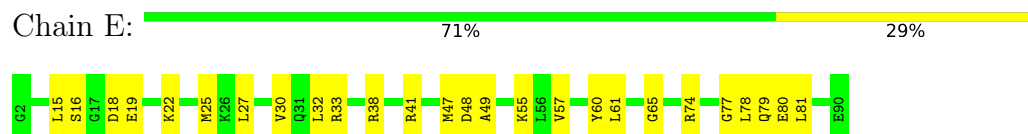
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

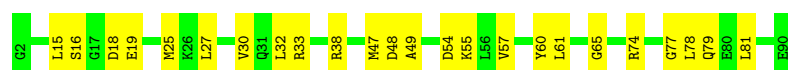


- Molecule 1: Apoptosis-associated speck-like protein



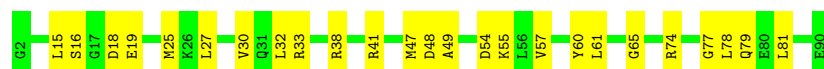
- Molecule 1: Apoptosis-associated speck-like protein

Chain F:  73% 27%



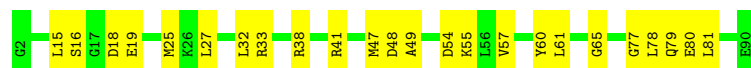
- Molecule 1: Apoptosis-associated speck-like protein

Chain G:  72% 28%



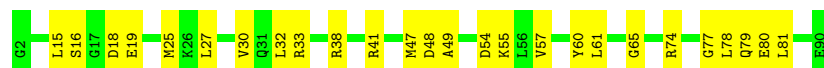
- Molecule 1: Apoptosis-associated speck-like protein

Chain H:  73% 27%



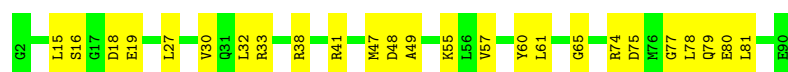
- Molecule 1: Apoptosis-associated speck-like protein

Chain I:  71% 29%



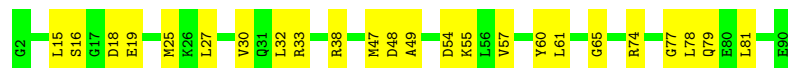
- Molecule 1: Apoptosis-associated speck-like protein

Chain J:  72% 28%



- Molecule 1: Apoptosis-associated speck-like protein

Chain K:  73% 27%



- Molecule 1: Apoptosis-associated speck-like protein

Chain L:  71% 29%

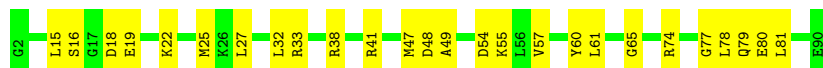


- Molecule 1: Apoptosis-associated speck-like protein

Chain M:  70% 30%



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

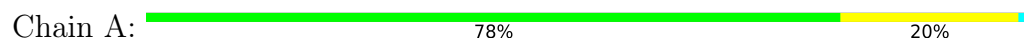


4.2 Scores per residue for each member of the ensemble

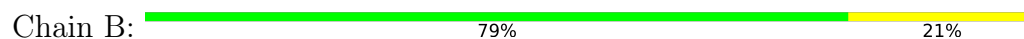
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

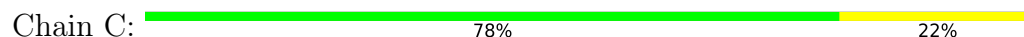
- Molecule 1: Apoptosis-associated speck-like protein



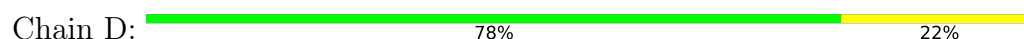
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

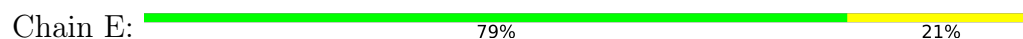


- Molecule 1: Apoptosis-associated speck-like protein

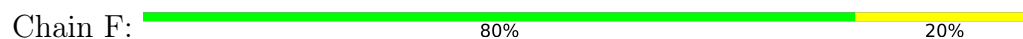




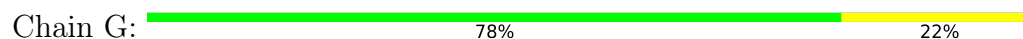
- Molecule 1: Apoptosis-associated speck-like protein



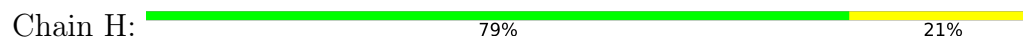
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



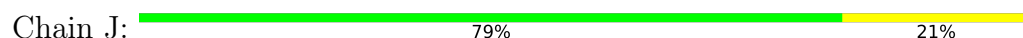
- Molecule 1: Apoptosis-associated speck-like protein



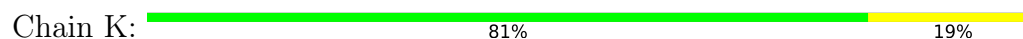
- Molecule 1: Apoptosis-associated speck-like protein



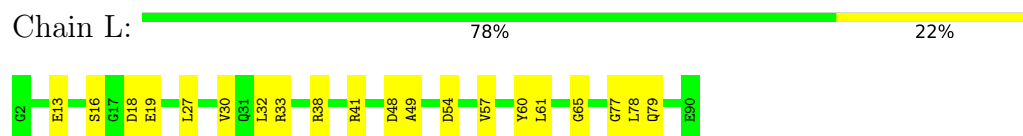
- Molecule 1: Apoptosis-associated speck-like protein



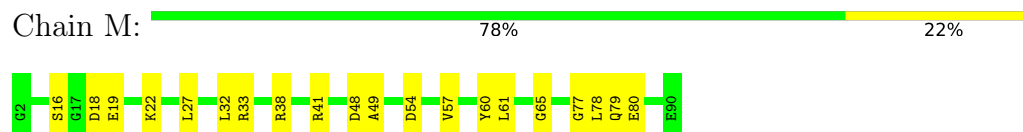
- Molecule 1: Apoptosis-associated speck-like protein



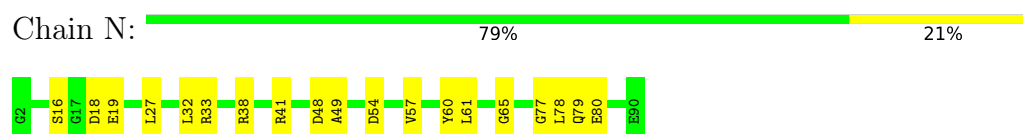
- Molecule 1: Apoptosis-associated speck-like protein



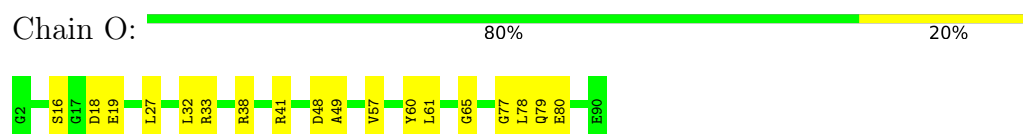
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

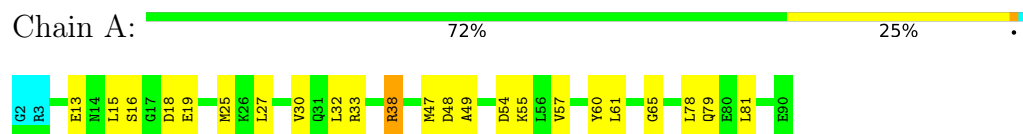


- Molecule 1: Apoptosis-associated speck-like protein

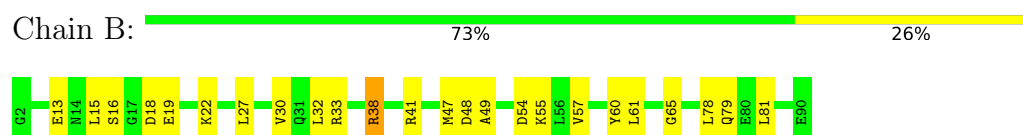


4.2.2 Score per residue for model 2

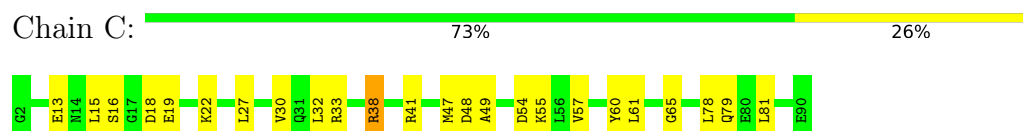
- Molecule 1: Apoptosis-associated speck-like protein



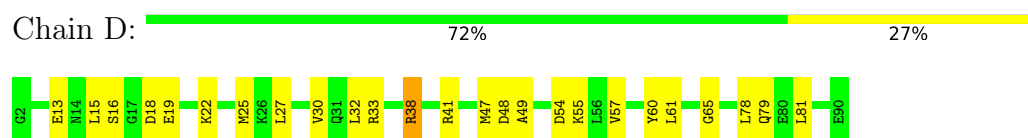
- Molecule 1: Apoptosis-associated speck-like protein



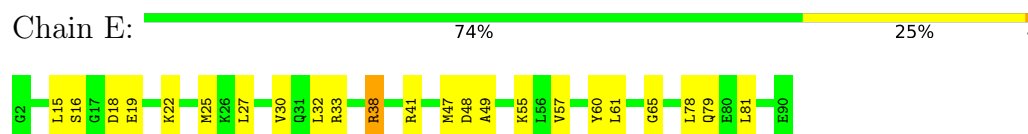
- Molecule 1: Apoptosis-associated speck-like protein



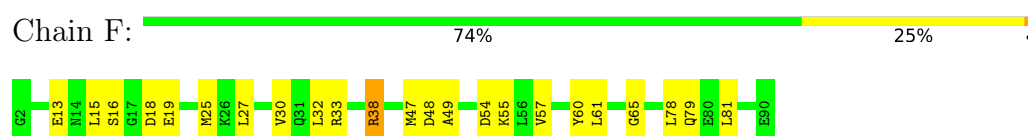
- Molecule 1: Apoptosis-associated speck-like protein



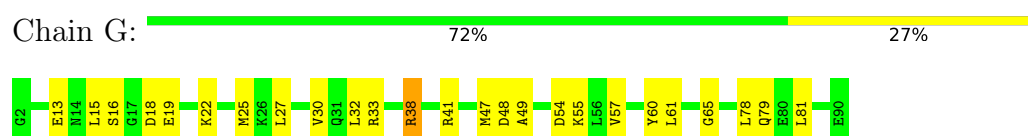
- Molecule 1: Apoptosis-associated speck-like protein



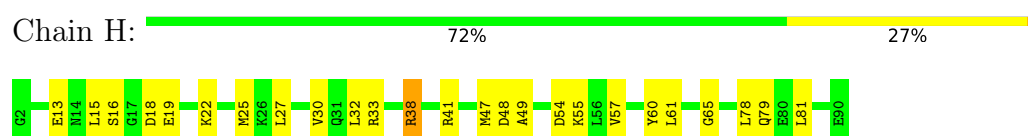
- Molecule 1: Apoptosis-associated speck-like protein



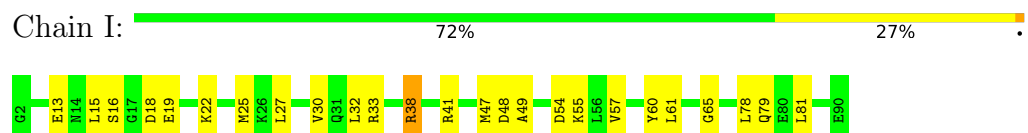
- Molecule 1: Apoptosis-associated speck-like protein



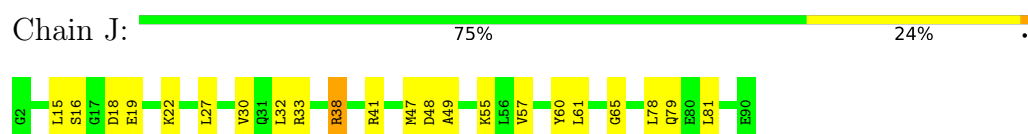
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



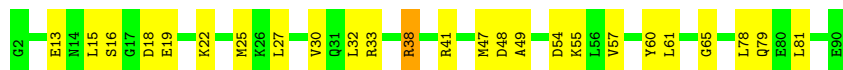
- Molecule 1: Apoptosis-associated speck-like protein





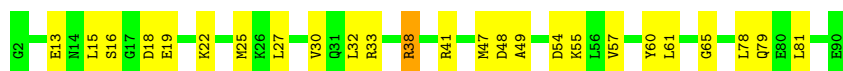
- Molecule 1: Apoptosis-associated speck-like protein

Chain L: 72% 27%



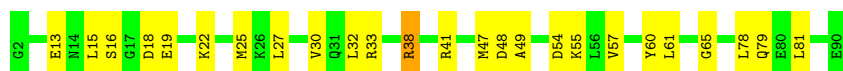
- Molecule 1: Apoptosis-associated speck-like protein

Chain M: 72% 27%



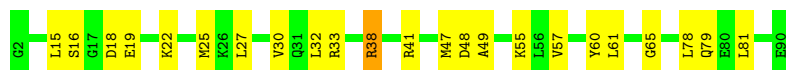
- Molecule 1: Apoptosis-associated speck-like protein

Chain N: 72% 27%



- Molecule 1: Apoptosis-associated speck-like protein

Chain O: 74% 25%



4.2.3 Score per residue for model 3

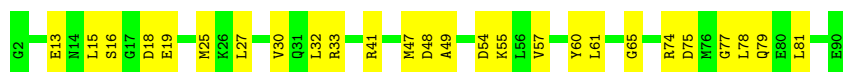
- Molecule 1: Apoptosis-associated speck-like protein

Chain A: 71% 27%



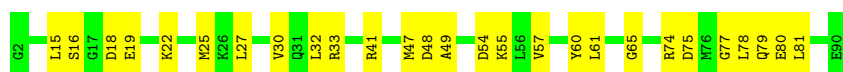
- Molecule 1: Apoptosis-associated speck-like protein

Chain B: 71% 29%

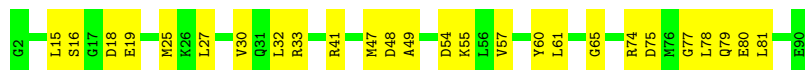


- Molecule 1: Apoptosis-associated speck-like protein

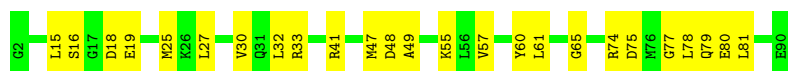
Chain C: 70% 30%



- Molecule 1: Apoptosis-associated speck-like protein



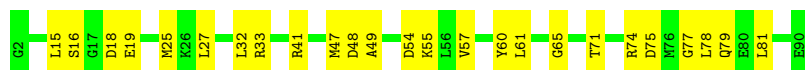
- Molecule 1: Apoptosis-associated speck-like protein



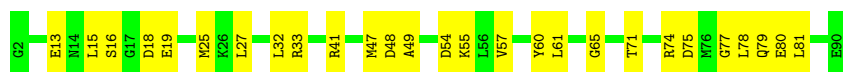
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



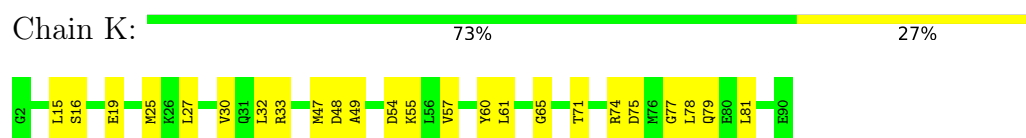
- Molecule 1: Apoptosis-associated speck-like protein



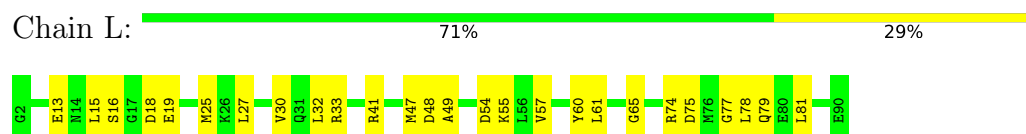
- Molecule 1: Apoptosis-associated speck-like protein



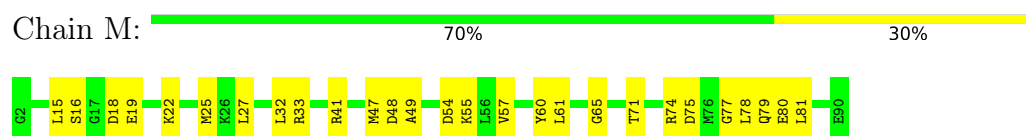
- Molecule 1: Apoptosis-associated speck-like protein



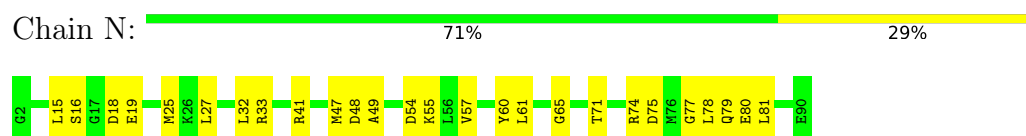
- Molecule 1: Apoptosis-associated speck-like protein



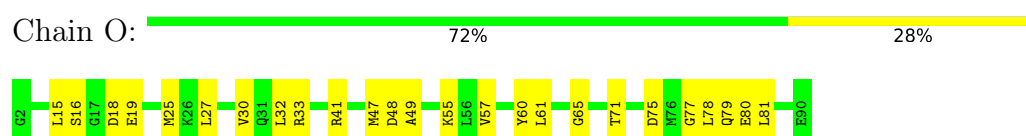
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

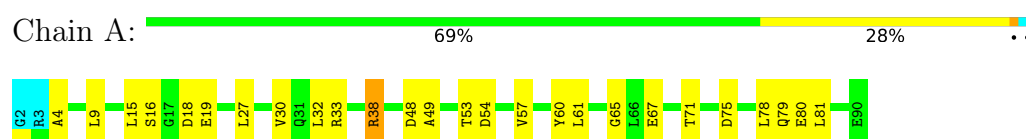


- Molecule 1: Apoptosis-associated speck-like protein

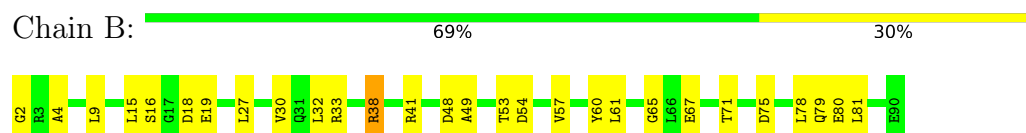


4.2.4 Score per residue for model 4

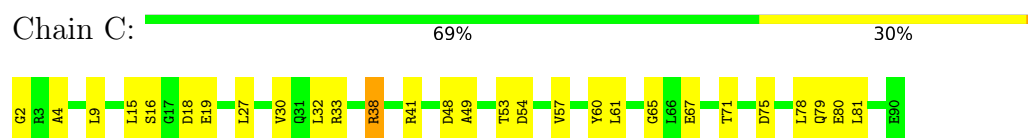
- Molecule 1: Apoptosis-associated speck-like protein



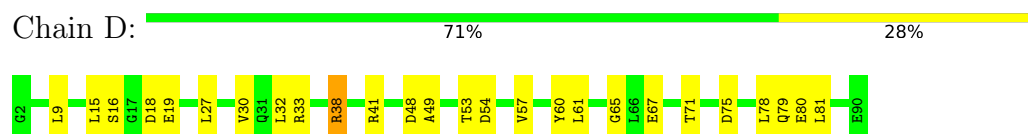
- Molecule 1: Apoptosis-associated speck-like protein



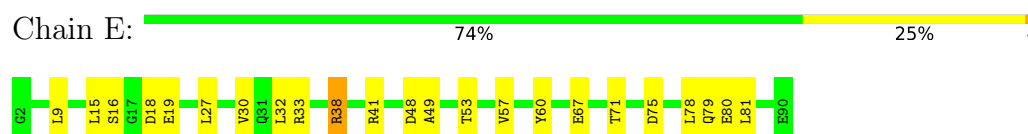
- Molecule 1: Apoptosis-associated speck-like protein



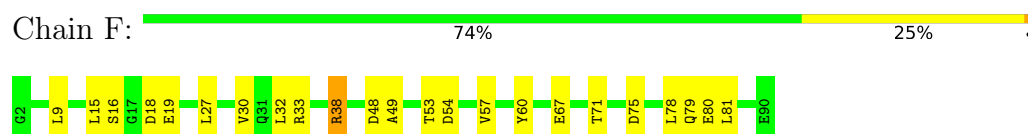
- Molecule 1: Apoptosis-associated speck-like protein



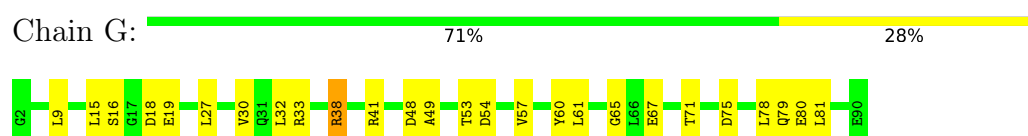
- Molecule 1: Apoptosis-associated speck-like protein



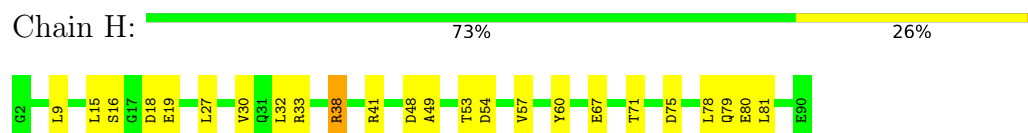
- Molecule 1: Apoptosis-associated speck-like protein



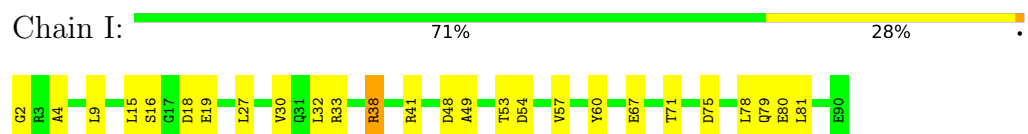
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

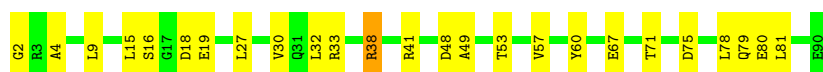


- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein





- Molecule 1: Apoptosis-associated speck-like protein

Chain K: 74% 25%



- Molecule 1: Apoptosis-associated speck-like protein

Chain L: 71% 28%



- Molecule 1: Apoptosis-associated speck-like protein

Chain M: 71% 28%



- Molecule 1: Apoptosis-associated speck-like protein

Chain N: 73% 26%



- Molecule 1: Apoptosis-associated speck-like protein

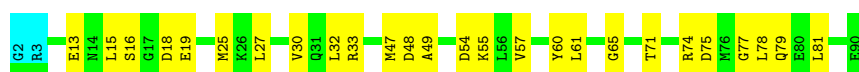
Chain O: 70% 29%



4.2.5 Score per residue for model 5

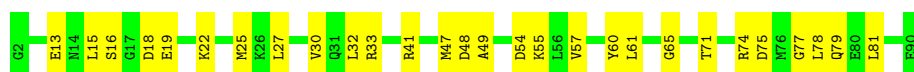
- Molecule 1: Apoptosis-associated speck-like protein

Chain A: 69% 29%

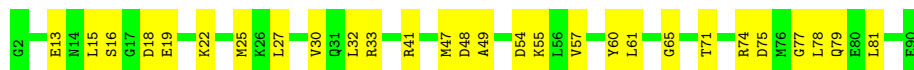


- Molecule 1: Apoptosis-associated speck-like protein

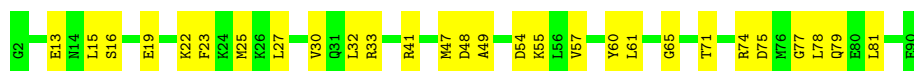
Chain B: 69% 31%



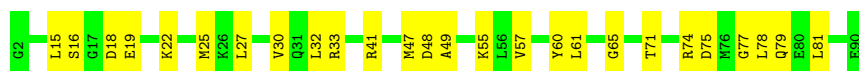
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



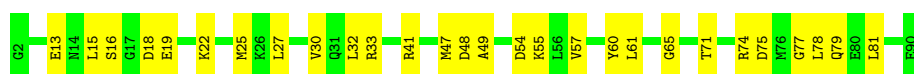
- Molecule 1: Apoptosis-associated speck-like protein



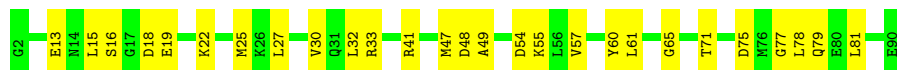
- Molecule 1: Apoptosis-associated speck-like protein



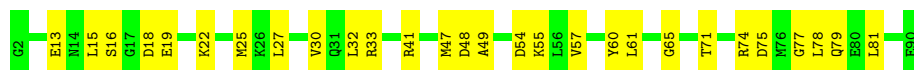
- Molecule 1: Apoptosis-associated speck-like protein



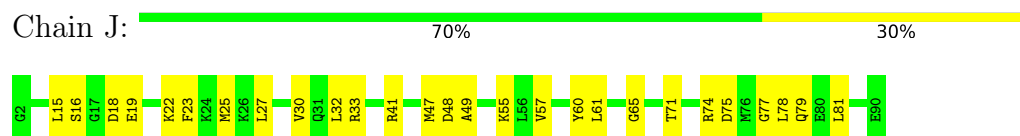
- Molecule 1: Apoptosis-associated speck-like protein



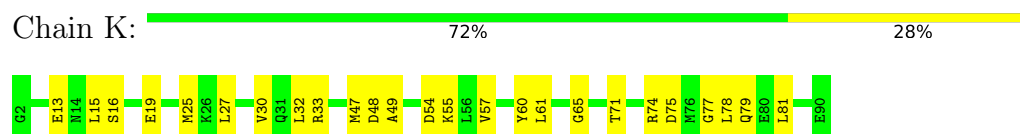
- Molecule 1: Apoptosis-associated speck-like protein



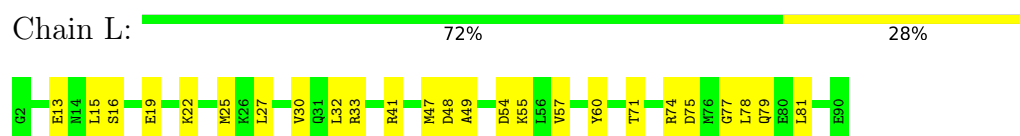
- Molecule 1: Apoptosis-associated speck-like protein



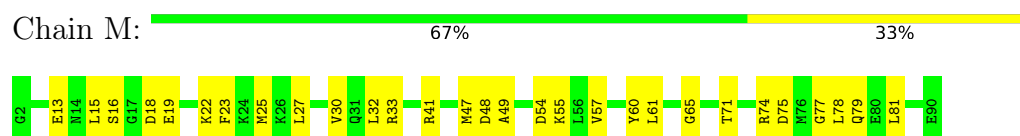
- Molecule 1: Apoptosis-associated speck-like protein



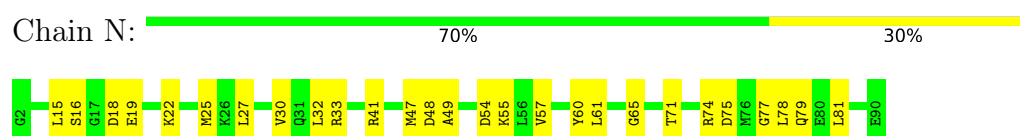
- Molecule 1: Apoptosis-associated speck-like protein



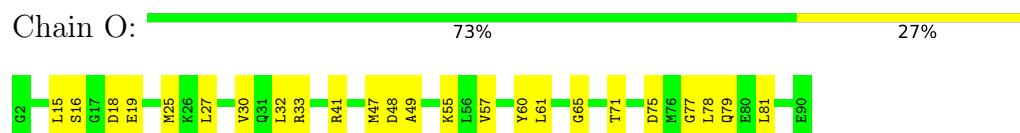
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

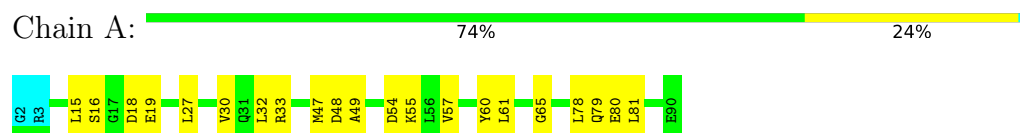


- Molecule 1: Apoptosis-associated speck-like protein

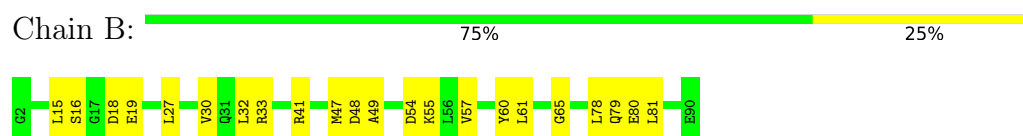


4.2.6 Score per residue for model 6

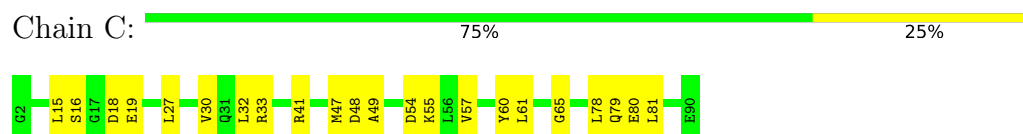
- Molecule 1: Apoptosis-associated speck-like protein



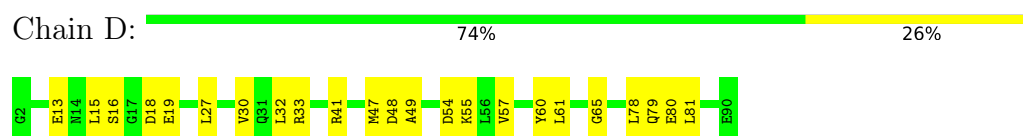
- Molecule 1: Apoptosis-associated speck-like protein



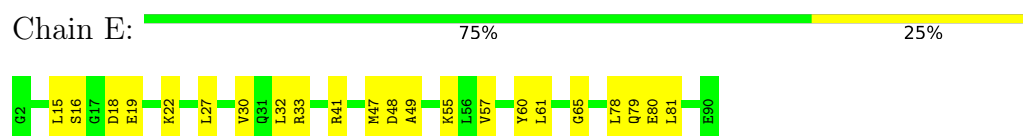
- Molecule 1: Apoptosis-associated speck-like protein



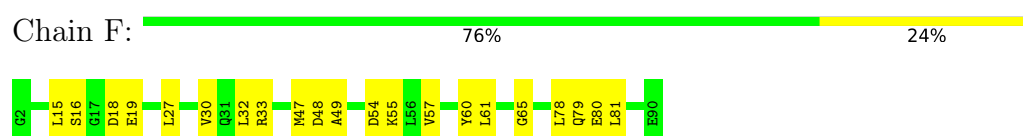
- Molecule 1: Apoptosis-associated speck-like protein



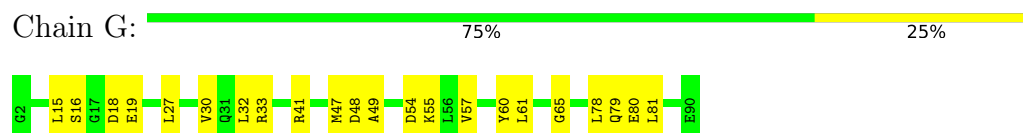
- Molecule 1: Apoptosis-associated speck-like protein



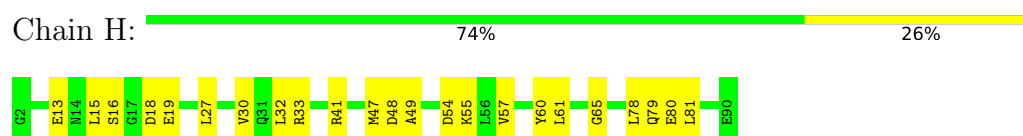
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

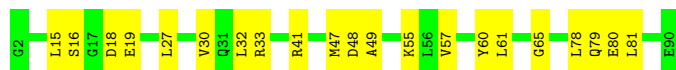


- Molecule 1: Apoptosis-associated speck-like protein

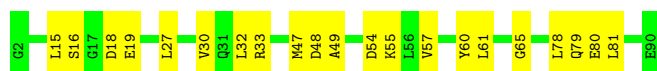
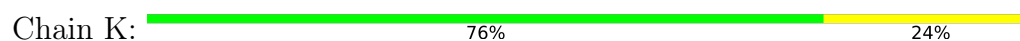




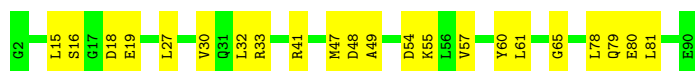
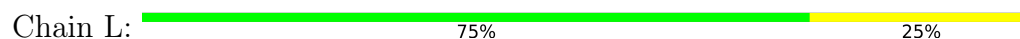
- Molecule 1: Apoptosis-associated speck-like protein



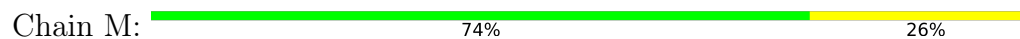
- Molecule 1: Apoptosis-associated speck-like protein



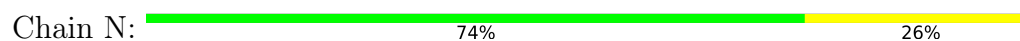
- Molecule 1: Apoptosis-associated speck-like protein



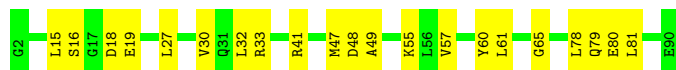
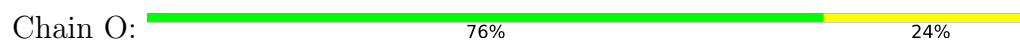
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



4.2.7 Score per residue for model 7

- Molecule 1: Apoptosis-associated speck-like protein





- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



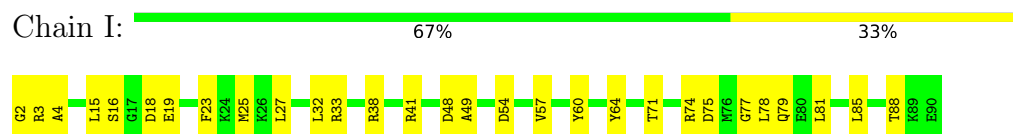
- Molecule 1: Apoptosis-associated speck-like protein



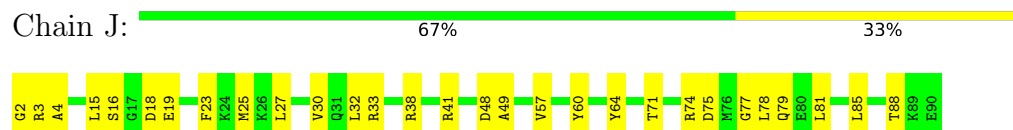
- Molecule 1: Apoptosis-associated speck-like protein



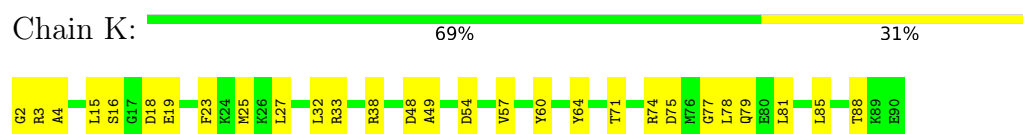
- Molecule 1: Apoptosis-associated speck-like protein



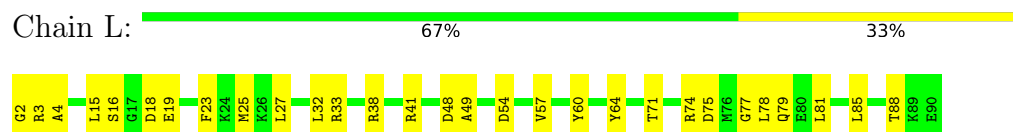
- Molecule 1: Apoptosis-associated speck-like protein



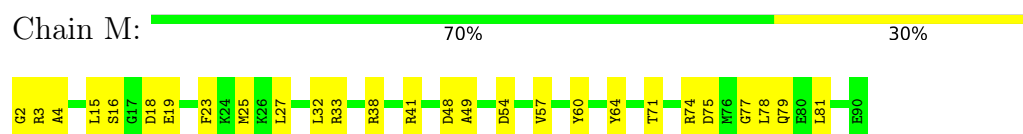
- Molecule 1: Apoptosis-associated speck-like protein



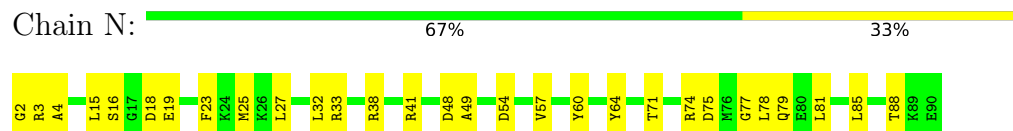
- Molecule 1: Apoptosis-associated speck-like protein



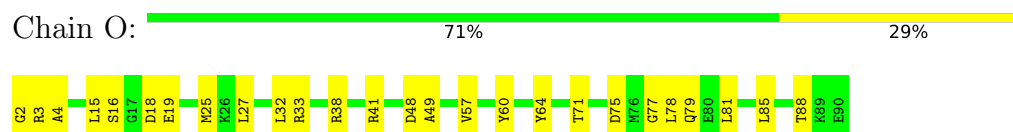
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



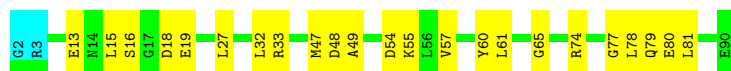
- Molecule 1: Apoptosis-associated speck-like protein



4.2.8 Score per residue for model 8

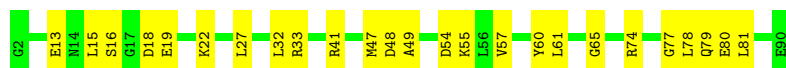
- Molecule 1: Apoptosis-associated speck-like protein

Chain A:  72% 26%



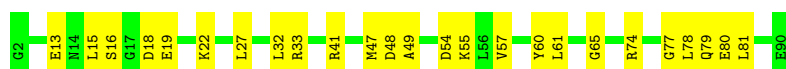
- Molecule 1: Apoptosis-associated speck-like protein

Chain B:  72% 28%



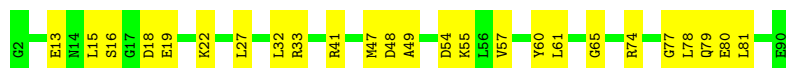
- Molecule 1: Apoptosis-associated speck-like protein

Chain C:  72% 28%



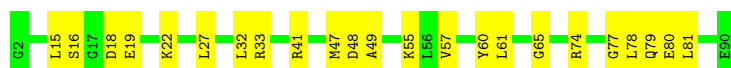
- Molecule 1: Apoptosis-associated speck-like protein

Chain D:  72% 28%



- Molecule 1: Apoptosis-associated speck-like protein

Chain E:  74% 26%



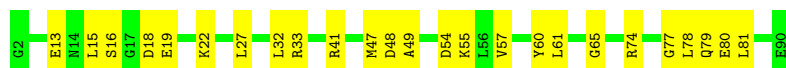
- Molecule 1: Apoptosis-associated speck-like protein

Chain F:  74% 26%

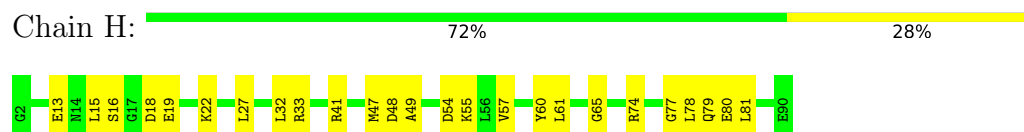


- Molecule 1: Apoptosis-associated speck-like protein

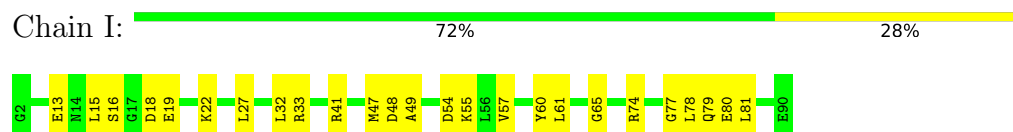
Chain G:  72% 28%



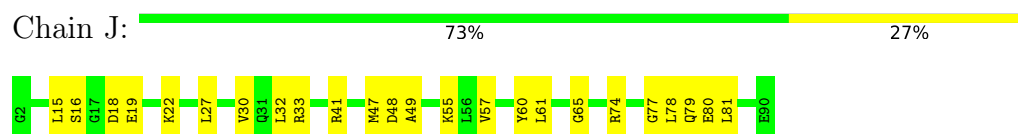
- Molecule 1: Apoptosis-associated speck-like protein



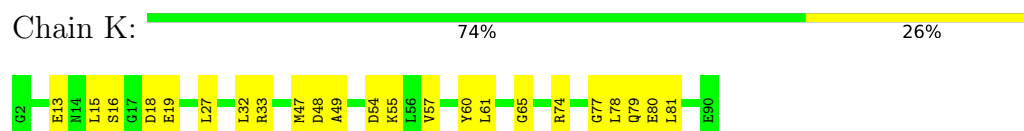
- Molecule 1: Apoptosis-associated speck-like protein



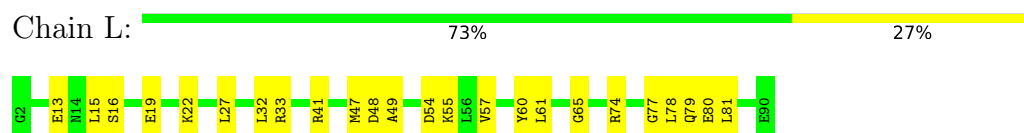
- Molecule 1: Apoptosis-associated speck-like protein



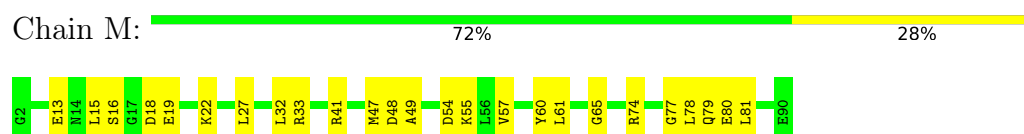
- Molecule 1: Apoptosis-associated speck-like protein



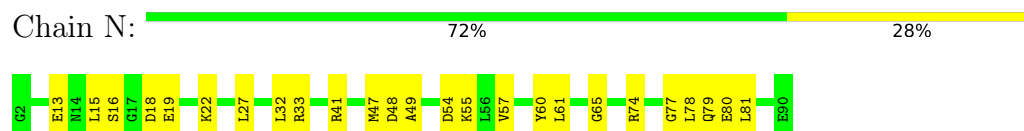
- Molecule 1: Apoptosis-associated speck-like protein



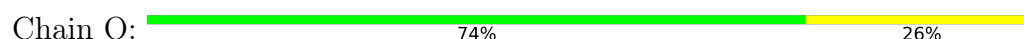
- Molecule 1: Apoptosis-associated speck-like protein

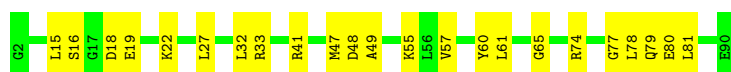


- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein





4.2.9 Score per residue for model 9

- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



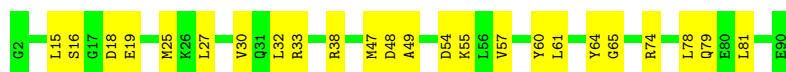
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

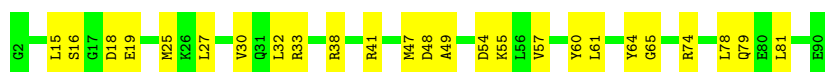


- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein





- Molecule 1: Apoptosis-associated speck-like protein



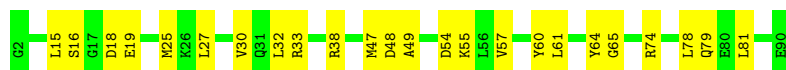
- Molecule 1: Apoptosis-associated speck-like protein



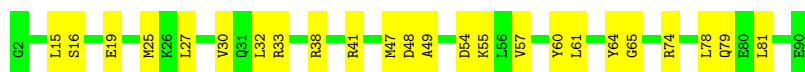
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein



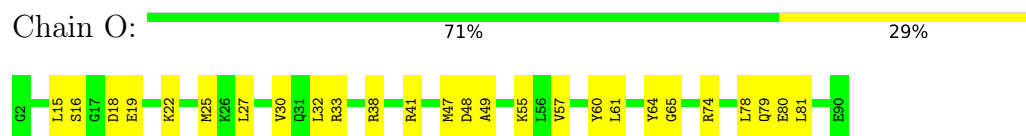
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

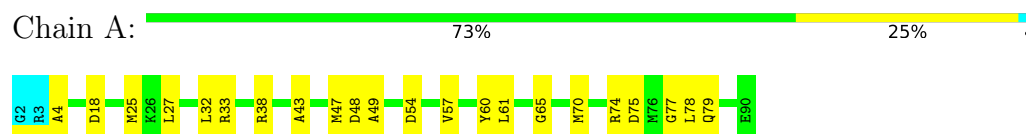


- Molecule 1: Apoptosis-associated speck-like protein

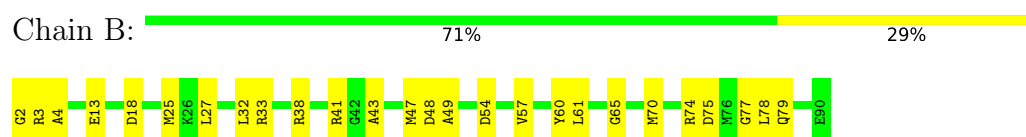


4.2.10 Score per residue for model 10

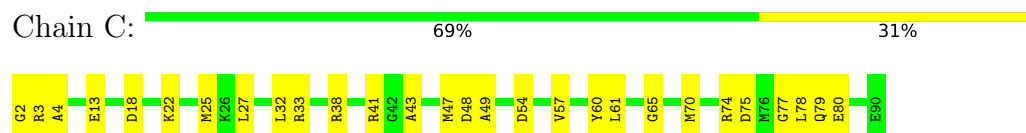
- Molecule 1: Apoptosis-associated speck-like protein



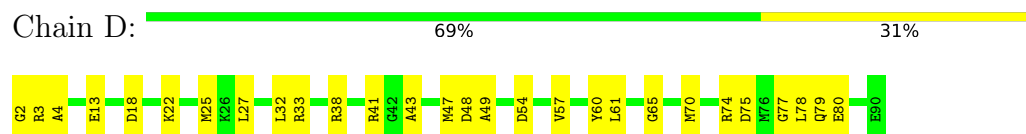
- Molecule 1: Apoptosis-associated speck-like protein



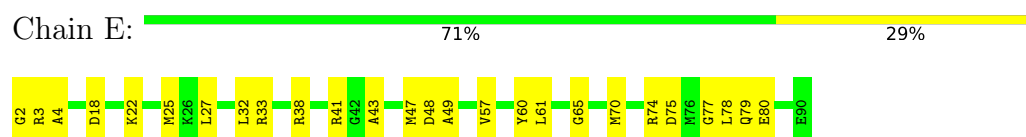
- Molecule 1: Apoptosis-associated speck-like protein



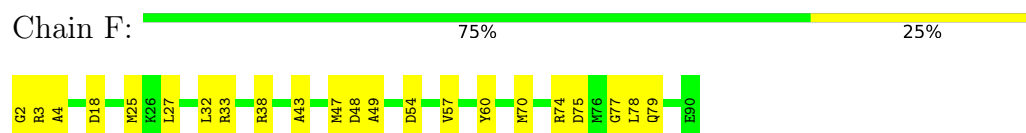
- Molecule 1: Apoptosis-associated speck-like protein



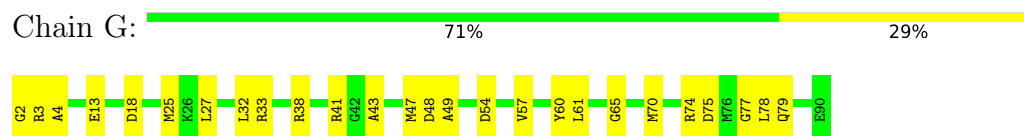
- Molecule 1: Apoptosis-associated speck-like protein



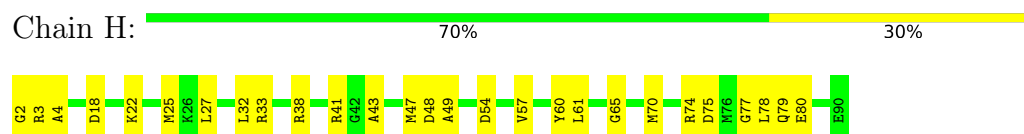
- Molecule 1: Apoptosis-associated speck-like protein



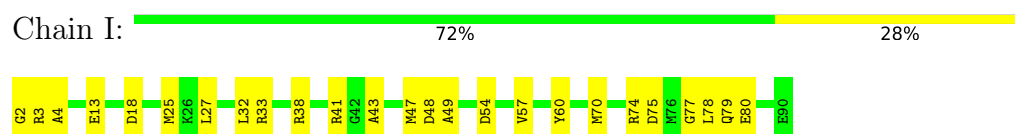
- Molecule 1: Apoptosis-associated speck-like protein



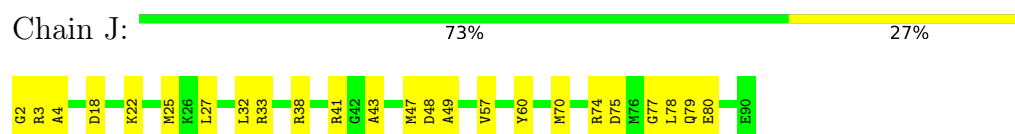
- Molecule 1: Apoptosis-associated speck-like protein



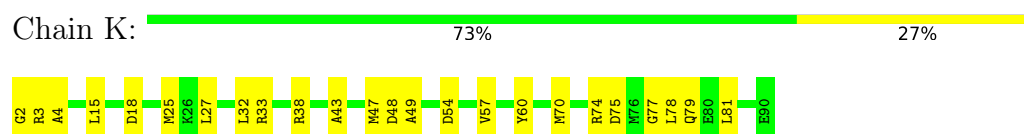
- Molecule 1: Apoptosis-associated speck-like protein



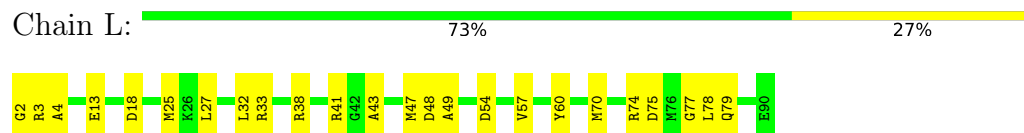
- Molecule 1: Apoptosis-associated speck-like protein



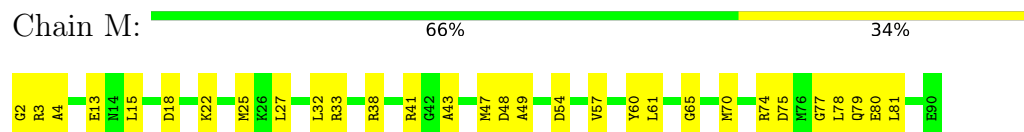
- Molecule 1: Apoptosis-associated speck-like protein



- Molecule 1: Apoptosis-associated speck-like protein

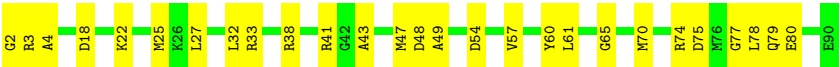


- Molecule 1: Apoptosis-associated speck-like protein

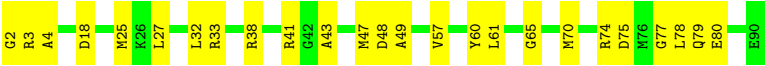


- Molecule 1: Apoptosis-associated speck-like protein





● Molecule 1: Apoptosis-associated speck-like protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *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
CYANA	structure solution	
XPLOR-NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	484
Number of shifts mapped to atoms	484
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	691	0	716	28±3
1	B	706	0	731	31±3
1	C	706	0	731	32±3
1	D	706	0	731	31±3
1	E	706	0	731	29±3
1	F	706	0	731	28±3
1	G	706	0	731	31±3
1	H	706	0	731	31±3
1	I	706	0	731	30±3
1	J	706	0	731	29±3
1	K	706	0	731	29±3
1	L	706	0	731	30±3
1	M	706	0	731	31±3
1	N	706	0	731	30±3
1	O	706	0	731	28±3
All	All	105750	0	109500	4208

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:L:54:ASP:OD2	1:M:41:ARG:NH2	1.30	1.65	5	4
1:F:54:ASP:OD2	1:G:41:ARG:NH2	1.29	1.66	5	4
1:M:54:ASP:OD2	1:N:41:ARG:NH2	1.28	1.63	5	4
1:A:54:ASP:OD2	1:B:41:ARG:NH2	1.28	1.66	5	5
1:C:54:ASP:OD2	1:D:41:ARG:NH2	1.28	1.67	5	4
1:D:54:ASP:OD2	1:E:41:ARG:NH2	1.26	1.67	5	5
1:G:54:ASP:OD2	1:H:41:ARG:NH2	1.26	1.68	5	4
1:H:54:ASP:OD2	1:I:41:ARG:NH2	1.25	1.66	5	5
1:K:54:ASP:OD2	1:L:41:ARG:NH2	1.25	1.66	5	4
1:N:54:ASP:OD2	1:O:41:ARG:NH2	1.24	1.71	5	4
1:B:54:ASP:OD2	1:C:41:ARG:NH2	1.24	1.70	5	4
1:I:54:ASP:OD2	1:J:41:ARG:NH2	1.24	1.68	5	4
1:D:54:ASP:OD1	1:E:41:ARG:NH2	1.11	1.84	4	5
1:L:54:ASP:OD1	1:M:41:ARG:NH2	1.10	1.85	4	5
1:I:54:ASP:OD1	1:J:41:ARG:NH2	1.08	1.86	4	5
1:B:13:GLU:OE2	1:C:22:LYS:NZ	1.07	1.87	8	1
1:I:13:GLU:OE2	1:J:22:LYS:NZ	1.06	1.88	8	1
1:N:13:GLU:OE2	1:O:22:LYS:NZ	1.06	1.88	8	1
1:D:13:GLU:OE2	1:E:22:LYS:NZ	1.06	1.89	8	1
1:H:13:GLU:OE2	1:I:22:LYS:NZ	1.06	1.89	8	1
1:G:54:ASP:OD1	1:H:41:ARG:NH2	1.05	1.89	4	5
1:G:13:GLU:OE2	1:H:22:LYS:NZ	1.05	1.89	8	1
1:L:13:GLU:OE2	1:M:22:LYS:NZ	1.05	1.89	8	1
1:C:13:GLU:OE2	1:D:22:LYS:NZ	1.05	1.89	8	1
1:F:54:ASP:OD1	1:G:41:ARG:NH2	1.05	1.88	4	5
1:M:54:ASP:OD1	1:N:41:ARG:NH2	1.05	1.89	4	5
1:A:13:GLU:OE2	1:B:22:LYS:NZ	1.04	1.90	8	1
1:B:54:ASP:OD1	1:C:41:ARG:NH2	1.04	1.91	4	5
1:H:54:ASP:OD1	1:I:41:ARG:NH2	1.04	1.89	4	5
1:C:54:ASP:OD1	1:D:41:ARG:NH2	1.04	1.90	4	5
1:A:54:ASP:OD1	1:B:41:ARG:NH2	1.04	1.90	4	5
1:M:13:GLU:OE2	1:N:22:LYS:NZ	1.04	1.90	8	1
1:K:54:ASP:OD1	1:L:41:ARG:NH2	1.03	1.90	8	5
1:K:13:GLU:OE2	1:L:22:LYS:NZ	1.03	1.92	8	1
1:F:13:GLU:OE2	1:G:22:LYS:NZ	1.02	1.92	8	1
1:N:54:ASP:OD1	1:O:41:ARG:NH2	1.01	1.90	4	5
1:E:16:SER:HB3	1:E:19:GLU:OE1	0.84	1.72	2	2
1:L:16:SER:HB3	1:L:19:GLU:OE1	0.84	1.72	2	2
1:D:16:SER:HB3	1:D:19:GLU:OE1	0.84	1.72	2	2
1:F:16:SER:HB3	1:F:19:GLU:OE1	0.84	1.72	2	2
1:M:16:SER:HB3	1:M:19:GLU:OE1	0.84	1.73	2	2
1:L:16:SER:HB2	1:L:19:GLU:OE1	0.84	1.73	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:K:16:SER:HB3	1:K:19:GLU:OE1	0.84	1.73	5	2
1:N:16:SER:HB3	1:N:19:GLU:OE1	0.84	1.73	2	2
1:E:16:SER:HB2	1:E:19:GLU:OE1	0.84	1.73	9	7
1:D:16:SER:HB2	1:D:19:GLU:OE1	0.84	1.73	9	7
1:F:16:SER:HB2	1:F:19:GLU:OE1	0.84	1.73	9	7
1:B:16:SER:HB3	1:B:19:GLU:OE1	0.84	1.73	5	2
1:M:16:SER:HB2	1:M:19:GLU:OE1	0.83	1.73	9	7
1:C:16:SER:HB3	1:C:19:GLU:OE1	0.83	1.73	5	2
1:G:16:SER:HB3	1:G:19:GLU:OE1	0.83	1.72	2	2
1:J:16:SER:HB3	1:J:19:GLU:OE1	0.83	1.72	2	2
1:A:16:SER:HB3	1:A:19:GLU:OE1	0.83	1.73	5	2
1:K:16:SER:HB2	1:K:19:GLU:OE1	0.83	1.73	9	7
1:N:16:SER:HB2	1:N:19:GLU:OE1	0.83	1.73	9	7
1:I:16:SER:HB3	1:I:19:GLU:OE1	0.83	1.72	2	2
1:B:16:SER:HB2	1:B:19:GLU:OE1	0.83	1.73	9	7
1:C:16:SER:HB2	1:C:19:GLU:OE1	0.83	1.73	9	7
1:G:16:SER:HB2	1:G:19:GLU:OE1	0.83	1.73	9	7
1:O:16:SER:HB3	1:O:19:GLU:OE1	0.82	1.72	2	2
1:H:16:SER:HB3	1:H:19:GLU:OE1	0.82	1.73	2	2
1:J:16:SER:HB2	1:J:19:GLU:OE1	0.82	1.73	9	7
1:I:16:SER:HB2	1:I:19:GLU:OE1	0.82	1.73	9	7
1:A:16:SER:HB2	1:A:19:GLU:OE1	0.82	1.73	9	7
1:H:16:SER:HB2	1:H:19:GLU:OE1	0.82	1.73	9	7
1:O:16:SER:HB2	1:O:19:GLU:OE1	0.82	1.73	9	7
1:A:13:GLU:CD	1:B:22:LYS:NZ	0.76	2.44	8	1
1:C:13:GLU:CD	1:D:22:LYS:NZ	0.76	2.44	8	1
1:D:13:GLU:CD	1:E:22:LYS:NZ	0.75	2.44	8	1
1:L:13:GLU:CD	1:M:22:LYS:NZ	0.75	2.44	8	1
1:N:13:GLU:CD	1:O:22:LYS:NZ	0.75	2.45	8	1
1:B:13:GLU:CD	1:C:22:LYS:NZ	0.74	2.45	8	1
1:G:13:GLU:CD	1:H:22:LYS:NZ	0.74	2.45	8	1
1:M:13:GLU:CD	1:N:22:LYS:NZ	0.74	2.45	8	1
1:I:13:GLU:CD	1:J:22:LYS:NZ	0.74	2.45	8	1
1:H:13:GLU:CD	1:I:22:LYS:NZ	0.74	2.46	8	1
1:K:13:GLU:CD	1:L:22:LYS:NZ	0.74	2.46	8	1
1:K:32:LEU:C	1:K:32:LEU:HD12	0.74	2.08	4	10
1:D:32:LEU:C	1:D:32:LEU:HD12	0.73	2.08	7	10
1:B:32:LEU:HD12	1:B:32:LEU:C	0.73	2.08	4	10
1:E:32:LEU:HD12	1:E:32:LEU:C	0.73	2.08	4	10
1:C:32:LEU:C	1:C:32:LEU:HD12	0.73	2.08	4	10
1:J:32:LEU:HD12	1:J:32:LEU:C	0.73	2.08	7	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:M:32:LEU:C	1:M:32:LEU:HD12	0.73	2.08	4	10
1:I:32:LEU:C	1:I:32:LEU:HD12	0.73	2.08	4	10
1:L:32:LEU:HD12	1:L:32:LEU:C	0.73	2.08	7	10
1:N:32:LEU:C	1:N:32:LEU:HD12	0.73	2.08	7	10
1:O:32:LEU:C	1:O:32:LEU:HD12	0.73	2.08	7	10
1:H:32:LEU:C	1:H:32:LEU:HD12	0.72	2.08	4	10
1:A:32:LEU:C	1:A:32:LEU:HD12	0.72	2.08	7	10
1:F:32:LEU:C	1:F:32:LEU:HD12	0.72	2.08	4	10
1:G:32:LEU:HD12	1:G:32:LEU:C	0.72	2.08	4	10
1:F:13:GLU:CD	1:G:22:LYS:NZ	0.71	2.49	8	1
1:B:78:LEU:C	1:B:78:LEU:HD23	0.69	2.13	7	10
1:E:78:LEU:C	1:E:78:LEU:HD23	0.69	2.13	10	10
1:I:78:LEU:C	1:I:78:LEU:HD23	0.69	2.13	10	10
1:C:78:LEU:HD23	1:C:78:LEU:C	0.69	2.13	7	10
1:D:78:LEU:C	1:D:78:LEU:HD23	0.69	2.13	10	10
1:L:78:LEU:C	1:L:78:LEU:HD23	0.69	2.13	10	10
1:M:78:LEU:HD23	1:M:78:LEU:C	0.69	2.13	7	10
1:F:32:LEU:CD1	1:F:33:ARG:O	0.69	2.41	5	10
1:J:32:LEU:CD1	1:J:33:ARG:O	0.69	2.41	5	10
1:F:78:LEU:HD23	1:F:78:LEU:C	0.69	2.13	10	10
1:J:78:LEU:C	1:J:78:LEU:HD23	0.69	2.13	10	10
1:K:78:LEU:C	1:K:78:LEU:HD23	0.69	2.13	8	10
1:O:70:MET:HE3	1:O:74:ARG:NH2	0.69	2.04	10	1
1:G:78:LEU:C	1:G:78:LEU:HD23	0.68	2.13	7	10
1:E:70:MET:HE3	1:E:74:ARG:NH2	0.68	2.04	10	1
1:E:32:LEU:CD1	1:E:33:ARG:O	0.68	2.41	5	10
1:H:78:LEU:HD23	1:H:78:LEU:C	0.68	2.13	7	10
1:K:32:LEU:CD1	1:K:33:ARG:O	0.68	2.41	5	10
1:H:70:MET:HE3	1:H:74:ARG:NH2	0.68	2.04	10	1
1:M:70:MET:HE3	1:M:74:ARG:NH2	0.68	2.04	10	1
1:A:78:LEU:HD23	1:A:78:LEU:C	0.68	2.13	10	10
1:L:32:LEU:CD1	1:L:33:ARG:O	0.68	2.41	5	10
1:I:32:LEU:CD1	1:I:33:ARG:O	0.68	2.41	5	10
1:B:70:MET:HE3	1:B:74:ARG:NH2	0.68	2.04	10	1
1:F:70:MET:HE3	1:F:74:ARG:NH2	0.68	2.04	10	1
1:D:32:LEU:CD1	1:D:33:ARG:O	0.68	2.41	5	10
1:G:32:LEU:CD1	1:G:33:ARG:O	0.68	2.41	5	10
1:O:32:LEU:CD1	1:O:33:ARG:O	0.68	2.41	5	10
1:M:61:LEU:N	1:M:61:LEU:HD12	0.68	2.03	3	1
1:A:32:LEU:CD1	1:A:33:ARG:O	0.68	2.41	5	10
1:N:78:LEU:C	1:N:78:LEU:HD23	0.68	2.13	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:O:61:LEU:HD12	1:O:61:LEU:N	0.68	2.03	3	1
1:A:70:MET:HE3	1:A:74:ARG:NH2	0.68	2.03	10	1
1:A:61:LEU:N	1:A:61:LEU:HD12	0.68	2.03	3	1
1:H:61:LEU:N	1:H:61:LEU:HD12	0.68	2.03	3	1
1:J:61:LEU:HD12	1:J:61:LEU:N	0.68	2.03	3	1
1:D:70:MET:HE3	1:D:74:ARG:NH2	0.68	2.04	10	1
1:C:32:LEU:CD1	1:C:33:ARG:O	0.68	2.41	5	10
1:M:32:LEU:CD1	1:M:33:ARG:O	0.68	2.41	5	10
1:J:70:MET:HE3	1:J:74:ARG:NH2	0.68	2.03	10	1
1:B:32:LEU:CD1	1:B:33:ARG:O	0.68	2.41	5	10
1:O:78:LEU:C	1:O:78:LEU:HD23	0.68	2.14	4	10
1:B:61:LEU:HD12	1:B:61:LEU:N	0.68	2.03	3	1
1:K:61:LEU:N	1:K:61:LEU:HD12	0.68	2.03	3	1
1:H:32:LEU:CD1	1:H:33:ARG:O	0.67	2.41	5	10
1:N:32:LEU:CD1	1:N:33:ARG:O	0.67	2.41	5	10
1:F:61:LEU:N	1:F:61:LEU:HD12	0.67	2.03	3	1
1:C:61:LEU:N	1:C:61:LEU:HD12	0.67	2.03	3	1
1:E:61:LEU:HD12	1:E:61:LEU:N	0.67	2.03	3	1
1:N:61:LEU:N	1:N:61:LEU:HD12	0.67	2.03	3	1
1:I:70:MET:HE3	1:I:74:ARG:NH2	0.67	2.04	10	1
1:K:70:MET:HE3	1:K:74:ARG:NH2	0.67	2.04	10	1
1:D:61:LEU:N	1:D:61:LEU:HD12	0.67	2.03	3	1
1:I:61:LEU:N	1:I:61:LEU:HD12	0.67	2.03	3	1
1:G:61:LEU:HD12	1:G:61:LEU:N	0.67	2.03	3	1
1:L:61:LEU:HD12	1:L:61:LEU:N	0.67	2.03	3	1
1:L:70:MET:HE3	1:L:74:ARG:NH2	0.67	2.03	10	1
1:G:70:MET:HE3	1:G:74:ARG:NH2	0.67	2.04	10	1
1:N:70:MET:HE3	1:N:74:ARG:NH2	0.67	2.04	10	1
1:J:61:LEU:HD12	1:J:61:LEU:H	0.67	1.50	3	1
1:C:70:MET:HE3	1:C:74:ARG:NH2	0.67	2.04	10	1
1:A:61:LEU:HD12	1:A:61:LEU:H	0.67	1.50	3	1
1:D:61:LEU:HD12	1:D:61:LEU:H	0.66	1.50	3	1
1:K:61:LEU:HD12	1:K:61:LEU:H	0.66	1.50	3	1
1:O:61:LEU:HD12	1:O:61:LEU:H	0.66	1.50	3	1
1:I:61:LEU:HD12	1:I:61:LEU:H	0.65	1.50	3	1
1:B:61:LEU:HD12	1:B:61:LEU:H	0.65	1.51	3	1
1:G:61:LEU:HD12	1:G:61:LEU:H	0.65	1.50	3	1
1:C:61:LEU:HD12	1:C:61:LEU:H	0.65	1.50	3	1
1:E:61:LEU:HD12	1:E:61:LEU:H	0.65	1.50	3	1
1:H:27:LEU:C	1:H:27:LEU:HD23	0.65	2.17	10	10
1:N:27:LEU:HD23	1:N:27:LEU:C	0.65	2.17	10	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:27:LEU:C	1:G:27:LEU:HD23	0.65	2.17	10	9
1:M:27:LEU:C	1:M:27:LEU:HD23	0.65	2.17	10	8
1:F:61:LEU:HD12	1:F:61:LEU:H	0.65	1.50	3	1
1:H:61:LEU:HD12	1:H:61:LEU:H	0.65	1.50	3	1
1:E:27:LEU:C	1:E:27:LEU:HD23	0.65	2.17	10	9
1:B:27:LEU:HD23	1:B:27:LEU:C	0.65	2.17	10	10
1:D:27:LEU:HD23	1:D:27:LEU:C	0.64	2.17	10	10
1:A:27:LEU:C	1:A:27:LEU:HD23	0.64	2.17	10	9
1:C:27:LEU:C	1:C:27:LEU:HD23	0.64	2.17	10	9
1:B:27:LEU:HD23	1:B:27:LEU:O	0.64	1.93	1	10
1:I:27:LEU:HD23	1:I:27:LEU:O	0.64	1.93	1	10
1:F:27:LEU:C	1:F:27:LEU:HD23	0.64	2.17	10	9
1:I:27:LEU:HD23	1:I:27:LEU:C	0.64	2.17	10	10
1:N:61:LEU:HD12	1:N:61:LEU:H	0.64	1.50	3	1
1:M:27:LEU:O	1:M:27:LEU:HD23	0.64	1.93	8	2
1:N:27:LEU:HD23	1:N:27:LEU:O	0.64	1.93	1	10
1:E:27:LEU:HD23	1:E:27:LEU:O	0.64	1.93	1	10
1:M:27:LEU:HD23	1:M:27:LEU:O	0.64	1.93	10	8
1:O:27:LEU:C	1:O:27:LEU:HD23	0.64	2.17	10	9
1:D:27:LEU:HD23	1:D:27:LEU:O	0.63	1.93	8	10
1:G:27:LEU:HD23	1:G:27:LEU:O	0.63	1.93	8	10
1:L:27:LEU:C	1:L:27:LEU:HD23	0.63	2.17	10	8
1:M:61:LEU:HD12	1:M:61:LEU:H	0.63	1.50	3	1
1:I:33:ARG:NH2	1:I:64:TYR:CD1	0.63	2.67	9	2
1:O:33:ARG:NH2	1:O:64:TYR:CD1	0.63	2.67	9	2
1:K:27:LEU:HD23	1:K:27:LEU:O	0.63	1.93	1	10
1:M:27:LEU:HD23	1:M:27:LEU:C	0.63	2.18	8	2
1:F:27:LEU:HD23	1:F:27:LEU:O	0.63	1.93	8	9
1:L:61:LEU:HD12	1:L:61:LEU:H	0.63	1.50	3	1
1:A:33:ARG:NH2	1:A:64:TYR:CD1	0.63	2.67	9	2
1:J:33:ARG:NH2	1:J:64:TYR:CD1	0.63	2.67	9	2
1:B:33:ARG:NH2	1:B:64:TYR:CD1	0.63	2.66	9	2
1:L:27:LEU:HD23	1:L:27:LEU:O	0.63	1.93	8	10
1:C:27:LEU:O	1:C:27:LEU:HD23	0.63	1.93	1	1
1:F:27:LEU:O	1:F:27:LEU:HD23	0.63	1.93	1	1
1:J:27:LEU:C	1:J:27:LEU:HD23	0.63	2.17	10	8
1:C:33:ARG:NH2	1:C:64:TYR:CD1	0.63	2.67	9	2
1:G:33:ARG:NH2	1:G:64:TYR:CD1	0.63	2.66	9	2
1:A:27:LEU:O	1:A:27:LEU:HD23	0.63	1.93	1	1
1:J:27:LEU:O	1:J:27:LEU:HD23	0.63	1.93	8	2
1:O:32:LEU:HD12	1:O:32:LEU:O	0.63	1.94	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:K:27:LEU:C	1:K:27:LEU:HD23	0.63	2.17	10	7
1:K:33:ARG:NH2	1:K:64:TYR:CD1	0.63	2.67	9	2
1:G:27:LEU:HD23	1:G:27:LEU:C	0.63	2.19	1	1
1:H:27:LEU:HD23	1:H:27:LEU:O	0.63	1.92	1	10
1:C:27:LEU:HD23	1:C:27:LEU:O	0.63	1.93	10	9
1:O:27:LEU:O	1:O:27:LEU:HD23	0.63	1.93	1	1
1:O:27:LEU:HD23	1:O:27:LEU:O	0.63	1.93	10	9
1:C:32:LEU:HD12	1:C:32:LEU:O	0.62	1.94	4	10
1:E:32:LEU:HD12	1:E:32:LEU:O	0.62	1.94	4	10
1:G:32:LEU:HD12	1:G:32:LEU:O	0.62	1.94	4	10
1:A:27:LEU:HD23	1:A:27:LEU:O	0.62	1.93	10	9
1:J:27:LEU:HD23	1:J:27:LEU:O	0.62	1.93	10	8
1:E:33:ARG:NH2	1:E:64:TYR:CD1	0.62	2.67	9	2
1:M:33:ARG:NH2	1:M:64:TYR:CD1	0.62	2.66	9	2
1:C:47:MET:HE1	1:C:55:LYS:NZ	0.62	2.09	2	2
1:F:33:ARG:NH2	1:F:64:TYR:CD1	0.62	2.66	9	2
1:H:33:ARG:NH2	1:H:64:TYR:CD1	0.62	2.67	9	2
1:N:33:ARG:NH2	1:N:64:TYR:CD1	0.62	2.67	9	2
1:A:27:LEU:HD23	1:A:27:LEU:C	0.62	2.19	1	1
1:E:27:LEU:HD23	1:E:27:LEU:C	0.62	2.19	1	1
1:L:27:LEU:HD23	1:L:27:LEU:C	0.62	2.18	8	2
1:C:27:LEU:HD23	1:C:27:LEU:C	0.62	2.19	1	1
1:J:27:LEU:HD23	1:J:27:LEU:C	0.62	2.18	8	2
1:D:47:MET:HE1	1:D:55:LYS:NZ	0.62	2.09	2	2
1:H:32:LEU:HD12	1:H:32:LEU:O	0.62	1.94	4	10
1:L:32:LEU:HD12	1:L:32:LEU:O	0.62	1.94	4	10
1:E:47:MET:HE1	1:E:55:LYS:NZ	0.62	2.10	2	2
1:F:47:MET:HE1	1:F:55:LYS:NZ	0.62	2.10	2	2
1:M:32:LEU:HD12	1:M:32:LEU:O	0.62	1.94	4	10
1:N:47:MET:HE1	1:N:55:LYS:NZ	0.62	2.10	2	2
1:D:33:ARG:NH2	1:D:64:TYR:CD1	0.62	2.67	9	2
1:F:27:LEU:HD23	1:F:27:LEU:C	0.62	2.19	1	1
1:O:47:MET:HE1	1:O:55:LYS:NZ	0.62	2.09	2	2
1:K:27:LEU:HD23	1:K:27:LEU:C	0.62	2.18	2	3
1:I:47:MET:HE1	1:I:55:LYS:NZ	0.62	2.10	2	2
1:O:27:LEU:HD23	1:O:27:LEU:C	0.62	2.19	1	1
1:L:47:MET:HE1	1:L:55:LYS:NZ	0.62	2.09	2	2
1:M:47:MET:HE1	1:M:55:LYS:NZ	0.62	2.09	2	2
1:F:32:LEU:HD12	1:F:32:LEU:O	0.62	1.94	4	10
1:B:47:MET:HE1	1:B:55:LYS:NZ	0.62	2.09	2	2
1:H:47:MET:HE1	1:H:55:LYS:NZ	0.62	2.09	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:L:33:ARG:NH2	1:L:64:TYR:CD1	0.61	2.67	9	2
1:I:32:LEU:HD12	1:I:32:LEU:O	0.61	1.94	4	10
1:K:32:LEU:HD12	1:K:32:LEU:O	0.61	1.94	4	10
1:D:32:LEU:HD12	1:D:32:LEU:O	0.61	1.94	4	10
1:A:47:MET:HE1	1:A:55:LYS:NZ	0.61	2.10	2	2
1:K:47:MET:HE1	1:K:55:LYS:NZ	0.61	2.09	2	2
1:N:32:LEU:HD12	1:N:32:LEU:O	0.61	1.94	4	10
1:B:47:MET:HE1	1:B:55:LYS:HZ2	0.61	1.55	2	1
1:G:47:MET:HE1	1:G:55:LYS:NZ	0.61	2.09	2	2
1:B:32:LEU:HD12	1:B:32:LEU:O	0.61	1.94	4	10
1:G:78:LEU:HD23	1:G:79:GLN:N	0.61	2.11	8	10
1:N:78:LEU:HD23	1:N:79:GLN:N	0.61	2.11	8	10
1:A:32:LEU:HD12	1:A:32:LEU:O	0.61	1.94	4	10
1:J:32:LEU:HD12	1:J:32:LEU:O	0.61	1.94	4	10
1:A:78:LEU:HD23	1:A:79:GLN:N	0.60	2.11	8	10
1:J:47:MET:HE1	1:J:55:LYS:NZ	0.60	2.09	2	2
1:I:32:LEU:HD12	1:I:33:ARG:O	0.60	1.97	5	8
1:K:78:LEU:HD23	1:K:79:GLN:N	0.60	2.11	8	10
1:D:78:LEU:HD23	1:D:79:GLN:N	0.60	2.11	8	10
1:G:32:LEU:HD12	1:G:33:ARG:O	0.60	1.97	5	8
1:J:78:LEU:HD23	1:J:79:GLN:N	0.60	2.11	8	10
1:C:78:LEU:HD23	1:C:79:GLN:N	0.60	2.11	8	10
1:H:78:LEU:HD23	1:H:79:GLN:N	0.60	2.11	8	10
1:N:32:LEU:HD12	1:N:33:ARG:O	0.60	1.97	5	8
1:O:32:LEU:HD12	1:O:33:ARG:O	0.60	1.97	5	8
1:E:32:LEU:HD12	1:E:33:ARG:O	0.60	1.97	5	8
1:E:78:LEU:HD23	1:E:79:GLN:N	0.60	2.11	8	10
1:L:78:LEU:HD23	1:L:79:GLN:N	0.60	2.11	8	10
1:A:32:LEU:HD12	1:A:33:ARG:O	0.60	1.97	5	8
1:B:32:LEU:HD12	1:B:33:ARG:O	0.60	1.97	5	8
1:C:32:LEU:HD12	1:C:33:ARG:O	0.60	1.97	5	8
1:H:32:LEU:HD12	1:H:33:ARG:O	0.60	1.97	5	8
1:F:32:LEU:HD12	1:F:33:ARG:O	0.59	1.97	5	8
1:K:32:LEU:HD12	1:K:33:ARG:O	0.59	1.97	5	8
1:D:54:ASP:CG	1:E:41:ARG:NH2	0.59	2.61	7	3
1:I:78:LEU:HD23	1:I:79:GLN:N	0.59	2.11	8	10
1:J:32:LEU:HD12	1:J:33:ARG:O	0.59	1.97	5	8
1:M:32:LEU:HD12	1:M:33:ARG:O	0.59	1.97	5	8
1:H:54:ASP:CG	1:I:41:ARG:NH2	0.59	2.61	7	2
1:O:78:LEU:HD23	1:O:79:GLN:N	0.59	2.11	8	10
1:B:78:LEU:HD23	1:B:79:GLN:N	0.59	2.11	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:L:32:LEU:HD12	1:L:33:ARG:O	0.59	1.97	5	8
1:F:78:LEU:HD23	1:F:79:GLN:N	0.58	2.11	8	10
1:M:78:LEU:HD23	1:M:79:GLN:N	0.58	2.11	8	10
1:K:9:LEU:HD12	1:K:53:THR:HG21	0.58	1.76	4	1
1:J:9:LEU:HD12	1:J:53:THR:HG21	0.58	1.76	4	1
1:A:54:ASP:CG	1:B:41:ARG:NH2	0.58	2.62	7	2
1:D:32:LEU:HD12	1:D:33:ARG:O	0.58	1.97	5	8
1:D:9:LEU:HD12	1:D:53:THR:HG21	0.58	1.76	4	1
1:L:9:LEU:HD12	1:L:53:THR:HG21	0.58	1.76	4	1
1:C:9:LEU:HD12	1:C:53:THR:HG21	0.58	1.76	4	1
1:I:9:LEU:HD12	1:I:53:THR:HG21	0.58	1.76	4	1
1:J:47:MET:HE1	1:J:55:LYS:HZ2	0.58	1.59	2	1
1:B:9:LEU:HD12	1:B:53:THR:HG21	0.58	1.76	4	1
1:B:33:ARG:NH2	1:B:64:TYR:CE1	0.58	2.72	9	1
1:C:33:ARG:NH2	1:C:64:TYR:CE1	0.58	2.72	9	1
1:J:33:ARG:NH2	1:J:64:TYR:CE1	0.58	2.72	9	1
1:N:33:ARG:NH2	1:N:64:TYR:CE1	0.58	2.72	9	1
1:E:9:LEU:HD12	1:E:53:THR:HG21	0.57	1.76	4	1
1:A:9:LEU:HD12	1:A:53:THR:HG21	0.57	1.76	4	1
1:A:33:ARG:NH2	1:A:64:TYR:CE1	0.57	2.72	9	1
1:G:33:ARG:NH2	1:G:64:TYR:CE1	0.57	2.72	9	1
1:L:33:ARG:NH2	1:L:64:TYR:CE1	0.57	2.72	9	1
1:O:33:ARG:NH2	1:O:64:TYR:CE1	0.57	2.72	9	1
1:H:9:LEU:HD12	1:H:53:THR:HG21	0.57	1.76	4	1
1:D:33:ARG:NH2	1:D:64:TYR:CE1	0.57	2.72	9	1
1:E:33:ARG:NH2	1:E:64:TYR:CE1	0.57	2.72	9	1
1:F:33:ARG:NH2	1:F:64:TYR:CE1	0.57	2.72	9	1
1:K:33:ARG:NH2	1:K:64:TYR:CE1	0.57	2.72	9	1
1:M:9:LEU:HD12	1:M:53:THR:HG21	0.57	1.76	4	1
1:O:9:LEU:HD12	1:O:53:THR:HG21	0.57	1.76	4	1
1:M:33:ARG:NH2	1:M:64:TYR:CE1	0.57	2.72	9	1
1:E:43:ALA:O	1:E:47:MET:HG3	0.57	2.00	10	1
1:M:43:ALA:O	1:M:47:MET:HG3	0.57	2.00	10	1
1:B:43:ALA:O	1:B:47:MET:HG3	0.57	2.00	10	1
1:I:43:ALA:O	1:I:47:MET:HG3	0.57	2.00	10	1
1:O:47:MET:HE1	1:O:55:LYS:CD	0.57	2.30	6	4
1:F:43:ALA:O	1:F:47:MET:HG3	0.57	2.00	10	1
1:I:33:ARG:NH2	1:I:64:TYR:CE1	0.57	2.72	9	1
1:N:47:MET:HE1	1:N:55:LYS:CD	0.57	2.30	6	4
1:B:80:GLU:CD	1:B:80:GLU:H	0.57	2.08	8	3
1:F:9:LEU:HD12	1:F:53:THR:HG21	0.57	1.76	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:MET:HE1	1:A:55:LYS:CD	0.57	2.30	6	4
1:A:43:ALA:O	1:A:47:MET:HG3	0.57	2.00	10	1
1:I:47:MET:HE1	1:I:55:LYS:CD	0.56	2.30	6	4
1:J:80:GLU:CD	1:J:80:GLU:H	0.56	2.08	6	3
1:J:47:MET:HE1	1:J:55:LYS:CD	0.56	2.30	6	4
1:K:80:GLU:CD	1:K:80:GLU:H	0.56	2.08	6	3
1:I:54:ASP:CG	1:J:41:ARG:NH2	0.56	2.64	7	2
1:L:43:ALA:O	1:L:47:MET:HG3	0.56	2.00	10	1
1:B:47:MET:HE1	1:B:55:LYS:CD	0.56	2.30	6	4
1:C:47:MET:HE1	1:C:55:LYS:CD	0.56	2.30	6	4
1:K:47:MET:HE1	1:K:55:LYS:CD	0.56	2.30	6	4
1:L:54:ASP:CG	1:M:41:ARG:NH2	0.56	2.63	7	2
1:B:33:ARG:NH2	1:B:64:TYR:CG	0.56	2.74	7	1
1:H:33:ARG:NH2	1:H:64:TYR:CG	0.56	2.74	7	1
1:J:33:ARG:NH2	1:J:64:TYR:CG	0.56	2.74	7	1
1:G:43:ALA:O	1:G:47:MET:HG3	0.56	2.00	10	1
1:H:43:ALA:O	1:H:47:MET:HG3	0.56	2.00	10	1
1:J:43:ALA:O	1:J:47:MET:HG3	0.56	2.00	10	1
1:N:43:ALA:O	1:N:47:MET:HG3	0.56	2.00	10	1
1:O:43:ALA:O	1:O:47:MET:HG3	0.56	2.00	10	1
1:H:80:GLU:H	1:H:80:GLU:CD	0.56	2.08	6	3
1:C:33:ARG:NH2	1:C:64:TYR:CG	0.56	2.74	7	1
1:G:33:ARG:NH2	1:G:64:TYR:CG	0.56	2.74	7	1
1:I:33:ARG:NH2	1:I:64:TYR:CG	0.56	2.74	7	1
1:H:33:ARG:NH2	1:H:64:TYR:CE1	0.56	2.72	9	1
1:D:43:ALA:O	1:D:47:MET:HG3	0.56	2.00	10	1
1:G:47:MET:HE1	1:G:55:LYS:HZ2	0.56	1.60	2	1
1:D:47:MET:HE1	1:D:55:LYS:CD	0.56	2.30	6	4
1:F:47:MET:HE1	1:F:55:LYS:CD	0.56	2.30	6	4
1:H:47:MET:HE1	1:H:55:LYS:CD	0.56	2.30	6	4
1:L:47:MET:HE1	1:L:55:LYS:CD	0.56	2.30	6	4
1:M:47:MET:HE1	1:M:55:LYS:CD	0.56	2.30	6	4
1:G:9:LEU:HD12	1:G:53:THR:HG21	0.56	1.76	4	1
1:A:33:ARG:NH2	1:A:64:TYR:CG	0.56	2.74	7	1
1:E:47:MET:HE1	1:E:55:LYS:CD	0.56	2.30	6	4
1:N:9:LEU:HD12	1:N:53:THR:HG21	0.56	1.76	4	1
1:M:54:ASP:CG	1:N:41:ARG:NH2	0.56	2.64	7	2
1:O:33:ARG:NH2	1:O:64:TYR:CG	0.56	2.74	7	1
1:C:43:ALA:O	1:C:47:MET:HG3	0.56	2.00	10	1
1:K:43:ALA:O	1:K:47:MET:HG3	0.56	2.00	10	1
1:D:80:GLU:CD	1:D:80:GLU:H	0.56	2.08	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:L:80:GLU:CD	1:L:80:GLU:H	0.56	2.08	6	3
1:O:80:GLU:CD	1:O:80:GLU:H	0.56	2.08	8	3
1:M:33:ARG:NH2	1:M:64:TYR:CG	0.56	2.74	7	1
1:G:61:LEU:O	1:G:65:GLY:N	0.56	2.39	6	9
1:C:80:GLU:H	1:C:80:GLU:CD	0.56	2.08	8	3
1:E:80:GLU:OE2	1:M:57:VAL:O	0.56	2.24	6	3
1:D:33:ARG:NH2	1:D:64:TYR:CG	0.56	2.74	7	1
1:N:33:ARG:NH2	1:N:64:TYR:CG	0.56	2.74	7	1
1:D:61:LEU:O	1:D:65:GLY:N	0.56	2.39	6	9
1:G:47:MET:HE1	1:G:55:LYS:CD	0.56	2.30	6	4
1:I:80:GLU:CD	1:I:80:GLU:H	0.56	2.08	8	3
1:C:54:ASP:CG	1:D:41:ARG:NH2	0.56	2.63	7	2
1:H:2:GLY:C	1:H:4:ALA:N	0.56	2.64	10	2
1:M:61:LEU:O	1:M:65:GLY:N	0.56	2.39	6	9
1:F:47:MET:HE1	1:F:55:LYS:HZ2	0.56	1.60	2	1
1:N:80:GLU:CD	1:N:80:GLU:H	0.56	2.08	8	3
1:F:33:ARG:NH2	1:F:64:TYR:CG	0.56	2.74	7	1
1:A:80:GLU:H	1:A:80:GLU:CD	0.55	2.08	6	3
1:K:33:ARG:NH2	1:K:64:TYR:CG	0.55	2.74	7	1
1:M:80:GLU:H	1:M:80:GLU:CD	0.55	2.08	8	3
1:K:54:ASP:CG	1:L:41:ARG:NH2	0.55	2.64	7	3
1:D:2:GLY:C	1:D:4:ALA:N	0.55	2.64	10	2
1:N:2:GLY:C	1:N:4:ALA:N	0.55	2.64	10	2
1:C:61:LEU:O	1:C:65:GLY:N	0.55	2.39	6	9
1:J:2:GLY:C	1:J:4:ALA:N	0.55	2.64	10	3
1:A:61:LEU:O	1:A:65:GLY:N	0.55	2.39	6	9
1:O:61:LEU:O	1:O:65:GLY:N	0.55	2.39	6	9
1:E:80:GLU:CD	1:E:80:GLU:H	0.55	2.08	6	3
1:F:80:GLU:H	1:F:80:GLU:CD	0.55	2.08	6	3
1:G:80:GLU:CD	1:G:80:GLU:H	0.55	2.09	4	3
1:E:2:GLY:C	1:E:4:ALA:N	0.55	2.64	10	2
1:I:47:MET:HE1	1:I:55:LYS:HZ2	0.55	1.60	2	2
1:M:25:MET:SD	1:M:25:MET:C	0.55	2.90	9	6
1:N:25:MET:SD	1:N:25:MET:C	0.55	2.90	9	6
1:F:25:MET:C	1:F:25:MET:SD	0.55	2.90	9	5
1:I:25:MET:SD	1:I:25:MET:C	0.55	2.90	9	5
1:E:33:ARG:NH2	1:E:64:TYR:CG	0.55	2.74	7	1
1:K:2:GLY:C	1:K:4:ALA:N	0.55	2.64	10	2
1:L:61:LEU:O	1:L:65:GLY:N	0.55	2.39	6	6
1:E:25:MET:SD	1:E:25:MET:C	0.55	2.90	7	6
1:G:25:MET:SD	1:G:25:MET:C	0.55	2.90	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:25:MET:SD	1:B:25:MET:C	0.55	2.90	9	5
1:N:54:ASP:CG	1:O:41:ARG:NH2	0.55	2.64	7	2
1:H:2:GLY:O	1:H:4:ALA:N	0.55	2.40	7	2
1:I:2:GLY:O	1:I:4:ALA:N	0.55	2.40	7	2
1:B:61:LEU:O	1:B:65:GLY:N	0.55	2.39	6	9
1:O:25:MET:SD	1:O:25:MET:C	0.55	2.90	9	6
1:L:25:MET:SD	1:L:25:MET:C	0.55	2.90	9	5
1:B:2:GLY:C	1:B:4:ALA:N	0.55	2.64	10	3
1:L:2:GLY:C	1:L:4:ALA:N	0.55	2.64	10	3
1:F:61:LEU:O	1:F:65:GLY:N	0.55	2.39	6	7
1:I:48:ASP:OD1	1:I:49:ALA:N	0.55	2.40	3	10
1:H:25:MET:SD	1:H:25:MET:C	0.55	2.90	9	6
1:D:25:MET:SD	1:D:25:MET:C	0.55	2.90	9	5
1:J:25:MET:SD	1:J:25:MET:C	0.55	2.90	7	5
1:C:2:GLY:O	1:C:4:ALA:N	0.55	2.40	10	2
1:G:2:GLY:O	1:G:4:ALA:N	0.55	2.40	10	2
1:L:33:ARG:NH2	1:L:64:TYR:CG	0.55	2.74	7	1
1:M:2:GLY:O	1:M:4:ALA:N	0.55	2.40	7	2
1:B:48:ASP:OD1	1:B:49:ALA:N	0.55	2.40	3	10
1:H:48:ASP:OD1	1:H:49:ALA:N	0.55	2.40	4	10
1:N:47:MET:HE1	1:N:55:LYS:HD2	0.55	1.79	6	5
1:I:2:GLY:C	1:I:4:ALA:N	0.55	2.65	7	3
1:D:2:GLY:O	1:D:4:ALA:N	0.55	2.40	7	2
1:J:2:GLY:C	1:J:4:ALA:H	0.55	2.10	10	2
1:N:2:GLY:C	1:N:4:ALA:H	0.55	2.10	10	2
1:A:48:ASP:OD1	1:A:49:ALA:N	0.55	2.40	3	10
1:F:47:MET:HE1	1:F:55:LYS:HD2	0.55	1.79	6	5
1:C:2:GLY:C	1:C:4:ALA:N	0.55	2.65	7	3
1:B:2:GLY:O	1:B:4:ALA:N	0.55	2.40	10	2
1:G:2:GLY:C	1:G:4:ALA:H	0.55	2.10	10	2
1:A:32:LEU:C	1:A:32:LEU:CD1	0.54	2.81	7	10
1:J:48:ASP:OD1	1:J:49:ALA:N	0.54	2.40	4	10
1:A:25:MET:SD	1:A:25:MET:C	0.54	2.90	9	6
1:G:47:MET:HE1	1:G:55:LYS:HD2	0.54	1.79	6	5
1:I:2:GLY:C	1:I:4:ALA:H	0.54	2.10	10	2
1:J:2:GLY:O	1:J:4:ALA:N	0.54	2.40	7	2
1:H:32:LEU:C	1:H:32:LEU:CD1	0.54	2.81	7	10
1:C:25:MET:SD	1:C:25:MET:C	0.54	2.90	7	5
1:F:54:ASP:CG	1:G:41:ARG:NH2	0.54	2.66	7	2
1:E:2:GLY:C	1:E:4:ALA:H	0.54	2.10	10	2
1:F:2:GLY:O	1:F:4:ALA:N	0.54	2.40	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:O:2:GLY:O	1:O:4:ALA:N	0.54	2.40	10	2
1:O:32:LEU:C	1:O:32:LEU:CD1	0.54	2.81	7	10
1:K:25:MET:C	1:K:25:MET:SD	0.54	2.90	7	6
1:M:47:MET:HE1	1:M:55:LYS:HD2	0.54	1.79	6	5
1:L:61:LEU:H	1:L:61:LEU:CD1	0.54	2.15	3	1
1:M:61:LEU:H	1:M:61:LEU:CD1	0.54	2.15	3	1
1:G:2:GLY:C	1:G:4:ALA:N	0.54	2.65	7	2
1:K:2:GLY:O	1:K:4:ALA:N	0.54	2.40	7	2
1:K:2:GLY:C	1:K:4:ALA:H	0.54	2.10	10	2
1:L:2:GLY:O	1:L:4:ALA:N	0.54	2.40	10	2
1:M:2:GLY:C	1:M:4:ALA:N	0.54	2.65	7	2
1:G:48:ASP:OD1	1:G:49:ALA:N	0.54	2.40	4	10
1:N:32:LEU:C	1:N:32:LEU:CD1	0.54	2.80	4	10
1:N:48:ASP:OD1	1:N:49:ALA:N	0.54	2.40	4	10
1:O:48:ASP:OD1	1:O:49:ALA:N	0.54	2.40	4	10
1:E:47:MET:HE1	1:E:55:LYS:HD2	0.54	1.79	6	5
1:L:2:GLY:C	1:L:4:ALA:H	0.54	2.10	10	2
1:G:57:VAL:O	1:N:80:GLU:OE2	0.54	2.25	6	3
1:C:48:ASP:OD1	1:C:49:ALA:N	0.54	2.40	3	10
1:D:48:ASP:OD1	1:D:49:ALA:N	0.54	2.40	3	10
1:F:48:ASP:OD1	1:F:49:ALA:N	0.54	2.40	3	10
1:H:2:GLY:C	1:H:4:ALA:H	0.54	2.10	10	2
1:E:48:ASP:OD1	1:E:49:ALA:N	0.54	2.40	3	10
1:G:32:LEU:C	1:G:32:LEU:CD1	0.54	2.81	1	10
1:O:47:MET:HE1	1:O:55:LYS:HD2	0.54	1.79	6	5
1:I:61:LEU:H	1:I:61:LEU:CD1	0.54	2.15	3	1
1:O:2:GLY:C	1:O:4:ALA:N	0.54	2.65	7	3
1:E:2:GLY:O	1:E:4:ALA:N	0.54	2.40	7	2
1:N:61:LEU:O	1:N:65:GLY:N	0.54	2.39	6	8
1:N:2:GLY:O	1:N:4:ALA:N	0.54	2.40	7	2
1:E:61:LEU:O	1:E:65:GLY:N	0.54	2.39	6	8
1:C:47:MET:HE1	1:C:55:LYS:HD2	0.54	1.79	6	5
1:J:47:MET:HE1	1:J:55:LYS:HD2	0.54	1.79	6	5
1:M:47:MET:HE1	1:M:55:LYS:HZ2	0.54	1.63	2	1
1:D:2:GLY:C	1:D:4:ALA:H	0.54	2.10	10	2
1:M:2:GLY:C	1:M:4:ALA:H	0.54	2.10	10	2
1:K:61:LEU:O	1:K:65:GLY:N	0.54	2.39	6	7
1:D:47:MET:HE1	1:D:55:LYS:HD2	0.54	1.80	6	5
1:K:47:MET:HE1	1:K:55:LYS:HD2	0.54	1.79	6	5
1:L:47:MET:HE1	1:L:55:LYS:HD2	0.54	1.80	6	5
1:C:2:GLY:C	1:C:4:ALA:H	0.54	2.10	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:H	1:A:61:LEU:CD1	0.53	2.15	3	1
1:K:48:ASP:OD1	1:K:49:ALA:N	0.53	2.40	4	10
1:B:47:MET:HE1	1:B:55:LYS:HD2	0.53	1.80	6	5
1:A:57:VAL:O	1:H:80:GLU:OE2	0.53	2.25	6	3
1:O:2:GLY:C	1:O:4:ALA:H	0.53	2.11	10	2
1:B:32:LEU:C	1:B:32:LEU:CD1	0.53	2.80	4	10
1:L:48:ASP:OD1	1:L:49:ALA:N	0.53	2.40	4	10
1:I:47:MET:HE1	1:I:55:LYS:HD2	0.53	1.79	6	5
1:O:61:LEU:H	1:O:61:LEU:CD1	0.53	2.15	3	1
1:C:80:GLU:OE2	1:K:57:VAL:O	0.53	2.25	6	3
1:M:48:ASP:OD1	1:M:49:ALA:N	0.53	2.40	3	10
1:H:47:MET:HE1	1:H:55:LYS:HD2	0.53	1.80	6	5
1:B:2:GLY:C	1:B:4:ALA:H	0.53	2.10	10	2
1:D:32:LEU:C	1:D:32:LEU:CD1	0.53	2.81	7	9
1:N:61:LEU:H	1:N:61:LEU:CD1	0.53	2.15	3	1
1:F:2:GLY:C	1:F:4:ALA:N	0.53	2.65	7	2
1:K:32:LEU:C	1:K:32:LEU:CD1	0.53	2.81	7	10
1:C:32:LEU:C	1:C:32:LEU:CD1	0.53	2.81	7	9
1:I:32:LEU:C	1:I:32:LEU:CD1	0.53	2.80	4	10
1:J:61:LEU:O	1:J:65:GLY:N	0.53	2.39	6	7
1:L:32:LEU:C	1:L:32:LEU:CD1	0.53	2.81	7	10
1:A:47:MET:HE1	1:A:55:LYS:HD2	0.53	1.79	6	5
1:C:61:LEU:H	1:C:61:LEU:CD1	0.53	2.15	3	1
1:F:2:GLY:C	1:F:4:ALA:H	0.53	2.10	10	2
1:I:61:LEU:O	1:I:65:GLY:N	0.53	2.39	6	7
1:J:32:LEU:C	1:J:32:LEU:CD1	0.53	2.81	9	10
1:H:61:LEU:O	1:H:65:GLY:N	0.53	2.39	6	8
1:G:61:LEU:H	1:G:61:LEU:CD1	0.53	2.15	3	1
1:H:61:LEU:H	1:H:61:LEU:CD1	0.53	2.15	3	1
1:C:57:VAL:O	1:J:80:GLU:OE2	0.53	2.27	6	3
1:L:77:GLY:C	1:L:79:GLN:HE21	0.53	2.12	7	5
1:M:77:GLY:C	1:M:79:GLN:HE21	0.53	2.12	7	5
1:B:61:LEU:H	1:B:61:LEU:CD1	0.53	2.15	3	1
1:F:32:LEU:C	1:F:32:LEU:CD1	0.52	2.80	4	10
1:N:77:GLY:C	1:N:79:GLN:HE21	0.52	2.12	7	5
1:J:61:LEU:H	1:J:61:LEU:CD1	0.52	2.15	3	1
1:D:61:LEU:H	1:D:61:LEU:CD1	0.52	2.15	3	1
1:B:54:ASP:CG	1:C:41:ARG:NH2	0.52	2.67	7	2
1:A:77:GLY:C	1:A:79:GLN:HE21	0.52	2.12	7	5
1:D:78:LEU:C	1:D:78:LEU:CD2	0.52	2.83	10	10
1:J:78:LEU:C	1:J:78:LEU:CD2	0.52	2.83	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:K:78:LEU:C	1:K:78:LEU:CD2	0.52	2.83	8	10
1:M:78:LEU:C	1:M:78:LEU:CD2	0.52	2.83	9	10
1:B:78:LEU:C	1:B:78:LEU:CD2	0.52	2.83	9	10
1:C:78:LEU:C	1:C:78:LEU:CD2	0.52	2.83	10	10
1:E:77:GLY:C	1:E:79:GLN:HE21	0.52	2.12	7	5
1:F:77:GLY:C	1:F:79:GLN:HE21	0.52	2.12	7	5
1:F:78:LEU:C	1:F:78:LEU:CD2	0.52	2.83	8	10
1:G:77:GLY:C	1:G:79:GLN:HE21	0.52	2.12	7	5
1:I:78:LEU:C	1:I:78:LEU:CD2	0.52	2.83	8	10
1:K:77:GLY:C	1:K:79:GLN:HE21	0.52	2.12	7	5
1:K:61:LEU:H	1:K:61:LEU:CD1	0.52	2.15	3	1
1:E:78:LEU:C	1:E:78:LEU:CD2	0.52	2.83	8	10
1:H:77:GLY:C	1:H:79:GLN:HE21	0.52	2.12	7	5
1:I:77:GLY:C	1:I:79:GLN:HE21	0.52	2.12	7	5
1:D:61:LEU:N	1:D:61:LEU:CD1	0.52	2.73	3	1
1:L:61:LEU:N	1:L:61:LEU:CD1	0.52	2.73	3	1
1:A:78:LEU:C	1:A:78:LEU:CD2	0.52	2.83	9	10
1:L:78:LEU:C	1:L:78:LEU:CD2	0.52	2.83	8	10
1:E:61:LEU:N	1:E:61:LEU:CD1	0.52	2.73	3	1
1:E:61:LEU:H	1:E:61:LEU:CD1	0.52	2.15	3	1
1:F:61:LEU:N	1:F:61:LEU:CD1	0.52	2.73	3	1
1:N:78:LEU:C	1:N:78:LEU:CD2	0.52	2.83	9	10
1:M:61:LEU:N	1:M:61:LEU:CD1	0.52	2.73	3	1
1:B:77:GLY:C	1:B:79:GLN:HE21	0.52	2.12	7	5
1:O:77:GLY:C	1:O:79:GLN:HE21	0.52	2.12	7	5
1:O:78:LEU:C	1:O:78:LEU:CD2	0.52	2.83	9	10
1:K:61:LEU:N	1:K:61:LEU:CD1	0.52	2.73	3	1
1:G:78:LEU:C	1:G:78:LEU:CD2	0.51	2.83	8	10
1:H:78:LEU:C	1:H:78:LEU:CD2	0.51	2.83	8	10
1:C:61:LEU:N	1:C:61:LEU:CD1	0.51	2.73	3	1
1:M:32:LEU:C	1:M:32:LEU:CD1	0.51	2.81	2	10
1:J:61:LEU:N	1:J:61:LEU:CD1	0.51	2.73	3	1
1:C:77:GLY:C	1:C:79:GLN:HE21	0.51	2.12	7	5
1:D:16:SER:HB2	1:D:19:GLU:CD	0.51	2.30	7	5
1:D:77:GLY:C	1:D:79:GLN:HE21	0.51	2.12	7	5
1:H:16:SER:HB2	1:H:19:GLU:CD	0.51	2.31	7	5
1:J:77:GLY:C	1:J:79:GLN:HE21	0.51	2.12	7	5
1:O:16:SER:HB2	1:O:19:GLU:CD	0.51	2.31	7	5
1:E:47:MET:HE1	1:E:55:LYS:HZ2	0.51	1.64	2	1
1:O:47:MET:HE1	1:O:55:LYS:HZ2	0.51	1.65	2	1
1:A:16:SER:HB2	1:A:19:GLU:CD	0.51	2.31	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:19:GLU:CD	1:D:19:GLU:H	0.51	2.14	7	3
1:L:16:SER:HB2	1:L:19:GLU:CD	0.51	2.30	7	5
1:F:61:LEU:H	1:F:61:LEU:CD1	0.51	2.15	3	1
1:J:19:GLU:H	1:J:19:GLU:CD	0.51	2.14	7	3
1:A:13:GLU:OE1	1:B:22:LYS:NZ	0.51	2.42	8	4
1:F:57:VAL:O	1:M:80:GLU:OE2	0.51	2.29	6	3
1:M:19:GLU:H	1:M:19:GLU:CD	0.51	2.14	7	3
1:E:16:SER:HB2	1:E:19:GLU:CD	0.51	2.30	7	5
1:G:16:SER:HB2	1:G:19:GLU:CD	0.51	2.31	7	5
1:K:16:SER:HB2	1:K:19:GLU:CD	0.51	2.31	7	5
1:N:16:SER:HB2	1:N:19:GLU:CD	0.51	2.31	7	5
1:C:47:MET:HE1	1:C:55:LYS:HZ2	0.51	1.63	2	1
1:K:13:GLU:OE1	1:L:22:LYS:NZ	0.51	2.44	8	3
1:B:19:GLU:H	1:B:19:GLU:CD	0.51	2.14	7	3
1:C:16:SER:HB2	1:C:19:GLU:CD	0.51	2.31	7	5
1:K:19:GLU:CD	1:K:19:GLU:H	0.51	2.14	7	3
1:G:54:ASP:CG	1:H:41:ARG:NH2	0.51	2.68	7	1
1:F:16:SER:HB2	1:F:19:GLU:CD	0.51	2.31	7	5
1:I:16:SER:HB2	1:I:19:GLU:CD	0.51	2.30	7	5
1:M:16:SER:HB2	1:M:19:GLU:CD	0.51	2.31	7	5
1:H:19:GLU:CD	1:H:19:GLU:H	0.51	2.14	7	5
1:J:16:SER:HB2	1:J:19:GLU:CD	0.51	2.31	7	5
1:B:16:SER:HB2	1:B:19:GLU:CD	0.50	2.31	7	5
1:D:80:GLU:OE2	1:L:57:VAL:O	0.50	2.29	8	3
1:A:57:VAL:O	1:A:60:TYR:O	0.50	2.30	1	10
1:E:32:LEU:C	1:E:32:LEU:CD1	0.50	2.80	4	10
1:A:61:LEU:N	1:A:61:LEU:CD1	0.50	2.73	3	1
1:D:19:GLU:H	1:D:19:GLU:CD	0.50	2.15	4	2
1:I:57:VAL:O	1:I:60:TYR:O	0.50	2.30	1	10
1:O:19:GLU:CD	1:O:19:GLU:H	0.50	2.14	7	3
1:C:13:GLU:OE1	1:D:22:LYS:NZ	0.50	2.43	8	5
1:M:13:GLU:OE1	1:N:22:LYS:NZ	0.50	2.44	5	6
1:K:19:GLU:H	1:K:19:GLU:CD	0.50	2.15	4	2
1:B:57:VAL:O	1:B:60:TYR:O	0.50	2.30	1	10
1:G:19:GLU:CD	1:G:19:GLU:H	0.50	2.14	7	3
1:H:57:VAL:O	1:H:60:TYR:O	0.50	2.30	5	10
1:O:57:VAL:O	1:O:60:TYR:O	0.50	2.30	1	10
1:L:47:MET:HE1	1:L:55:LYS:HZ2	0.50	1.65	2	1
1:C:57:VAL:O	1:C:60:TYR:O	0.49	2.30	5	10
1:H:61:LEU:N	1:H:61:LEU:CD1	0.49	2.73	3	1
1:G:57:VAL:O	1:G:60:TYR:O	0.49	2.30	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:J:57:VAL:O	1:J:60:TYR:O	0.49	2.30	5	10
1:E:19:GLU:CD	1:E:19:GLU:H	0.49	2.14	7	3
1:E:57:VAL:O	1:E:60:TYR:O	0.49	2.30	1	10
1:N:57:VAL:O	1:N:60:TYR:O	0.49	2.30	5	10
1:G:19:GLU:H	1:G:19:GLU:CD	0.49	2.15	4	3
1:H:57:VAL:O	1:O:80:GLU:OE2	0.49	2.28	6	3
1:K:57:VAL:O	1:K:60:TYR:O	0.49	2.30	5	10
1:B:57:VAL:O	1:I:80:GLU:OE2	0.49	2.30	6	3
1:O:19:GLU:H	1:O:19:GLU:CD	0.49	2.15	4	2
1:O:74:ARG:O	1:O:77:GLY:N	0.49	2.45	10	2
1:L:57:VAL:O	1:L:60:TYR:O	0.49	2.30	1	10
1:M:57:VAL:O	1:M:60:TYR:O	0.49	2.30	1	10
1:D:57:VAL:O	1:D:60:TYR:O	0.49	2.30	1	10
1:F:57:VAL:O	1:F:60:TYR:O	0.49	2.30	1	10
1:I:19:GLU:CD	1:I:19:GLU:H	0.49	2.14	7	3
1:O:61:LEU:N	1:O:61:LEU:CD1	0.49	2.73	3	1
1:C:80:GLU:OE2	1:K:57:VAL:HG12	0.49	2.08	3	4
1:H:74:ARG:O	1:H:77:GLY:N	0.49	2.45	10	3
1:J:74:ARG:O	1:J:77:GLY:N	0.49	2.45	10	5
1:M:67:GLU:C	1:M:67:GLU:CD	0.49	2.81	4	1
1:E:19:GLU:H	1:E:19:GLU:CD	0.49	2.15	4	2
1:A:47:MET:HE1	1:A:55:LYS:HZ2	0.49	1.68	2	1
1:L:67:GLU:C	1:L:67:GLU:CD	0.49	2.81	4	1
1:H:47:MET:HE1	1:H:55:LYS:HZ2	0.49	1.67	2	1
1:N:67:GLU:C	1:N:67:GLU:CD	0.49	2.81	4	1
1:I:19:GLU:H	1:I:19:GLU:CD	0.48	2.15	4	2
1:C:19:GLU:CD	1:C:19:GLU:H	0.48	2.14	7	4
1:L:19:GLU:CD	1:L:19:GLU:H	0.48	2.14	7	5
1:A:19:GLU:CD	1:A:19:GLU:H	0.48	2.14	7	5
1:E:48:ASP:CG	1:E:49:ALA:N	0.48	2.71	3	10
1:A:74:ARG:O	1:A:77:GLY:N	0.48	2.45	10	5
1:I:67:GLU:C	1:I:67:GLU:CD	0.48	2.81	4	1
1:A:18:ASP:OD1	1:A:18:ASP:C	0.48	2.57	2	10
1:D:48:ASP:CG	1:D:49:ALA:N	0.48	2.71	3	10
1:G:13:GLU:OE1	1:H:22:LYS:NZ	0.48	2.45	8	4
1:C:74:ARG:O	1:C:77:GLY:N	0.48	2.45	10	5
1:D:67:GLU:C	1:D:67:GLU:CD	0.48	2.81	4	1
1:K:67:GLU:C	1:K:67:GLU:CD	0.48	2.81	4	1
1:H:18:ASP:OD1	1:H:18:ASP:C	0.48	2.57	2	10
1:I:18:ASP:C	1:I:18:ASP:OD1	0.48	2.57	2	10
1:M:18:ASP:OD1	1:M:18:ASP:C	0.48	2.57	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:O:18:ASP:OD1	1:O:18:ASP:C	0.48	2.57	2	10
1:K:19:GLU:OE1	1:K:19:GLU:N	0.48	2.40	7	8
1:B:18:ASP:C	1:B:18:ASP:OD1	0.48	2.57	2	7
1:F:18:ASP:OD1	1:F:18:ASP:C	0.48	2.57	2	10
1:L:18:ASP:C	1:L:18:ASP:OD1	0.48	2.57	2	6
1:E:67:GLU:CD	1:E:67:GLU:C	0.48	2.81	4	1
1:F:67:GLU:C	1:F:67:GLU:CD	0.48	2.81	4	1
1:H:67:GLU:CD	1:H:67:GLU:C	0.48	2.81	4	1
1:D:18:ASP:OD1	1:D:18:ASP:C	0.48	2.57	2	7
1:F:48:ASP:CG	1:F:49:ALA:N	0.48	2.72	2	10
1:G:18:ASP:C	1:G:18:ASP:OD1	0.48	2.57	2	10
1:H:57:VAL:HG12	1:O:80:GLU:OE2	0.48	2.09	3	4
1:J:18:ASP:C	1:J:18:ASP:OD1	0.48	2.57	2	10
1:M:48:ASP:CG	1:M:49:ALA:N	0.48	2.71	3	10
1:N:18:ASP:C	1:N:18:ASP:OD1	0.48	2.57	2	10
1:N:19:GLU:CD	1:N:19:GLU:H	0.48	2.14	7	5
1:E:18:ASP:C	1:E:18:ASP:OD1	0.48	2.57	2	6
1:B:61:LEU:N	1:B:61:LEU:CD1	0.48	2.73	3	1
1:J:67:GLU:CD	1:J:67:GLU:C	0.48	2.81	4	1
1:A:48:ASP:CG	1:A:49:ALA:N	0.48	2.71	3	10
1:C:18:ASP:OD1	1:C:18:ASP:C	0.48	2.57	2	9
1:K:18:ASP:OD1	1:K:18:ASP:C	0.48	2.57	2	8
1:C:19:GLU:H	1:C:19:GLU:CD	0.48	2.15	6	2
1:B:67:GLU:C	1:B:67:GLU:CD	0.48	2.81	4	1
1:E:80:GLU:OE2	1:M:57:VAL:HG12	0.47	2.09	1	4
1:F:19:GLU:CD	1:F:19:GLU:H	0.47	2.14	7	5
1:N:48:ASP:CG	1:N:49:ALA:N	0.47	2.71	3	9
1:C:67:GLU:CD	1:C:67:GLU:C	0.47	2.81	4	1
1:O:67:GLU:CD	1:O:67:GLU:C	0.47	2.81	4	1
1:C:48:ASP:CG	1:C:49:ALA:N	0.47	2.71	3	9
1:L:48:ASP:CG	1:L:49:ALA:N	0.47	2.71	3	9
1:N:19:GLU:OE1	1:N:19:GLU:N	0.47	2.40	7	7
1:J:48:ASP:CG	1:J:49:ALA:N	0.47	2.71	3	10
1:I:61:LEU:N	1:I:61:LEU:CD1	0.47	2.73	3	1
1:A:67:GLU:C	1:A:67:GLU:CD	0.47	2.81	4	1
1:G:67:GLU:C	1:G:67:GLU:CD	0.47	2.81	4	1
1:H:48:ASP:CG	1:H:49:ALA:N	0.47	2.72	2	10
1:B:48:ASP:CG	1:B:49:ALA:N	0.47	2.72	2	10
1:G:48:ASP:CG	1:G:49:ALA:N	0.47	2.72	2	10
1:H:13:GLU:OE1	1:I:22:LYS:NZ	0.47	2.47	8	5
1:C:27:LEU:C	1:C:27:LEU:CD2	0.47	2.88	10	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:K:27:LEU:C	1:K:27:LEU:CD2	0.47	2.88	10	10
1:B:13:GLU:OE1	1:C:22:LYS:NZ	0.47	2.48	5	6
1:M:19:GLU:OE1	1:M:19:GLU:N	0.47	2.41	8	3
1:K:74:ARG:O	1:K:77:GLY:N	0.47	2.45	10	5
1:N:74:ARG:O	1:N:77:GLY:N	0.47	2.45	10	5
1:C:19:GLU:OE1	1:C:19:GLU:N	0.47	2.40	7	9
1:D:27:LEU:C	1:D:27:LEU:CD2	0.47	2.88	10	10
1:H:27:LEU:C	1:H:27:LEU:CD2	0.47	2.88	10	9
1:I:48:ASP:CG	1:I:49:ALA:N	0.47	2.71	3	9
1:J:27:LEU:C	1:J:27:LEU:CD2	0.47	2.88	10	10
1:K:48:ASP:CG	1:K:49:ALA:N	0.47	2.72	2	9
1:L:27:LEU:C	1:L:27:LEU:CD2	0.47	2.88	10	10
1:O:48:ASP:CG	1:O:49:ALA:N	0.47	2.72	2	10
1:B:27:LEU:C	1:B:27:LEU:CD2	0.47	2.88	10	10
1:D:49:ALA:O	1:D:53:THR:HG23	0.47	2.10	4	1
1:K:49:ALA:O	1:K:53:THR:HG23	0.47	2.10	4	1
1:A:27:LEU:C	1:A:27:LEU:CD2	0.47	2.88	10	10
1:B:57:VAL:HG12	1:I:80:GLU:OE2	0.47	2.10	3	4
1:N:47:MET:HE1	1:N:55:LYS:HZ2	0.47	1.69	2	1
1:C:49:ALA:O	1:C:53:THR:HG23	0.47	2.10	4	1
1:J:49:ALA:O	1:J:53:THR:HG23	0.47	2.10	4	1
1:L:49:ALA:O	1:L:53:THR:HG23	0.47	2.10	4	1
1:A:19:GLU:OE1	1:A:19:GLU:N	0.47	2.40	7	7
1:J:19:GLU:CD	1:J:19:GLU:H	0.47	2.19	3	2
1:I:27:LEU:C	1:I:27:LEU:CD2	0.46	2.88	10	10
1:L:13:GLU:OE1	1:M:22:LYS:NZ	0.46	2.44	8	6
1:E:49:ALA:O	1:E:53:THR:HG23	0.46	2.10	4	1
1:M:19:GLU:CD	1:M:19:GLU:H	0.46	2.19	3	2
1:B:19:GLU:CD	1:B:19:GLU:H	0.46	2.19	3	2
1:D:13:GLU:OE1	1:E:22:LYS:NZ	0.46	2.49	9	6
1:B:49:ALA:O	1:B:53:THR:HG23	0.46	2.10	4	1
1:I:13:GLU:OE1	1:J:22:LYS:NZ	0.46	2.47	8	5
1:M:49:ALA:O	1:M:53:THR:HG23	0.46	2.10	4	1
1:O:49:ALA:O	1:O:53:THR:HG23	0.46	2.10	4	1
1:G:74:ARG:O	1:G:77:GLY:N	0.46	2.45	10	6
1:I:49:ALA:O	1:I:53:THR:HG23	0.46	2.10	4	1
1:F:49:ALA:O	1:F:53:THR:HG23	0.46	2.10	4	1
1:G:70:MET:HE3	1:G:74:ARG:HH21	0.46	1.69	10	1
1:D:27:LEU:O	1:D:30:VAL:HG12	0.46	2.11	9	7
1:A:27:LEU:O	1:A:30:VAL:HG12	0.46	2.11	9	7
1:I:74:ARG:O	1:I:77:GLY:N	0.46	2.45	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:19:GLU:OE1	1:E:19:GLU:N	0.46	2.41	8	4
1:F:13:GLU:OE1	1:G:22:LYS:NZ	0.46	2.49	5	3
1:K:47:MET:HE1	1:K:55:LYS:HZ2	0.46	1.69	2	1
1:G:61:LEU:N	1:G:61:LEU:CD1	0.46	2.73	3	1
1:N:70:MET:HE3	1:N:74:ARG:HH21	0.46	1.69	10	1
1:C:27:LEU:O	1:C:30:VAL:HG12	0.45	2.11	9	7
1:I:27:LEU:O	1:I:30:VAL:HG12	0.45	2.11	9	7
1:H:27:LEU:O	1:H:30:VAL:HG12	0.45	2.11	9	5
1:K:27:LEU:O	1:K:30:VAL:HG12	0.45	2.12	9	5
1:H:49:ALA:O	1:H:53:THR:HG23	0.45	2.10	4	1
1:O:70:MET:HE3	1:O:74:ARG:HH21	0.45	1.69	10	1
1:B:27:LEU:O	1:B:30:VAL:HG12	0.45	2.11	9	7
1:J:27:LEU:O	1:J:30:VAL:HG12	0.45	2.11	9	8
1:L:27:LEU:O	1:L:30:VAL:HG12	0.45	2.11	9	7
1:J:19:GLU:OE1	1:J:19:GLU:N	0.45	2.40	7	8
1:A:49:ALA:O	1:A:53:THR:HG23	0.45	2.10	4	1
1:G:27:LEU:O	1:G:30:VAL:HG12	0.45	2.11	9	6
1:G:19:GLU:OE1	1:G:19:GLU:N	0.45	2.41	8	7
1:D:74:ARG:O	1:D:77:GLY:N	0.45	2.45	10	5
1:L:74:ARG:O	1:L:77:GLY:N	0.45	2.45	10	5
1:N:49:ALA:O	1:N:53:THR:HG23	0.45	2.10	4	1
1:E:18:ASP:OD1	1:E:18:ASP:C	0.45	2.60	1	4
1:E:27:LEU:C	1:E:27:LEU:CD2	0.45	2.88	10	10
1:G:27:LEU:C	1:G:27:LEU:CD2	0.45	2.88	10	10
1:E:74:ARG:O	1:E:77:GLY:N	0.45	2.45	10	5
1:E:80:GLU:CD	1:E:80:GLU:N	0.45	2.75	8	3
1:N:27:LEU:C	1:N:27:LEU:CD2	0.45	2.88	9	9
1:L:80:GLU:CD	1:L:80:GLU:N	0.45	2.75	4	3
1:M:80:GLU:CD	1:M:80:GLU:N	0.45	2.75	8	3
1:H:70:MET:HE3	1:H:74:ARG:HH21	0.45	1.69	10	1
1:H:19:GLU:OE1	1:H:19:GLU:N	0.45	2.40	7	7
1:D:80:GLU:CD	1:D:80:GLU:N	0.45	2.75	4	3
1:F:80:GLU:CD	1:F:80:GLU:N	0.45	2.75	8	3
1:A:70:MET:HE3	1:A:74:ARG:HH21	0.45	1.68	10	1
1:C:57:VAL:HG12	1:J:80:GLU:OE2	0.45	2.12	1	4
1:N:27:LEU:O	1:N:30:VAL:HG12	0.45	2.12	9	4
1:D:30:VAL:O	1:D:38:ARG:NH2	0.45	2.50	4	3
1:G:30:VAL:O	1:G:38:ARG:NH2	0.45	2.50	4	3
1:J:30:VAL:O	1:J:38:ARG:NH2	0.45	2.50	4	3
1:G:80:GLU:CD	1:G:80:GLU:N	0.45	2.75	4	3
1:O:80:GLU:CD	1:O:80:GLU:N	0.45	2.75	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:23:PHE:CD1	1:F:23:PHE:C	0.45	2.95	7	1
1:F:70:MET:HE3	1:F:74:ARG:HH21	0.45	1.69	10	1
1:F:27:LEU:O	1:F:30:VAL:HG12	0.45	2.11	9	6
1:I:30:VAL:O	1:I:38:ARG:NH2	0.45	2.50	4	3
1:N:30:VAL:O	1:N:38:ARG:NH2	0.45	2.50	4	3
1:O:27:LEU:O	1:O:30:VAL:HG12	0.45	2.11	9	5
1:B:80:GLU:CD	1:B:80:GLU:N	0.45	2.75	8	3
1:G:49:ALA:O	1:G:53:THR:HG23	0.45	2.10	4	1
1:H:80:GLU:CD	1:H:80:GLU:N	0.45	2.75	4	3
1:B:23:PHE:CD1	1:B:23:PHE:C	0.45	2.95	7	1
1:M:27:LEU:C	1:M:27:LEU:CD2	0.44	2.88	10	10
1:B:30:VAL:O	1:B:38:ARG:NH2	0.44	2.50	4	3
1:M:30:VAL:O	1:M:38:ARG:NH2	0.44	2.50	4	3
1:B:74:ARG:O	1:B:77:GLY:N	0.44	2.45	10	5
1:M:74:ARG:O	1:M:77:GLY:N	0.44	2.45	10	5
1:N:23:PHE:CD1	1:N:23:PHE:C	0.44	2.95	7	1
1:A:57:VAL:HG12	1:H:80:GLU:OE2	0.44	2.12	10	4
1:E:27:LEU:O	1:E:30:VAL:HG12	0.44	2.11	9	6
1:G:57:VAL:HG12	1:N:80:GLU:OE2	0.44	2.11	3	4
1:L:30:VAL:O	1:L:38:ARG:NH2	0.44	2.50	4	3
1:D:85:LEU:O	1:D:88:THR:OG1	0.44	2.35	7	1
1:C:30:VAL:O	1:C:38:ARG:NH2	0.44	2.50	4	3
1:F:30:VAL:O	1:F:38:ARG:NH2	0.44	2.50	4	3
1:I:80:GLU:CD	1:I:80:GLU:N	0.44	2.75	8	3
1:J:80:GLU:CD	1:J:80:GLU:N	0.44	2.75	8	3
1:E:23:PHE:CD1	1:E:23:PHE:C	0.44	2.95	7	1
1:F:27:LEU:C	1:F:27:LEU:CD2	0.44	2.89	5	10
1:E:30:VAL:O	1:E:38:ARG:NH2	0.44	2.50	4	3
1:J:71:THR:O	1:J:75:ASP:CG	0.44	2.61	7	4
1:M:27:LEU:O	1:M:30:VAL:HG12	0.44	2.11	9	4
1:O:30:VAL:O	1:O:38:ARG:NH2	0.44	2.50	4	3
1:F:74:ARG:O	1:F:77:GLY:N	0.44	2.45	10	5
1:L:18:ASP:OD1	1:L:18:ASP:C	0.44	2.61	3	1
1:A:80:GLU:CD	1:A:80:GLU:N	0.44	2.75	8	3
1:K:80:GLU:CD	1:K:80:GLU:N	0.44	2.75	4	3
1:M:70:MET:HE3	1:M:74:ARG:HH21	0.44	1.69	10	1
1:F:57:VAL:HG12	1:M:80:GLU:OE2	0.44	2.13	3	4
1:N:61:LEU:N	1:N:61:LEU:CD1	0.44	2.73	3	1
1:N:71:THR:O	1:N:75:ASP:CG	0.44	2.61	7	4
1:C:80:GLU:CD	1:C:80:GLU:N	0.44	2.75	8	3
1:N:80:GLU:CD	1:N:80:GLU:N	0.44	2.75	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:I:23:PHE:CD1	1:I:23:PHE:C	0.44	2.95	7	1
1:A:30:VAL:O	1:A:38:ARG:NH2	0.44	2.50	4	3
1:C:18:ASP:C	1:C:18:ASP:OD1	0.44	2.61	3	1
1:F:71:THR:O	1:F:75:ASP:CG	0.44	2.61	7	4
1:H:71:THR:O	1:H:75:ASP:CG	0.44	2.61	7	4
1:J:23:PHE:CD1	1:J:23:PHE:C	0.44	2.95	7	2
1:H:85:LEU:O	1:H:88:THR:OG1	0.44	2.35	7	1
1:E:15:LEU:HD21	1:E:81:LEU:CD1	0.43	2.43	4	7
1:K:15:LEU:HD21	1:K:81:LEU:CD1	0.43	2.43	6	8
1:K:30:VAL:O	1:K:38:ARG:NH2	0.43	2.50	4	3
1:M:15:LEU:HD21	1:M:81:LEU:CD1	0.43	2.43	4	8
1:G:71:THR:O	1:G:75:ASP:CG	0.43	2.61	7	4
1:K:71:THR:O	1:K:75:ASP:CG	0.43	2.61	7	4
1:O:71:THR:O	1:O:75:ASP:CG	0.43	2.61	7	4
1:I:71:THR:O	1:I:75:ASP:CG	0.43	2.61	7	3
1:E:70:MET:HE3	1:E:74:ARG:HH21	0.43	1.69	10	1
1:F:15:LEU:HD21	1:F:81:LEU:CD1	0.43	2.43	6	7
1:H:30:VAL:O	1:H:38:ARG:NH2	0.43	2.50	4	3
1:J:75:ASP:C	1:J:77:GLY:H	0.43	2.22	10	5
1:M:71:THR:O	1:M:75:ASP:CG	0.43	2.61	7	4
1:C:71:THR:O	1:C:75:ASP:CG	0.43	2.61	7	3
1:A:16:SER:CB	1:A:19:GLU:OE1	0.43	2.62	7	1
1:D:15:LEU:HD21	1:D:81:LEU:CD1	0.43	2.43	4	7
1:J:15:LEU:HD21	1:J:81:LEU:CD1	0.43	2.44	6	7
1:L:15:LEU:HD21	1:L:81:LEU:CD1	0.43	2.43	4	7
1:N:15:LEU:HD21	1:N:81:LEU:CD1	0.43	2.43	4	7
1:D:18:ASP:C	1:D:18:ASP:OD1	0.43	2.61	8	2
1:B:19:GLU:OE1	1:B:19:GLU:N	0.43	2.40	7	4
1:C:75:ASP:C	1:C:77:GLY:H	0.43	2.21	10	5
1:D:75:ASP:C	1:D:77:GLY:H	0.43	2.22	10	5
1:A:71:THR:O	1:A:75:ASP:CG	0.43	2.61	7	3
1:I:85:LEU:O	1:I:88:THR:OG1	0.43	2.35	7	1
1:K:23:PHE:CD1	1:K:23:PHE:C	0.43	2.95	7	1
1:L:70:MET:HE3	1:L:74:ARG:HH21	0.43	1.69	10	1
1:D:80:GLU:OE2	1:L:57:VAL:HG12	0.43	2.13	9	4
1:G:15:LEU:HD21	1:G:81:LEU:CD1	0.43	2.44	6	7
1:N:13:GLU:OE1	1:O:22:LYS:NZ	0.43	2.46	8	3
1:B:71:THR:O	1:B:75:ASP:CG	0.43	2.61	7	3
1:L:71:THR:O	1:L:75:ASP:CG	0.43	2.61	7	3
1:H:23:PHE:CD1	1:H:23:PHE:C	0.43	2.95	7	1
1:O:15:LEU:HD21	1:O:81:LEU:CD1	0.43	2.43	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:71:THR:O	1:D:75:ASP:CG	0.43	2.61	7	3
1:J:85:LEU:O	1:J:88:THR:OG1	0.43	2.35	7	1
1:D:70:MET:HE3	1:D:74:ARG:HH21	0.43	1.69	10	1
1:H:16:SER:CB	1:H:19:GLU:OE1	0.43	2.62	7	3
1:H:15:LEU:HD21	1:H:81:LEU:CD1	0.43	2.44	6	7
1:O:19:GLU:OE1	1:O:19:GLU:N	0.43	2.40	7	6
1:E:71:THR:O	1:E:75:ASP:CG	0.43	2.61	7	3
1:I:70:MET:HE3	1:I:74:ARG:HH21	0.43	1.69	10	1
1:A:15:LEU:HD21	1:A:81:LEU:CD1	0.43	2.43	6	7
1:I:75:ASP:C	1:I:77:GLY:H	0.43	2.22	10	4
1:L:19:GLU:OE1	1:L:19:GLU:N	0.43	2.40	7	4
1:L:75:ASP:C	1:L:77:GLY:H	0.43	2.21	10	4
1:D:23:PHE:CD1	1:D:23:PHE:C	0.43	2.95	7	2
1:M:23:PHE:CD1	1:M:23:PHE:C	0.43	2.95	7	2
1:N:32:LEU:HD13	1:N:33:ARG:O	0.43	2.14	5	1
1:K:85:LEU:O	1:K:88:THR:OG1	0.43	2.35	7	1
1:D:47:MET:HE1	1:D:55:LYS:HZ2	0.43	1.72	2	1
1:O:32:LEU:HD13	1:O:33:ARG:O	0.43	2.14	5	1
1:C:70:MET:HE3	1:C:74:ARG:HH21	0.43	1.69	10	1
1:B:15:LEU:HD21	1:B:81:LEU:CD1	0.43	2.44	6	7
1:C:15:LEU:HD21	1:C:81:LEU:CD1	0.43	2.43	4	7
1:B:18:ASP:OD1	1:B:18:ASP:C	0.43	2.59	4	3
1:E:85:LEU:O	1:E:88:THR:OG1	0.42	2.36	7	1
1:K:16:SER:CB	1:K:19:GLU:OE1	0.42	2.62	3	5
1:I:15:LEU:HD21	1:I:81:LEU:CD1	0.42	2.44	4	7
1:K:75:ASP:C	1:K:77:GLY:H	0.42	2.22	10	3
1:N:85:LEU:O	1:N:88:THR:OG1	0.42	2.35	7	1
1:D:19:GLU:OE1	1:D:19:GLU:N	0.42	2.41	8	3
1:B:70:MET:HE3	1:B:74:ARG:HH21	0.42	1.69	10	1
1:K:32:LEU:HD13	1:K:33:ARG:O	0.42	2.14	5	1
1:M:32:LEU:HD13	1:M:33:ARG:O	0.42	2.14	5	1
1:K:70:MET:HE3	1:K:74:ARG:HH21	0.42	1.69	10	1
1:G:32:LEU:HD13	1:G:33:ARG:O	0.42	2.14	5	1
1:H:32:LEU:HD13	1:H:33:ARG:O	0.42	2.14	5	1
1:O:16:SER:CB	1:O:19:GLU:OE1	0.42	2.62	3	5
1:F:85:LEU:O	1:F:88:THR:OG1	0.42	2.35	7	1
1:O:27:LEU:C	1:O:27:LEU:CD2	0.42	2.88	10	7
1:B:75:ASP:C	1:B:77:GLY:H	0.42	2.22	10	3
1:I:32:LEU:HD13	1:I:33:ARG:O	0.42	2.14	5	1
1:C:23:PHE:CD1	1:C:23:PHE:C	0.42	2.95	7	1
1:A:75:ASP:C	1:A:77:GLY:H	0.42	2.22	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:75:ASP:C	1:E:77:GLY:H	0.42	2.22	10	3
1:F:32:LEU:HD13	1:F:33:ARG:O	0.42	2.14	5	1
1:L:32:LEU:HD13	1:L:33:ARG:O	0.42	2.14	5	1
1:G:23:PHE:CD1	1:G:23:PHE:C	0.42	2.95	7	1
1:O:75:ASP:C	1:O:77:GLY:H	0.42	2.22	10	3
1:G:75:ASP:C	1:G:77:GLY:H	0.42	2.22	10	2
1:N:75:ASP:C	1:N:77:GLY:H	0.42	2.22	10	2
1:J:32:LEU:HD13	1:J:33:ARG:O	0.42	2.14	5	1
1:J:70:MET:HE3	1:J:74:ARG:HH21	0.42	1.69	10	1
1:B:15:LEU:HD21	1:B:81:LEU:CD2	0.41	2.45	7	1
1:G:16:SER:CB	1:G:19:GLU:OE1	0.41	2.62	7	5
1:M:15:LEU:HD21	1:M:81:LEU:CD2	0.41	2.45	7	1
1:M:75:ASP:C	1:M:77:GLY:H	0.41	2.22	10	2
1:O:15:LEU:HD21	1:O:81:LEU:CD2	0.41	2.45	7	1
1:G:15:LEU:HD21	1:G:81:LEU:CD2	0.41	2.46	7	1
1:L:19:GLU:H	1:L:19:GLU:CD	0.41	2.23	2	1
1:H:15:LEU:HD21	1:H:81:LEU:CD2	0.41	2.45	7	1
1:N:15:LEU:HD21	1:N:81:LEU:CD2	0.41	2.45	7	1
1:B:16:SER:CB	1:B:19:GLU:OE1	0.41	2.63	1	5
1:A:15:LEU:HD21	1:A:81:LEU:CD2	0.41	2.46	7	1
1:H:75:ASP:C	1:H:77:GLY:H	0.41	2.22	10	1
1:L:85:LEU:O	1:L:88:THR:OG1	0.41	2.35	7	1
1:C:16:SER:CB	1:C:19:GLU:OE1	0.41	2.63	1	5
1:C:15:LEU:HD21	1:C:81:LEU:CD2	0.41	2.46	7	1
1:L:15:LEU:HD21	1:L:81:LEU:CD2	0.41	2.46	7	1
1:L:16:SER:CB	1:L:19:GLU:OE1	0.41	2.62	3	5
1:F:19:GLU:H	1:F:19:GLU:CD	0.41	2.23	2	1
1:J:15:LEU:HD21	1:J:81:LEU:CD2	0.41	2.46	7	1
1:K:15:LEU:HD21	1:K:81:LEU:CD2	0.41	2.46	7	1
1:A:32:LEU:HD13	1:A:33:ARG:O	0.41	2.14	5	1
1:B:32:LEU:HD13	1:B:33:ARG:O	0.41	2.14	5	1
1:O:85:LEU:O	1:O:88:THR:OG1	0.41	2.35	7	1
1:F:25:MET:SD	1:F:25:MET:C	0.40	3.05	2	1
1:F:16:SER:CB	1:F:19:GLU:OE1	0.40	2.62	7	2
1:D:15:LEU:HD21	1:D:81:LEU:CD2	0.40	2.46	7	1
1:E:15:LEU:HD21	1:E:81:LEU:CD2	0.40	2.45	7	1
1:F:15:LEU:HD21	1:F:81:LEU:CD2	0.40	2.46	7	1
1:I:15:LEU:HD21	1:I:81:LEU:CD2	0.40	2.46	7	1
1:I:19:GLU:OE1	1:I:19:GLU:N	0.40	2.40	7	1
1:L:23:PHE:CD1	1:L:23:PHE:C	0.40	2.95	7	1
1:D:25:MET:C	1:D:25:MET:SD	0.40	3.05	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:L:25:MET:C	1:L:25:MET:SD	0.40	3.05	2	1
1:F:75:ASP:C	1:F:77:GLY:H	0.40	2.21	10	1
1:E:16:SER:CB	1:E:19:GLU:OE1	0.40	2.62	7	1
1:I:25:MET:C	1:I:25:MET:SD	0.40	3.05	2	1
1:F:19:GLU:OE1	1:F:19:GLU:N	0.40	2.40	7	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	86/89 (97%)	86±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	B	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	C	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	D	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	E	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	F	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	G	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	H	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	I	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	J	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	K	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	L	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	M	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	N	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
1	O	87/89 (98%)	87±0 (100±1%)	0±0 (0±0%)	0±0 (0±0%)	44	80
All	All	13040/13350 (98%)	12998 (100%)	14 (0%)	28 (0%)	44	80

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	3	ARG	2
1	C	3	ARG	2
1	D	3	ARG	2
1	E	3	ARG	2
1	F	3	ARG	2
1	G	3	ARG	2
1	H	3	ARG	2
1	I	3	ARG	2
1	J	3	ARG	2
1	K	3	ARG	2
1	L	3	ARG	2
1	M	3	ARG	2
1	N	3	ARG	2
1	O	3	ARG	2

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	75/76 (99%)	74±0 (99±1%)	1±0 (1±1%)	70	95
1	B	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	C	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	D	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	E	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	F	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	G	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	H	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	I	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	J	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	K	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	L	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	M	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	N	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95
1	O	76/76 (100%)	75±0 (99±1%)	1±0 (1±1%)	70	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	11390/11400 (100%)	11300 (99%)	90 (1%)	70 95

All 30 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	38	ARG	5
1	B	38	ARG	5
1	C	38	ARG	5
1	D	38	ARG	5
1	E	38	ARG	5
1	F	38	ARG	5
1	G	38	ARG	5
1	H	38	ARG	5
1	I	38	ARG	5
1	J	38	ARG	5
1	K	38	ARG	5
1	L	38	ARG	5
1	M	38	ARG	5
1	N	38	ARG	5
1	O	38	ARG	5
1	A	74	ARG	1
1	B	74	ARG	1
1	C	74	ARG	1
1	D	74	ARG	1
1	E	74	ARG	1
1	F	74	ARG	1
1	G	74	ARG	1
1	H	74	ARG	1
1	I	74	ARG	1
1	J	74	ARG	1
1	K	74	ARG	1
1	L	74	ARG	1
1	M	74	ARG	1
1	N	74	ARG	1
1	O	74	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% 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	484
Number of shifts mapped to atoms	484
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	81	-0.32 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	75	0.17 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	82	-0.25 ± 0.13	None needed (< 0.5 ppm)
^{15}N	81	0.60 ± 0.24	Should be applied

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 3%, i.e. 477 atoms were assigned a chemical shift out of a possible 18856. 0 out of 315 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	242/6739 (4%)	0/2755 (0%)	162/2666 (6%)	80/1318 (6%)
Sidechain	210/11427 (2%)	0/7429 (0%)	202/3551 (6%)	8/447 (2%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	25/690 (4%)	0/315 (0%)	25/375 (7%)	0/0 (—%)
Overall	477/18856 (3%)	0/10499 (0%)	389/6592 (6%)	88/1765 (5%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 478 atoms were assigned a chemical shift out of a possible 18885. 0 out of 315 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	243/6750 (4%)	0/2760 (0%)	163/2670 (6%)	80/1320 (6%)
Sidechain	210/11445 (2%)	0/7440 (0%)	202/3555 (6%)	8/450 (2%)
Aromatic	25/690 (4%)	0/315 (0%)	25/375 (7%)	0/0 (—%)
Overall	478/18885 (3%)	0/10515 (0%)	390/6600 (6%)	88/1770 (5%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

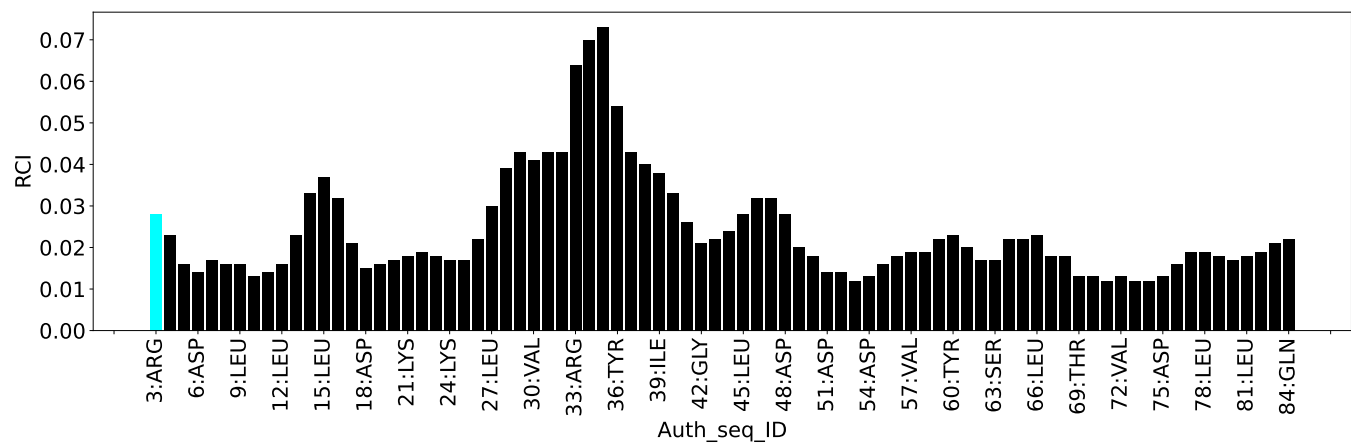
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain 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	9765
Intra-residue ($ i-j =0$)	285
Sequential ($ i-j =1$)	1335
Medium range ($ i-j >1$ and $ i-j <5$)	4440
Long range ($ i-j \geq 5$)	3000
Inter-chain	705
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	2100
Number of unmapped restraints	0
Number of restraints per residue	8.9
Number of long range restraints per residue ¹	2.2

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)	23.2	0.2
0.2-0.5 (Medium)	37.7	0.49
>0.5 (Large)	12.0	0.72

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)	185.6	10.0
10.0-20.0 (Medium)	17.4	13.95
>20.0 (Large)	None	None

9 Distance violation analysis

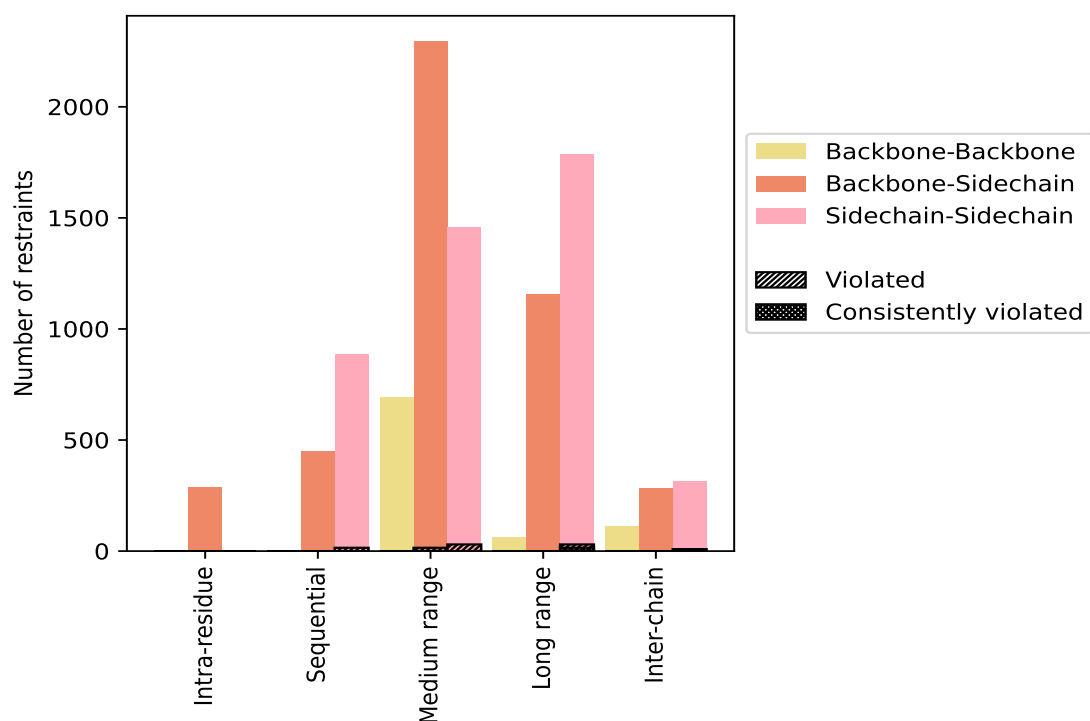
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	285	2.9	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	285	2.9	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
Sequential ($i-j =1$)	1335	13.7	15	1.1	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	450	4.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	885	9.1	15	1.7	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	4440	45.5	45	1.0	0.5	0	0.0	0.0
Backbone-Backbone	690	7.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2295	23.5	15	0.7	0.2	0	0.0	0.0
Sidechain-Sidechain	1455	14.9	30	2.1	0.3	0	0.0	0.0
Long range ($i-j \geq 5$)	3000	30.7	30	1.0	0.3	15	0.5	0.2
Backbone-Backbone	60	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1155	11.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1785	18.3	30	1.7	0.3	15	0.8	0.2
Inter-chain	705	7.2	9	1.3	0.1	0	0.0	0.0
Backbone-Backbone	111	1.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	282	2.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	312	3.2	9	2.9	0.1	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	9765	100.0	99	1.0	1.0	15	0.2	0.2
Backbone-Backbone	861	8.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4467	45.7	15	0.3	0.2	0	0.0	0.0
Sidechain-Sidechain	4437	45.4	84	1.9	0.9	15	0.3	0.2

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

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



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

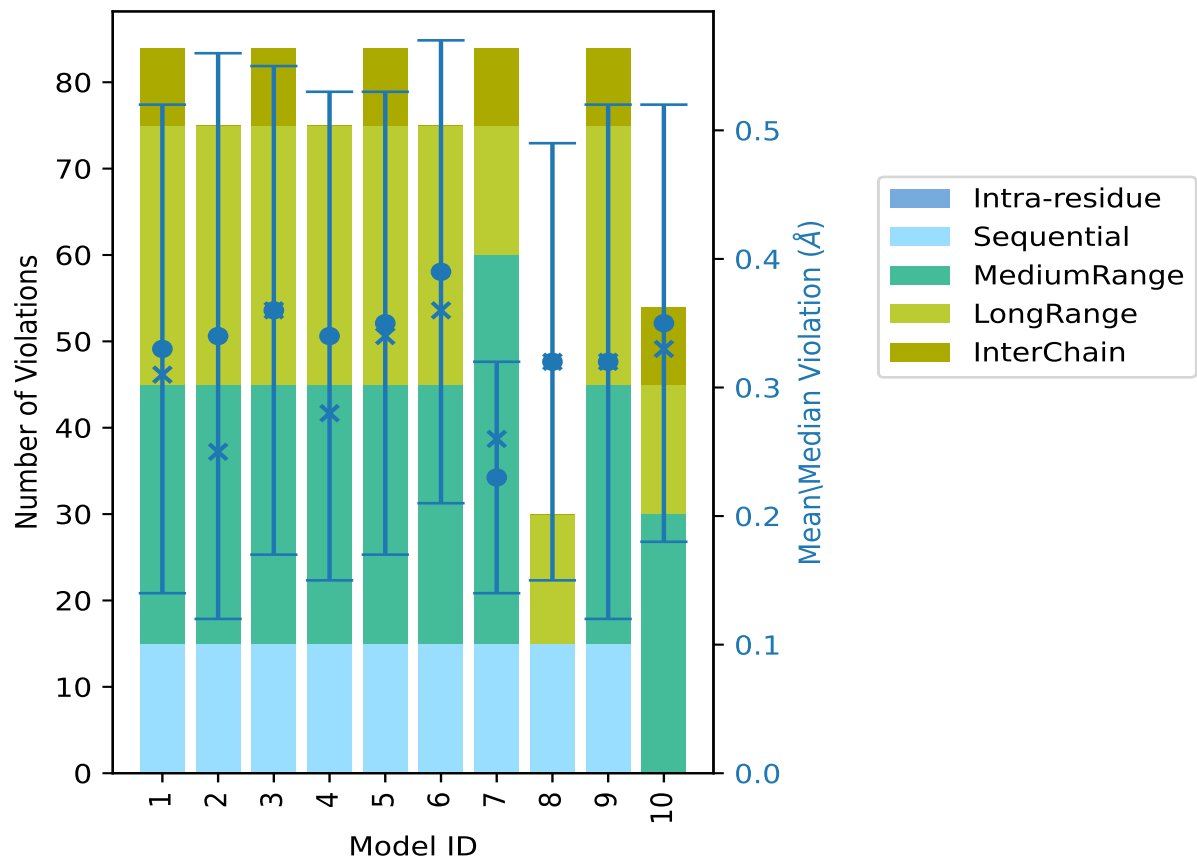
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	15	30	30	9	84	0.33	0.71	0.19	0.31
2	0	15	30	30	0	75	0.34	0.7	0.22	0.25
3	0	15	30	30	9	84	0.36	0.72	0.19	0.36
4	0	15	30	30	0	75	0.34	0.7	0.19	0.28
5	0	15	30	30	9	84	0.35	0.7	0.18	0.34
6	0	15	30	30	0	75	0.39	0.69	0.18	0.36
7	0	15	45	15	9	84	0.23	0.34	0.09	0.26
8	0	15	0	15	0	30	0.32	0.49	0.17	0.32
9	0	15	30	30	9	84	0.32	0.72	0.2	0.32
10	0	0	30	15	9	54	0.35	0.61	0.17	0.33

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 9666(IR:285, SQ:1320, MR:4395, LR:2970, IC:696) 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	0	15	0	0	15	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0

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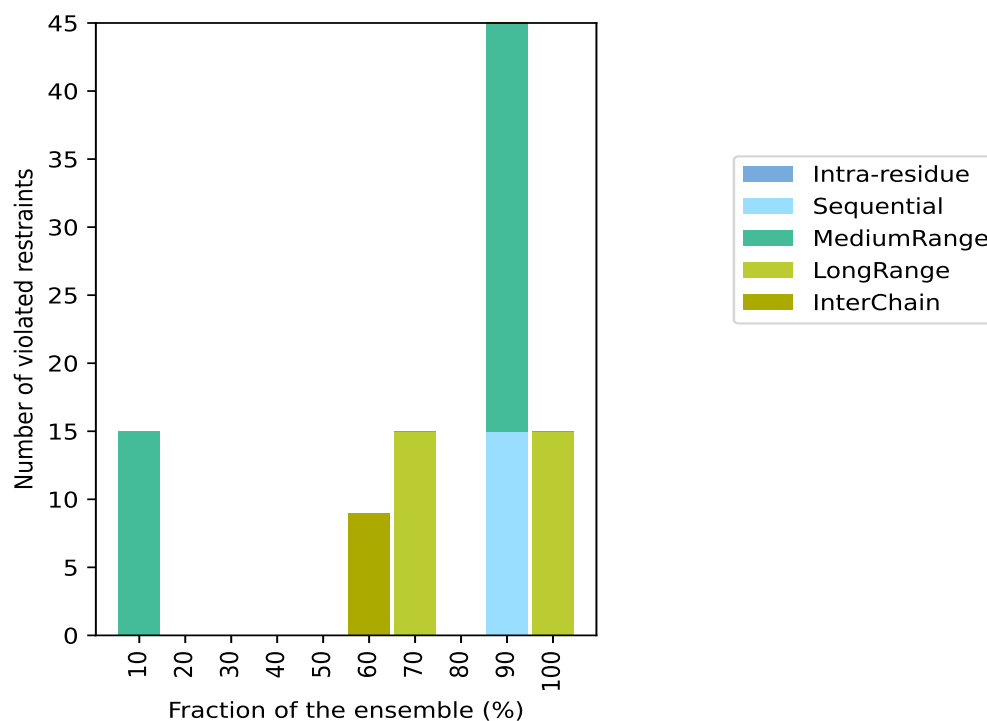
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	9	9	6	60.0
0	0	0	15	0	15	7	70.0
0	0	0	0	0	0	8	80.0
0	15	30	0	0	45	9	90.0
0	0	0	15	0	15	10	100.0

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 ⓘ

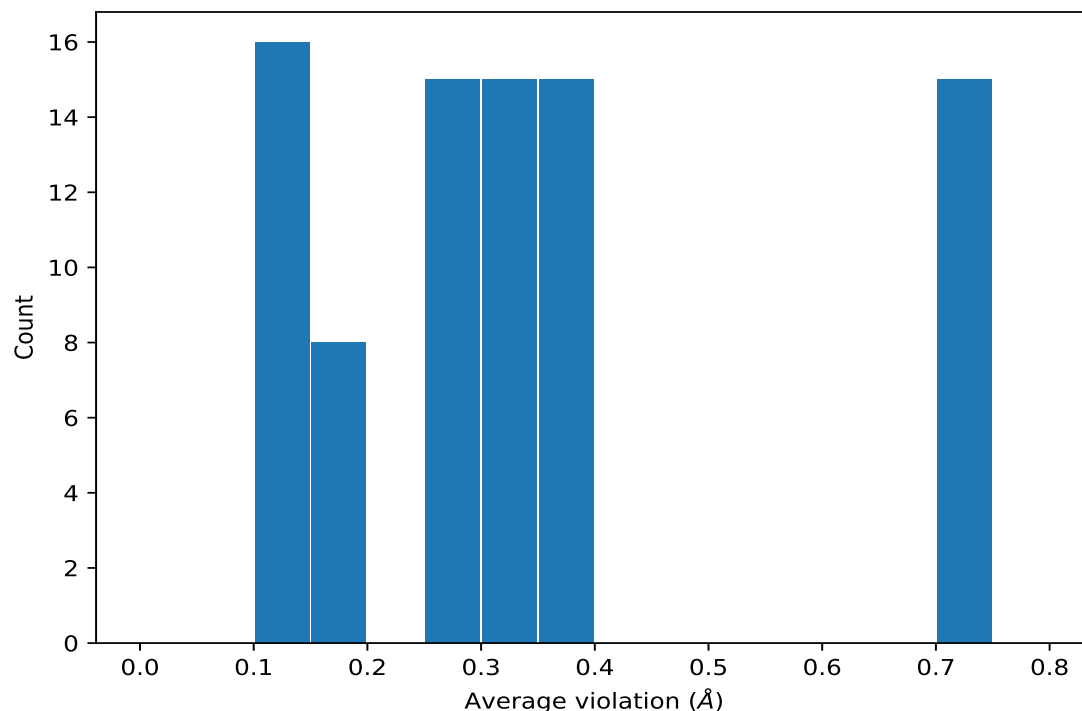


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	10	0.38	0.07	0.36
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	10	0.38	0.07	0.35
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	10	0.38	0.07	0.35
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	10	0.38	0.07	0.35
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	10	0.38	0.07	0.35
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	10	0.38	0.07	0.35
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	10	0.38	0.07	0.35
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	10	0.38	0.07	0.35
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	10	0.37	0.06	0.35
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	10	0.37	0.06	0.35
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	10	0.37	0.06	0.35
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	10	0.37	0.06	0.35
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	10	0.37	0.06	0.35
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	10	0.37	0.06	0.35
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	10	0.37	0.06	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	9	0.32	0.13	0.33
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	9	0.32	0.13	0.33
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	9	0.32	0.13	0.33
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	9	0.32	0.13	0.33
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	9	0.32	0.13	0.33
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	9	0.32	0.13	0.33
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	9	0.32	0.13	0.33
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	9	0.32	0.13	0.33
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	9	0.32	0.13	0.33
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	9	0.32	0.13	0.33
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	9	0.32	0.13	0.33
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	9	0.32	0.13	0.33
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	9	0.32	0.13	0.33
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	9	0.32	0.13	0.33
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	9	0.32	0.13	0.33
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	9	0.28	0.05	0.26
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	9	0.28	0.05	0.26
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	9	0.28	0.05	0.26
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	9	0.28	0.05	0.26
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	9	0.28	0.05	0.26
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	9	0.28	0.05	0.26
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	9	0.28	0.05	0.26
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	9	0.28	0.05	0.26
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	9	0.28	0.05	0.26
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	9	0.28	0.05	0.26
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	9	0.28	0.05	0.26
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	9	0.28	0.05	0.26
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	9	0.28	0.05	0.26
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	9	0.28	0.05	0.26
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	9	0.28	0.05	0.26
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	9	0.15	0.01	0.15
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	9	0.15	0.01	0.15
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	9	0.15	0.01	0.15
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	9	0.15	0.01	0.15
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	9	0.15	0.01	0.15
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	9	0.15	0.01	0.15
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	9	0.15	0.01	0.15
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	9	0.15	0.01	0.15
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	9	0.15	0.01	0.15
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	9	0.15	0.01	0.15
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	9	0.15	0.01	0.15
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	9	0.15	0.01	0.15

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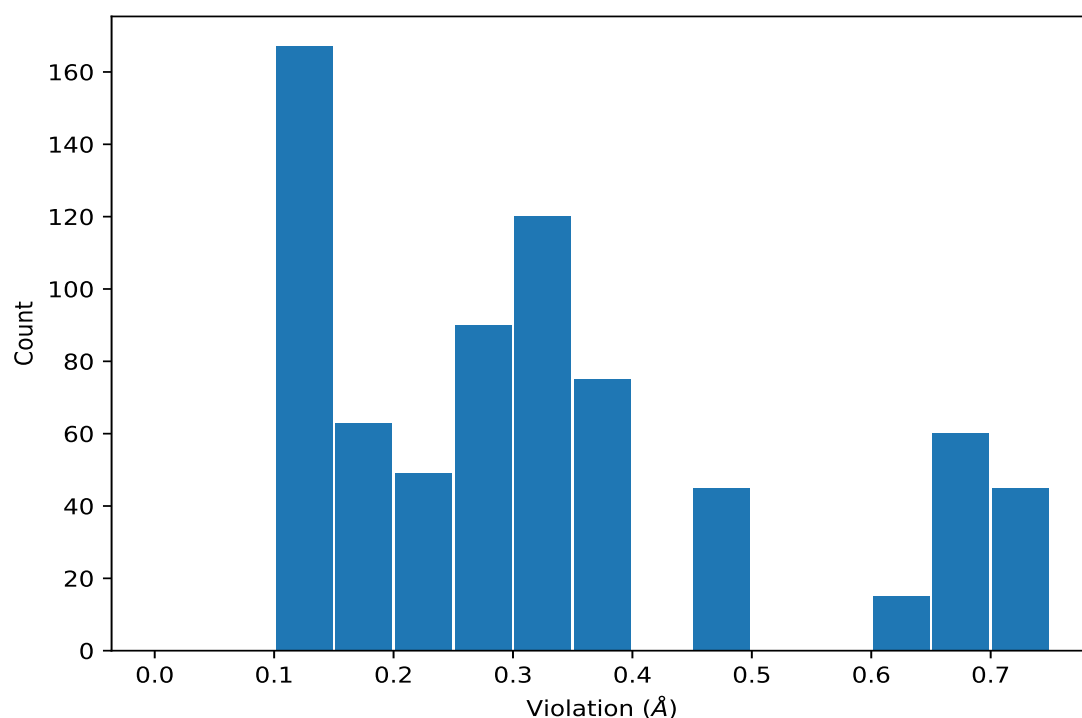
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	9	0.15	0.01	0.15
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	9	0.15	0.01	0.15
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	9	0.15	0.01	0.15
(1,891)	1:56:A:LEU:CB	1:69:A:THR:CG2	7	0.71	0.01	0.7
(1,1495)	1:56:B:LEU:CB	1:69:B:THR:CG2	7	0.71	0.01	0.7
(1,2099)	1:56:C:LEU:CB	1:69:C:THR:CG2	7	0.71	0.01	0.7
(1,2703)	1:56:D:LEU:CB	1:69:D:THR:CG2	7	0.71	0.01	0.7
(1,3307)	1:56:E:LEU:CB	1:69:E:THR:CG2	7	0.71	0.01	0.7
(1,3911)	1:56:F:LEU:CB	1:69:F:THR:CG2	7	0.71	0.01	0.7
(1,4515)	1:56:G:LEU:CB	1:69:G:THR:CG2	7	0.71	0.01	0.7
(1,5119)	1:56:H:LEU:CB	1:69:H:THR:CG2	7	0.71	0.01	0.7
(1,5723)	1:56:I:LEU:CB	1:69:I:THR:CG2	7	0.71	0.01	0.7
(1,6327)	1:56:J:LEU:CB	1:69:J:THR:CG2	7	0.71	0.01	0.7
(1,6931)	1:56:K:LEU:CB	1:69:K:THR:CG2	7	0.71	0.01	0.7
(1,7535)	1:56:L:LEU:CB	1:69:L:THR:CG2	7	0.71	0.01	0.7
(1,8139)	1:56:M:LEU:CB	1:69:M:THR:CG2	7	0.71	0.01	0.7
(1,8743)	1:56:N:LEU:CB	1:69:N:THR:CG2	7	0.71	0.01	0.7
(1,9347)	1:56:O:LEU:CB	1:69:O:THR:CG2	7	0.71	0.01	0.7
(1,574)	1:59:B:TYR:CB	1:79:I:GLN:CG	6	0.17	0.01	0.17
(1,699)	1:59:M:TYR:CB	1:79:E:GLN:CG	6	0.16	0.02	0.16
(1,499)	1:59:A:TYR:CB	1:79:H:GLN:CG	6	0.16	0.02	0.16
(1,674)	1:59:H:TYR:CB	1:79:O:GLN:CG	6	0.16	0.04	0.16
(1,599)	1:59:G:TYR:CB	1:79:N:GLN:CG	6	0.16	0.02	0.16
(1,524)	1:59:F:TYR:CB	1:79:M:GLN:CG	6	0.16	0.01	0.16
(1,549)	1:59:K:TYR:CB	1:79:C:GLN:CG	6	0.16	0.02	0.16
(1,624)	1:59:L:TYR:CB	1:79:D:GLN:CG	6	0.16	0.01	0.15
(1,649)	1:59:C:TYR:CB	1:79:J:GLN:CG	6	0.15	0.03	0.15

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9347)	1:56:O:LEU:CB	1:69:O:THR:CG2	3	0.72
(1,9347)	1:56:O:LEU:CB	1:69:O:THR:CG2	9	0.72
(1,8743)	1:56:N:LEU:CB	1:69:N:THR:CG2	3	0.72
(1,8743)	1:56:N:LEU:CB	1:69:N:THR:CG2	9	0.72
(1,8139)	1:56:M:LEU:CB	1:69:M:THR:CG2	3	0.72
(1,8139)	1:56:M:LEU:CB	1:69:M:THR:CG2	9	0.72
(1,7535)	1:56:L:LEU:CB	1:69:L:THR:CG2	3	0.72
(1,7535)	1:56:L:LEU:CB	1:69:L:THR:CG2	9	0.72
(1,6931)	1:56:K:LEU:CB	1:69:K:THR:CG2	3	0.72
(1,6931)	1:56:K:LEU:CB	1:69:K:THR:CG2	9	0.72
(1,6327)	1:56:J:LEU:CB	1:69:J:THR:CG2	3	0.72
(1,6327)	1:56:J:LEU:CB	1:69:J:THR:CG2	9	0.72
(1,5723)	1:56:I:LEU:CB	1:69:I:THR:CG2	3	0.72
(1,5723)	1:56:I:LEU:CB	1:69:I:THR:CG2	9	0.72
(1,5119)	1:56:H:LEU:CB	1:69:H:THR:CG2	3	0.72
(1,5119)	1:56:H:LEU:CB	1:69:H:THR:CG2	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4515)	1:56:G:LEU:CB	1:69:G:THR:CG2	3	0.72
(1,4515)	1:56:G:LEU:CB	1:69:G:THR:CG2	9	0.72
(1,3911)	1:56:F:LEU:CB	1:69:F:THR:CG2	3	0.72
(1,3911)	1:56:F:LEU:CB	1:69:F:THR:CG2	9	0.72
(1,3307)	1:56:E:LEU:CB	1:69:E:THR:CG2	3	0.72
(1,3307)	1:56:E:LEU:CB	1:69:E:THR:CG2	9	0.72
(1,2703)	1:56:D:LEU:CB	1:69:D:THR:CG2	3	0.72
(1,2703)	1:56:D:LEU:CB	1:69:D:THR:CG2	9	0.72
(1,2099)	1:56:C:LEU:CB	1:69:C:THR:CG2	3	0.72
(1,2099)	1:56:C:LEU:CB	1:69:C:THR:CG2	9	0.72
(1,1495)	1:56:B:LEU:CB	1:69:B:THR:CG2	3	0.72
(1,1495)	1:56:B:LEU:CB	1:69:B:THR:CG2	9	0.72
(1,891)	1:56:A:LEU:CB	1:69:A:THR:CG2	3	0.72
(1,891)	1:56:A:LEU:CB	1:69:A:THR:CG2	9	0.72
(1,9347)	1:56:O:LEU:CB	1:69:O:THR:CG2	1	0.71
(1,8743)	1:56:N:LEU:CB	1:69:N:THR:CG2	1	0.71
(1,8139)	1:56:M:LEU:CB	1:69:M:THR:CG2	1	0.71
(1,7535)	1:56:L:LEU:CB	1:69:L:THR:CG2	1	0.71
(1,6931)	1:56:K:LEU:CB	1:69:K:THR:CG2	1	0.71
(1,6327)	1:56:J:LEU:CB	1:69:J:THR:CG2	1	0.71
(1,5723)	1:56:I:LEU:CB	1:69:I:THR:CG2	1	0.71
(1,5119)	1:56:H:LEU:CB	1:69:H:THR:CG2	1	0.71
(1,4515)	1:56:G:LEU:CB	1:69:G:THR:CG2	1	0.71
(1,3911)	1:56:F:LEU:CB	1:69:F:THR:CG2	1	0.71
(1,3307)	1:56:E:LEU:CB	1:69:E:THR:CG2	1	0.71
(1,2703)	1:56:D:LEU:CB	1:69:D:THR:CG2	1	0.71
(1,2099)	1:56:C:LEU:CB	1:69:C:THR:CG2	1	0.71
(1,1495)	1:56:B:LEU:CB	1:69:B:THR:CG2	1	0.71
(1,891)	1:56:A:LEU:CB	1:69:A:THR:CG2	1	0.71
(1,9347)	1:56:O:LEU:CB	1:69:O:THR:CG2	2	0.7
(1,9347)	1:56:O:LEU:CB	1:69:O:THR:CG2	4	0.7
(1,9347)	1:56:O:LEU:CB	1:69:O:THR:CG2	5	0.7
(1,8743)	1:56:N:LEU:CB	1:69:N:THR:CG2	2	0.7
(1,8743)	1:56:N:LEU:CB	1:69:N:THR:CG2	4	0.7
(1,8743)	1:56:N:LEU:CB	1:69:N:THR:CG2	5	0.7
(1,8139)	1:56:M:LEU:CB	1:69:M:THR:CG2	2	0.7
(1,8139)	1:56:M:LEU:CB	1:69:M:THR:CG2	4	0.7
(1,8139)	1:56:M:LEU:CB	1:69:M:THR:CG2	5	0.7
(1,7535)	1:56:L:LEU:CB	1:69:L:THR:CG2	2	0.7
(1,7535)	1:56:L:LEU:CB	1:69:L:THR:CG2	4	0.7
(1,7535)	1:56:L:LEU:CB	1:69:L:THR:CG2	5	0.7
(1,6931)	1:56:K:LEU:CB	1:69:K:THR:CG2	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6931)	1:56:K:LEU:CB	1:69:K:THR:CG2	4	0.7
(1,6931)	1:56:K:LEU:CB	1:69:K:THR:CG2	5	0.7
(1,6327)	1:56:J:LEU:CB	1:69:J:THR:CG2	2	0.7
(1,6327)	1:56:J:LEU:CB	1:69:J:THR:CG2	4	0.7
(1,6327)	1:56:J:LEU:CB	1:69:J:THR:CG2	5	0.7
(1,5723)	1:56:I:LEU:CB	1:69:I:THR:CG2	2	0.7
(1,5723)	1:56:I:LEU:CB	1:69:I:THR:CG2	4	0.7
(1,5723)	1:56:I:LEU:CB	1:69:I:THR:CG2	5	0.7
(1,5119)	1:56:H:LEU:CB	1:69:H:THR:CG2	2	0.7
(1,5119)	1:56:H:LEU:CB	1:69:H:THR:CG2	4	0.7
(1,5119)	1:56:H:LEU:CB	1:69:H:THR:CG2	5	0.7
(1,4515)	1:56:G:LEU:CB	1:69:G:THR:CG2	2	0.7
(1,4515)	1:56:G:LEU:CB	1:69:G:THR:CG2	4	0.7
(1,4515)	1:56:G:LEU:CB	1:69:G:THR:CG2	5	0.7
(1,3911)	1:56:F:LEU:CB	1:69:F:THR:CG2	2	0.7
(1,3911)	1:56:F:LEU:CB	1:69:F:THR:CG2	4	0.7
(1,3911)	1:56:F:LEU:CB	1:69:F:THR:CG2	5	0.7
(1,3307)	1:56:E:LEU:CB	1:69:E:THR:CG2	2	0.7
(1,3307)	1:56:E:LEU:CB	1:69:E:THR:CG2	4	0.7
(1,3307)	1:56:E:LEU:CB	1:69:E:THR:CG2	5	0.7
(1,2703)	1:56:D:LEU:CB	1:69:D:THR:CG2	2	0.7
(1,2703)	1:56:D:LEU:CB	1:69:D:THR:CG2	4	0.7
(1,2703)	1:56:D:LEU:CB	1:69:D:THR:CG2	5	0.7
(1,2099)	1:56:C:LEU:CB	1:69:C:THR:CG2	2	0.7
(1,2099)	1:56:C:LEU:CB	1:69:C:THR:CG2	4	0.7
(1,2099)	1:56:C:LEU:CB	1:69:C:THR:CG2	5	0.7
(1,1495)	1:56:B:LEU:CB	1:69:B:THR:CG2	2	0.7
(1,1495)	1:56:B:LEU:CB	1:69:B:THR:CG2	4	0.7
(1,1495)	1:56:B:LEU:CB	1:69:B:THR:CG2	5	0.7
(1,891)	1:56:A:LEU:CB	1:69:A:THR:CG2	2	0.7
(1,891)	1:56:A:LEU:CB	1:69:A:THR:CG2	4	0.7
(1,891)	1:56:A:LEU:CB	1:69:A:THR:CG2	5	0.7
(1,9347)	1:56:O:LEU:CB	1:69:O:THR:CG2	6	0.69
(1,8743)	1:56:N:LEU:CB	1:69:N:THR:CG2	6	0.69
(1,8139)	1:56:M:LEU:CB	1:69:M:THR:CG2	6	0.69
(1,7535)	1:56:L:LEU:CB	1:69:L:THR:CG2	6	0.69
(1,6931)	1:56:K:LEU:CB	1:69:K:THR:CG2	6	0.69
(1,6327)	1:56:J:LEU:CB	1:69:J:THR:CG2	6	0.69
(1,5723)	1:56:I:LEU:CB	1:69:I:THR:CG2	6	0.69
(1,5119)	1:56:H:LEU:CB	1:69:H:THR:CG2	6	0.69
(1,4515)	1:56:G:LEU:CB	1:69:G:THR:CG2	6	0.69
(1,3911)	1:56:F:LEU:CB	1:69:F:THR:CG2	6	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3307)	1:56:E:LEU:CB	1:69:E:THR:CG2	6	0.69
(1,2703)	1:56:D:LEU:CB	1:69:D:THR:CG2	6	0.69
(1,2099)	1:56:C:LEU:CB	1:69:C:THR:CG2	6	0.69
(1,1495)	1:56:B:LEU:CB	1:69:B:THR:CG2	6	0.69
(1,891)	1:56:A:LEU:CB	1:69:A:THR:CG2	6	0.69
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	10	0.61
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	10	0.61
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	10	0.61
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	10	0.61
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	10	0.61
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	10	0.61
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	10	0.61
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	10	0.61
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	10	0.61
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	10	0.61
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	10	0.61
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	10	0.61
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	10	0.61
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	10	0.61
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	10	0.61
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	8	0.49
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	8	0.49
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	8	0.49
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	8	0.49
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	8	0.49
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	8	0.49
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	8	0.49
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	8	0.49
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	8	0.48
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	8	0.48
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	8	0.48
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	8	0.48
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	8	0.48
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	8	0.48
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	8	0.48
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	2	0.46
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	2	0.46
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	2	0.46
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	2	0.46
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	2	0.46
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	2	0.46
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	2	0.46
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	2	0.46
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	2	0.46
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	2	0.46
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	2	0.46
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	2	0.46
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	2	0.46
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	2	0.46
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	6	0.45
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	6	0.45
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	6	0.45
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	6	0.45
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	6	0.45
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	6	0.45
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	6	0.45
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	6	0.45
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	6	0.45
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	6	0.45
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	6	0.45
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	6	0.45
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	6	0.45
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	6	0.45
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	6	0.45
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	5	0.39
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	5	0.39
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	5	0.39
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	5	0.39
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	5	0.39
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	5	0.39
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	5	0.39
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	5	0.39
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	5	0.39
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	5	0.39
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	5	0.39
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	5	0.39
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	5	0.39
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	5	0.39
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	5	0.39
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	3	0.38
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	3	0.38
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	3	0.38
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	3	0.38
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	3	0.38
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	3	0.38
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	3	0.38
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	3	0.38
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	3	0.38
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	3	0.38
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	3	0.38
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	3	0.38
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	3	0.38
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	3	0.38
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	4	0.37
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	4	0.36
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	3	0.36
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	6	0.36
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	4	0.36
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	3	0.36
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	6	0.36
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	4	0.36
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	3	0.36
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	6	0.36
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	4	0.36
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	3	0.36
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	6	0.36
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	4	0.36
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	3	0.36
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	6	0.36
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	4	0.36
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	3	0.36
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	6	0.36
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	4	0.36
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	3	0.36
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	6	0.36
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	3	0.36
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	6	0.36
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	4	0.36
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	3	0.36
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	6	0.36
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	4	0.36
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	3	0.36
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	6	0.36
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	3	0.36
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	6	0.36
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	4	0.36
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	3	0.36
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	6	0.36
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	4	0.36
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	3	0.36
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	6	0.36
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	4	0.36
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	3	0.36
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	6	0.36
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	4	0.36
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	3	0.36
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	6	0.36
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	9	0.34
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	5	0.34
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	7	0.34
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	9	0.34
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	5	0.34
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	7	0.34
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	9	0.34
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	5	0.34
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	7	0.34
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	9	0.34
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	5	0.34
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	7	0.34
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	9	0.34
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	5	0.34
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	7	0.34
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	9	0.34
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	5	0.34
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	7	0.34
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	9	0.34
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	5	0.34
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	7	0.34
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	9	0.34
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	5	0.34
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	7	0.34
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	9	0.34
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	5	0.34
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	7	0.34
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	5	0.34
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	7	0.34
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	9	0.34
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	5	0.34
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	7	0.34
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	9	0.34
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	5	0.34
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	7	0.34
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	9	0.34
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	5	0.34
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	7	0.34
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	9	0.34
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	5	0.34
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	7	0.34
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	9	0.34
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	5	0.34
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	7	0.34
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	10	0.33
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	1	0.33
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	10	0.33
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	1	0.33
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	10	0.33
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	1	0.33
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	10	0.33
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	1	0.33
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	10	0.33
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	1	0.33
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	10	0.33
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	1	0.33
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	10	0.33
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	1	0.33
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	10	0.33
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	1	0.33
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	10	0.33
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	1	0.33
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	10	0.33
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	1	0.33
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	10	0.33
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	1	0.33
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	10	0.33
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	1	0.33
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	1	0.33
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	10	0.33
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	1	0.33
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	10	0.33
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	1	0.33
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	7	0.32
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	9	0.32
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	7	0.32
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	9	0.32
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	7	0.32
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	9	0.32
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	7	0.32
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	9	0.32
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	7	0.32
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	9	0.32
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	7	0.32
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	9	0.32
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	7	0.32
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	9	0.32
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	7	0.32
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	9	0.32
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	7	0.32
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	9	0.32
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	7	0.32
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	9	0.32
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	7	0.32
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	9	0.32
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	7	0.32
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	9	0.32
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	7	0.32
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	9	0.32
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	7	0.32
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	9	0.32
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	7	0.32
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	9	0.32
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	1	0.31
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	1	0.31
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	1	0.31
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	1	0.31
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	1	0.31
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	1	0.31
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	1	0.31
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	1	0.31
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	1	0.31
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	1	0.31
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	1	0.31
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	1	0.31
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	1	0.31
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	1	0.31
(1,9715)	1:22:O:LYS:CE	1:76:O:MET:CE	3	0.3
(1,9111)	1:22:N:LYS:CE	1:76:N:MET:CE	3	0.3
(1,8507)	1:22:M:LYS:CE	1:76:M:MET:CE	3	0.3
(1,7903)	1:22:L:LYS:CE	1:76:L:MET:CE	3	0.3
(1,7299)	1:22:K:LYS:CE	1:76:K:MET:CE	3	0.3
(1,6695)	1:22:J:LYS:CE	1:76:J:MET:CE	3	0.3
(1,6091)	1:22:I:LYS:CE	1:76:I:MET:CE	3	0.3
(1,5487)	1:22:H:LYS:CE	1:76:H:MET:CE	3	0.3
(1,4883)	1:22:G:LYS:CE	1:76:G:MET:CE	3	0.3
(1,4279)	1:22:F:LYS:CE	1:76:F:MET:CE	3	0.3
(1,3675)	1:22:E:LYS:CE	1:76:E:MET:CE	3	0.3
(1,3071)	1:22:D:LYS:CE	1:76:D:MET:CE	3	0.3
(1,2467)	1:22:C:LYS:CE	1:76:C:MET:CE	3	0.3
(1,1863)	1:22:B:LYS:CE	1:76:B:MET:CE	3	0.3
(1,1259)	1:22:A:LYS:CE	1:76:A:MET:CE	3	0.3
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	6	0.29
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	6	0.29
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	6	0.29
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	6	0.29
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	4	0.29
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	6	0.29
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	6	0.29
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	6	0.29
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	6	0.29
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	4	0.29
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	6	0.29
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	4	0.28
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	4	0.28
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	6	0.28
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	4	0.28
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	6	0.28
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	4	0.28
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	4	0.28
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	4	0.28
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	4	0.28
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	4	0.28
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	4	0.28
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	6	0.28
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	4	0.28
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	6	0.28
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	4	0.28
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	6	0.28
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	4	0.28
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	4	0.28
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	5	0.27
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	5	0.27
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	5	0.27
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	5	0.27
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	5	0.27
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	5	0.27
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	5	0.27
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	5	0.27
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	5	0.27
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	5	0.27
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	5	0.27
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	5	0.27
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	5	0.27
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	5	0.27
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	5	0.27
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	7	0.26
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	7	0.26
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	7	0.26
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	7	0.26
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	7	0.26
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	7	0.26
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	7	0.26
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	7	0.26
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	7	0.26
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	7	0.26
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	7	0.26
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	7	0.26
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	7	0.26
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	7	0.26
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	7	0.26
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	2	0.25
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	2	0.25
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	2	0.25
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	2	0.25
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	2	0.25
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	2	0.25
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	2	0.25
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	2	0.25
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	2	0.25
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	2	0.25
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	2	0.25
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	2	0.25
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	2	0.25
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	2	0.25
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	10	0.24
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	10	0.24
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	10	0.24
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	10	0.24
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	10	0.24
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	10	0.24
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	10	0.24
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	10	0.24
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	10	0.24
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	10	0.24
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	10	0.24
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	10	0.24
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	10	0.24
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	10	0.24
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	10	0.24
(1,674)	1:59:H:TYR:CB	1:79:O:GLN:CG	5	0.24
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	1	0.23
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	1	0.23
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	1	0.23
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	1	0.23
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	1	0.23
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	1	0.23
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	1	0.23
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	1	0.23
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	1	0.23
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	1	0.23
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	1	0.23
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	1	0.23
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	1	0.23
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	1	0.23
(1,9604)	1:29:O:THR:C	1:32:O:LEU:CD2	4	0.22
(1,9000)	1:29:N:THR:C	1:32:N:LEU:CD2	4	0.22
(1,8396)	1:29:M:THR:C	1:32:M:LEU:CD2	4	0.22
(1,7792)	1:29:L:THR:C	1:32:L:LEU:CD2	4	0.22
(1,7188)	1:29:K:THR:C	1:32:K:LEU:CD2	4	0.22
(1,6584)	1:29:J:THR:C	1:32:J:LEU:CD2	4	0.22
(1,5980)	1:29:I:THR:C	1:32:I:LEU:CD2	4	0.22
(1,5376)	1:29:H:THR:C	1:32:H:LEU:CD2	4	0.22
(1,4772)	1:29:G:THR:C	1:32:G:LEU:CD2	4	0.22
(1,4168)	1:29:F:THR:C	1:32:F:LEU:CD2	4	0.22
(1,3564)	1:29:E:THR:C	1:32:E:LEU:CD2	4	0.22
(1,2960)	1:29:D:THR:C	1:32:D:LEU:CD2	4	0.22
(1,2356)	1:29:C:THR:C	1:32:C:LEU:CD2	4	0.22
(1,1752)	1:29:B:THR:C	1:32:B:LEU:CD2	4	0.22
(1,1148)	1:29:A:THR:C	1:32:A:LEU:CD2	4	0.22
(1,499)	1:59:A:TYR:CB	1:79:H:GLN:CG	3	0.21
(1,699)	1:59:M:TYR:CB	1:79:E:GLN:CG	5	0.2
(1,649)	1:59:C:TYR:CB	1:79:J:GLN:CG	3	0.2
(1,599)	1:59:G:TYR:CB	1:79:N:GLN:CG	5	0.19
(1,574)	1:59:B:TYR:CB	1:79:I:GLN:CG	5	0.19
(1,549)	1:59:K:TYR:CB	1:79:C:GLN:CG	5	0.19
(1,699)	1:59:M:TYR:CB	1:79:E:GLN:CG	3	0.18
(1,624)	1:59:L:TYR:CB	1:79:D:GLN:CG	3	0.18
(1,599)	1:59:G:TYR:CB	1:79:N:GLN:CG	3	0.18
(1,574)	1:59:B:TYR:CB	1:79:I:GLN:CG	9	0.18
(1,524)	1:59:F:TYR:CB	1:79:M:GLN:CG	5	0.18
(1,699)	1:59:M:TYR:CB	1:79:E:GLN:CG	7	0.17
(1,649)	1:59:C:TYR:CB	1:79:J:GLN:CG	5	0.17
(1,624)	1:59:L:TYR:CB	1:79:D:GLN:CG	5	0.17
(1,574)	1:59:B:TYR:CB	1:79:I:GLN:CG	3	0.17
(1,574)	1:59:B:TYR:CB	1:79:I:GLN:CG	10	0.17
(1,549)	1:59:K:TYR:CB	1:79:C:GLN:CG	7	0.17
(1,524)	1:59:F:TYR:CB	1:79:M:GLN:CG	3	0.17
(1,499)	1:59:A:TYR:CB	1:79:H:GLN:CG	5	0.17
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	9	0.16
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	9	0.16
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	7	0.16
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	9	0.16
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	7	0.16
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	9	0.16
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	9	0.16
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	9	0.16
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	9	0.16
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	9	0.16
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	9	0.16
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	7	0.16
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	9	0.16
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	9	0.16
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	9	0.16
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	9	0.16
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	9	0.16
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	9	0.16
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	7	0.16
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	9	0.16
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	9	0.16
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	9	0.16
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	9	0.16
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	9	0.16
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	9	0.16
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	9	0.16
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	9	0.16
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	9	0.16
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	9	0.16
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	7	0.16
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	9	0.16
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	9	0.16
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	7	0.16
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	9	0.16
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	9	0.16
(1,699)	1:59:M:TYR:CB	1:79:E:GLN:CG	1	0.16
(1,699)	1:59:M:TYR:CB	1:79:E:GLN:CG	10	0.16
(1,674)	1:59:H:TYR:CB	1:79:O:GLN:CG	1	0.16
(1,674)	1:59:H:TYR:CB	1:79:O:GLN:CG	9	0.16
(1,674)	1:59:H:TYR:CB	1:79:O:GLN:CG	10	0.16
(1,599)	1:59:G:TYR:CB	1:79:N:GLN:CG	1	0.16
(1,574)	1:59:B:TYR:CB	1:79:I:GLN:CG	1	0.16
(1,574)	1:59:B:TYR:CB	1:79:I:GLN:CG	7	0.16
(1,549)	1:59:K:TYR:CB	1:79:C:GLN:CG	3	0.16
(1,524)	1:59:F:TYR:CB	1:79:M:GLN:CG	9	0.16
(1,499)	1:59:A:TYR:CB	1:79:H:GLN:CG	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	1	0.15
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	3	0.15
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	4	0.15
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	6	0.15
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	7	0.15
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	8	0.15
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	1	0.15
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	3	0.15
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	4	0.15
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	6	0.15
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	8	0.15
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	1	0.15
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	3	0.15
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	4	0.15
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	6	0.15
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	8	0.15
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	1	0.15
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	3	0.15
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	4	0.15
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	6	0.15
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	7	0.15
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	8	0.15
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	1	0.15
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	3	0.15
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	4	0.15
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	6	0.15
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	7	0.15
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	8	0.15
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	1	0.15
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	3	0.15
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	4	0.15
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	6	0.15
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	8	0.15
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	1	0.15
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	3	0.15
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	4	0.15
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	6	0.15
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	7	0.15
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	8	0.15
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	1	0.15
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	3	0.15
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	6	0.15
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	7	0.15
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	8	0.15
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	1	0.15
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	3	0.15
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	4	0.15
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	6	0.15
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	8	0.15
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	1	0.15
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	3	0.15
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	4	0.15
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	6	0.15
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	7	0.15
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	8	0.15
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	1	0.15
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	3	0.15
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	4	0.15
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	6	0.15
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	7	0.15
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	8	0.15
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	1	0.15
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	3	0.15
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	4	0.15
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	6	0.15
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	7	0.15
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	8	0.15
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	1	0.15
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	3	0.15
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	4	0.15
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	6	0.15
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	7	0.15
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	8	0.15
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	1	0.15
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	3	0.15
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	4	0.15
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	6	0.15
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	8	0.15
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	1	0.15
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	3	0.15
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	4	0.15
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	6	0.15
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:59:C:TYR:CB	1:79:J:GLN:CG	1	0.15
(1,649)	1:59:C:TYR:CB	1:79:J:GLN:CG	10	0.15
(1,624)	1:59:L:TYR:CB	1:79:D:GLN:CG	1	0.15
(1,624)	1:59:L:TYR:CB	1:79:D:GLN:CG	10	0.15
(1,599)	1:59:G:TYR:CB	1:79:N:GLN:CG	9	0.15
(1,599)	1:59:G:TYR:CB	1:79:N:GLN:CG	10	0.15
(1,549)	1:59:K:TYR:CB	1:79:C:GLN:CG	10	0.15
(1,524)	1:59:F:TYR:CB	1:79:M:GLN:CG	10	0.15
(1,499)	1:59:A:TYR:CB	1:79:H:GLN:CG	1	0.15
(1,499)	1:59:A:TYR:CB	1:79:H:GLN:CG	10	0.15
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	5	0.14
(1,9246)	1:19:O:GLU:CG	1:22:O:LYS:CE	2	0.14
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	5	0.14
(1,8642)	1:19:N:GLU:CG	1:22:N:LYS:CE	2	0.14
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	5	0.14
(1,8038)	1:19:M:GLU:CG	1:22:M:LYS:CE	2	0.14
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	5	0.14
(1,7434)	1:19:L:GLU:CG	1:22:L:LYS:CE	2	0.14
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	5	0.14
(1,6830)	1:19:K:GLU:CG	1:22:K:LYS:CE	2	0.14
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	5	0.14
(1,6226)	1:19:J:GLU:CG	1:22:J:LYS:CE	2	0.14
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	5	0.14
(1,5622)	1:19:I:GLU:CG	1:22:I:LYS:CE	2	0.14
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	5	0.14
(1,5018)	1:19:H:GLU:CG	1:22:H:LYS:CE	2	0.14
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	5	0.14
(1,4414)	1:19:G:GLU:CG	1:22:G:LYS:CE	2	0.14
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	5	0.14
(1,3810)	1:19:F:GLU:CG	1:22:F:LYS:CE	2	0.14
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	5	0.14
(1,3206)	1:19:E:GLU:CG	1:22:E:LYS:CE	2	0.14
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	5	0.14
(1,2602)	1:19:D:GLU:CG	1:22:D:LYS:CE	2	0.14
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	5	0.14
(1,1998)	1:19:C:GLU:CG	1:22:C:LYS:CE	2	0.14
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	5	0.14
(1,1394)	1:19:B:GLU:CG	1:22:B:LYS:CE	2	0.14
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	5	0.14
(1,790)	1:19:A:GLU:CG	1:22:A:LYS:CE	2	0.14
(1,674)	1:59:H:TYR:CB	1:79:O:GLN:CG	7	0.14
(1,649)	1:59:C:TYR:CB	1:79:J:GLN:CG	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:59:L:TYR:CB	1:79:D:GLN:CG	7	0.14
(1,624)	1:59:L:TYR:CB	1:79:D:GLN:CG	9	0.14
(1,549)	1:59:K:TYR:CB	1:79:C:GLN:CG	1	0.14
(1,524)	1:59:F:TYR:CB	1:79:M:GLN:CG	1	0.14
(1,524)	1:59:F:TYR:CB	1:79:M:GLN:CG	7	0.14
(1,499)	1:59:A:TYR:CB	1:79:H:GLN:CG	9	0.14
(1,9666)	1:70:O:MET:CG	1:71:O:THR:CG2	2	0.13
(1,9062)	1:70:N:MET:CG	1:71:N:THR:CG2	2	0.13
(1,8458)	1:70:M:MET:CG	1:71:M:THR:CG2	2	0.13
(1,7854)	1:70:L:MET:CG	1:71:L:THR:CG2	2	0.13
(1,7250)	1:70:K:MET:CG	1:71:K:THR:CG2	2	0.13
(1,6646)	1:70:J:MET:CG	1:71:J:THR:CG2	2	0.13
(1,6042)	1:70:I:MET:CG	1:71:I:THR:CG2	2	0.13
(1,5438)	1:70:H:MET:CG	1:71:H:THR:CG2	2	0.13
(1,4834)	1:70:G:MET:CG	1:71:G:THR:CG2	2	0.13
(1,4230)	1:70:F:MET:CG	1:71:F:THR:CG2	2	0.13
(1,3626)	1:70:E:MET:CG	1:71:E:THR:CG2	2	0.13
(1,3022)	1:70:D:MET:CG	1:71:D:THR:CG2	2	0.13
(1,2418)	1:70:C:MET:CG	1:71:C:THR:CG2	2	0.13
(1,1814)	1:70:B:MET:CG	1:71:B:THR:CG2	2	0.13
(1,1210)	1:70:A:MET:CG	1:71:A:THR:CG2	2	0.13
(1,599)	1:59:G:TYR:CB	1:79:N:GLN:CG	7	0.13
(1,549)	1:59:K:TYR:CB	1:79:C:GLN:CG	9	0.13
(1,699)	1:59:M:TYR:CB	1:79:E:GLN:CG	9	0.12
(1,674)	1:59:H:TYR:CB	1:79:O:GLN:CG	3	0.12
(1,9242)	1:68:O:LEU:CB	1:72:O:VAL:CB	7	0.11
(1,8638)	1:68:N:LEU:CB	1:72:N:VAL:CB	7	0.11
(1,8034)	1:68:M:LEU:CB	1:72:M:VAL:CB	7	0.11
(1,7430)	1:68:L:LEU:CB	1:72:L:VAL:CB	7	0.11
(1,6826)	1:68:K:LEU:CB	1:72:K:VAL:CB	7	0.11
(1,6222)	1:68:J:LEU:CB	1:72:J:VAL:CB	7	0.11
(1,5618)	1:68:I:LEU:CB	1:72:I:VAL:CB	7	0.11
(1,5014)	1:68:H:LEU:CB	1:72:H:VAL:CB	7	0.11
(1,4410)	1:68:G:LEU:CB	1:72:G:VAL:CB	7	0.11
(1,3806)	1:68:F:LEU:CB	1:72:F:VAL:CB	7	0.11
(1,3202)	1:68:E:LEU:CB	1:72:E:VAL:CB	7	0.11
(1,2598)	1:68:D:LEU:CB	1:72:D:VAL:CB	7	0.11
(1,1994)	1:68:C:LEU:CB	1:72:C:VAL:CB	7	0.11
(1,1390)	1:68:B:LEU:CB	1:72:B:VAL:CB	7	0.11
(1,786)	1:68:A:LEU:CB	1:72:A:VAL:CB	7	0.11
(1,649)	1:59:C:TYR:CB	1:79:J:GLN:CG	9	0.11

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

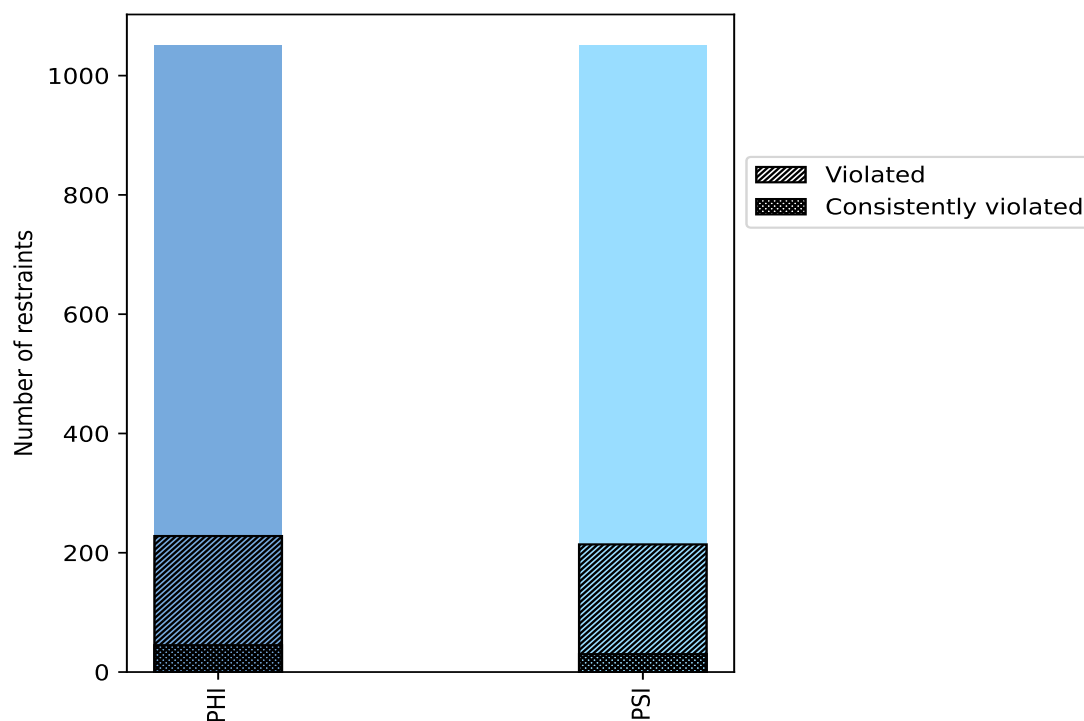
10.1 Summary of dihedral-angle violations [i](#)

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	1050	50.0	228	21.7	10.9	45	4.3	2.1
PSI	1050	50.0	214	20.4	10.2	30	2.9	1.4
Total	2100	100.0	442	21.0	21.0	75	3.6	3.6

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](#)



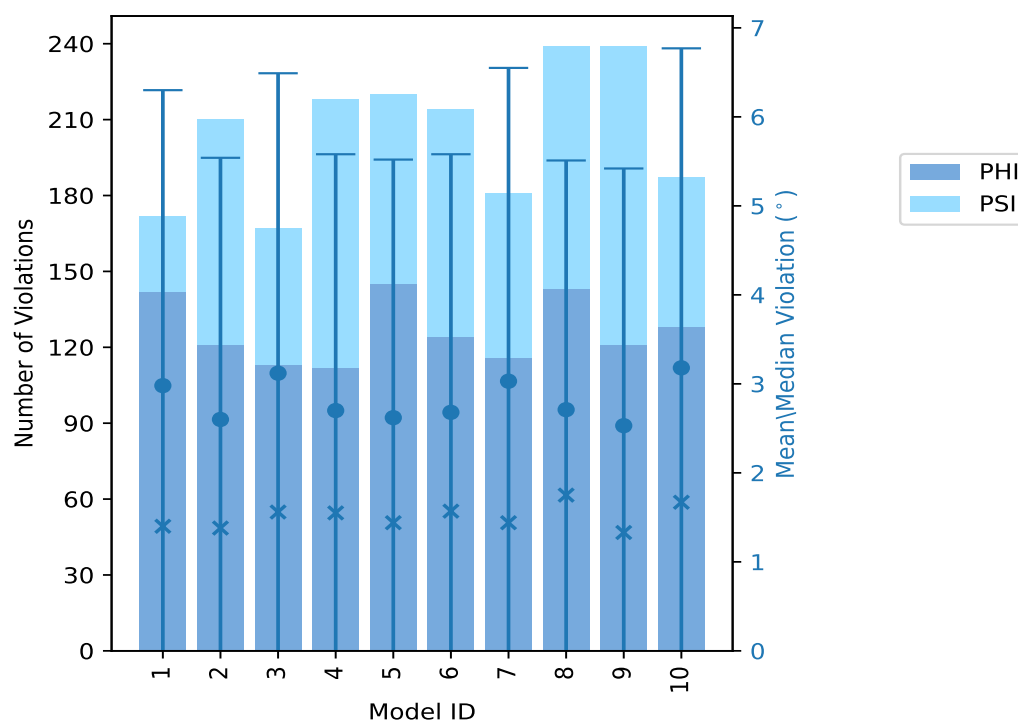
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	142	30	172	2.98	10.34	3.32	1.4
2	121	89	210	2.6	10.14	2.94	1.38
3	113	54	167	3.12	10.5	3.37	1.56
4	112	106	218	2.7	10.11	2.88	1.55
5	145	75	220	2.62	10.24	2.9	1.44
6	124	90	214	2.68	10.12	2.9	1.57
7	116	65	181	3.03	13.11	3.52	1.44
8	143	96	239	2.71	10.4	2.8	1.75
9	121	118	239	2.53	10.36	2.89	1.33
10	128	59	187	3.18	13.95	3.59	1.67

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

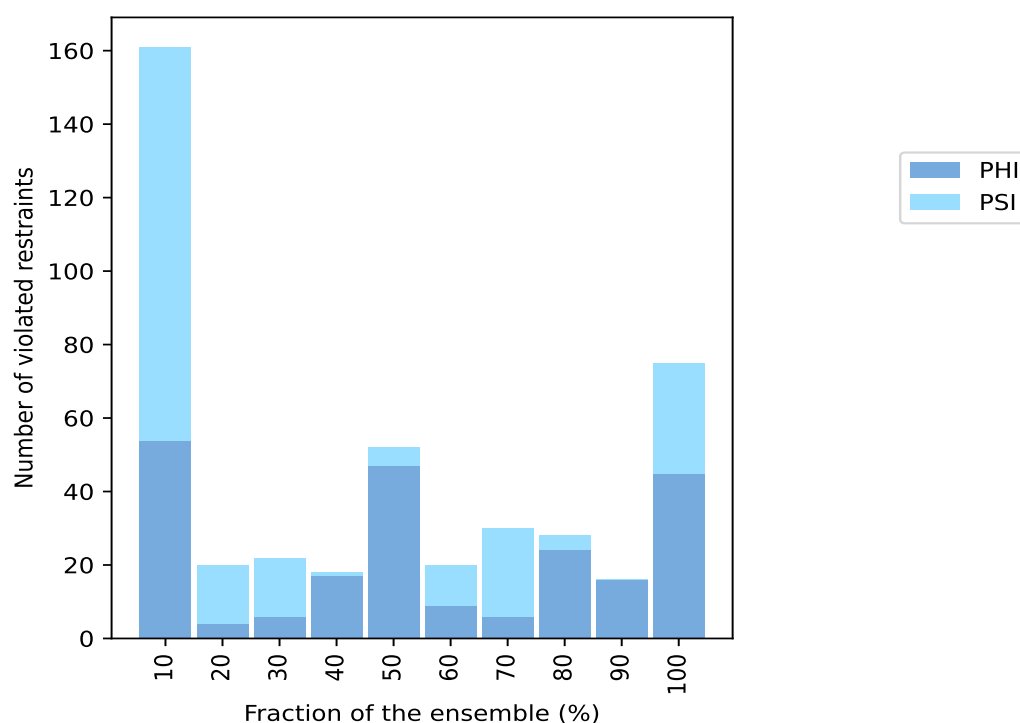
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
54	107	161	1	10.0
4	16	20	2	20.0
6	16	22	3	30.0
17	1	18	4	40.0
47	5	52	5	50.0
9	11	20	6	60.0
6	24	30	7	70.0
24	4	28	8	80.0
16	0	16	9	90.0
45	30	75	10	100.0

¹ Number of models with violations

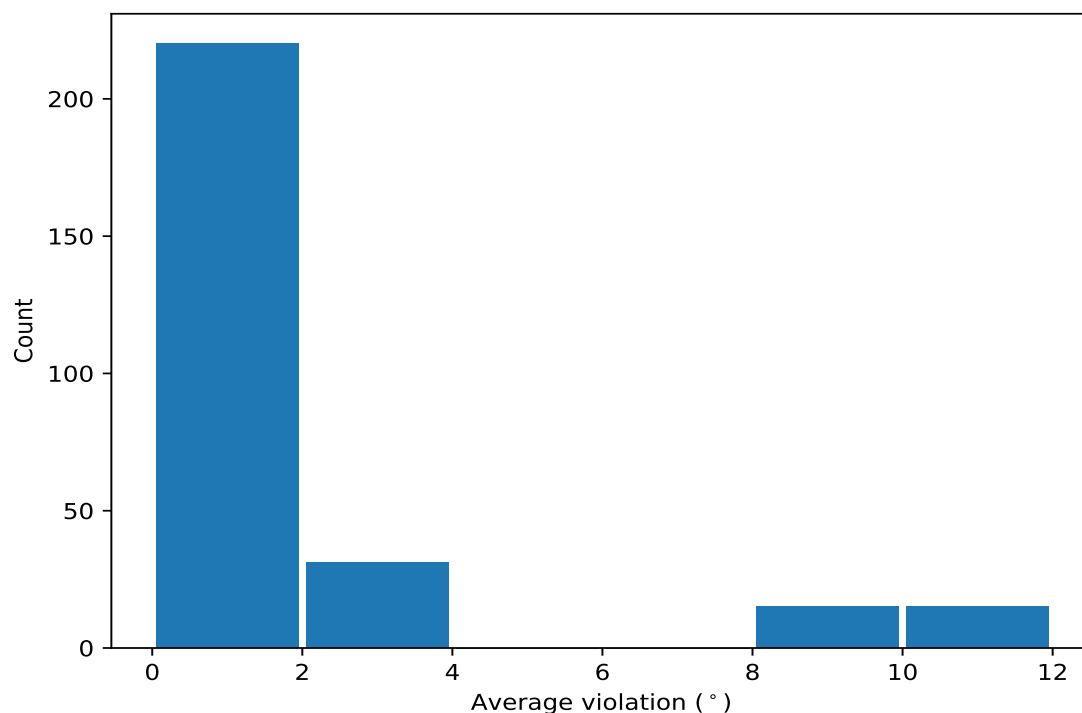
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	10	10.91	1.32	10.3
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	10	10.9	1.32	10.33
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	10	10.89	1.31	10.34
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	10	10.89	1.32	10.3
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	10	10.88	1.29	10.33
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	10	10.88	1.31	10.3
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	10	10.87	1.33	10.28
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	10	10.87	1.3	10.26
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	10	10.87	1.33	10.32
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	10	10.87	1.31	10.3
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	10	10.87	1.31	10.26
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	10	10.87	1.31	10.28
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	10	10.86	1.31	10.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	10	10.85	1.32	10.27
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	10	10.83	1.31	10.27
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	10	9.37	0.78	9.6
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	10	9.34	0.77	9.57
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	10	9.34	0.77	9.59
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	10	9.33	0.75	9.54
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	10	9.31	0.76	9.51
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	10	9.3	0.78	9.54
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	10	9.3	0.76	9.51
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	10	9.3	0.78	9.54
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	10	9.3	0.77	9.52
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	10	9.3	0.75	9.52
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	10	9.28	0.75	9.48
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	10	9.28	0.77	9.48
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	10	9.28	0.79	9.51
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	10	9.28	0.77	9.51
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	10	9.28	0.77	9.54
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	10	2.41	0.28	2.41
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	10	2.41	0.27	2.41
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	10	2.41	0.29	2.42
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	10	2.41	0.27	2.42
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	10	2.41	0.29	2.42
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	10	2.4	0.26	2.42
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	10	2.4	0.28	2.44
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	10	2.4	0.27	2.38
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	10	2.4	0.28	2.42
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	10	2.39	0.28	2.38
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	10	2.38	0.29	2.4
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	10	2.38	0.28	2.42
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	10	2.37	0.29	2.4
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	10	2.37	0.28	2.37
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	10	2.36	0.29	2.34
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	10	1.83	0.32	1.84
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	10	1.82	0.32	1.84
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	10	1.82	0.32	1.81
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	10	1.81	0.33	1.82
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	10	1.79	0.28	1.66
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	10	1.78	0.26	1.69
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	10	1.78	0.26	1.73
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	10	1.78	0.25	1.72
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	10	1.77	0.25	1.72
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	10	1.76	0.27	1.67
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	10	1.76	0.33	1.76
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	10	1.76	0.26	1.67
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	10	1.75	0.28	1.65
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	10	1.75	0.24	1.67
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	10	1.74	0.26	1.65
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	10	1.74	0.25	1.66
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	10	1.74	0.31	1.73
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	10	1.73	0.32	1.69
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	10	1.73	0.32	1.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	10	1.73	0.33	1.71
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	10	1.72	0.31	1.72
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	10	1.72	0.34	1.7
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	10	1.72	0.34	1.7
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	10	1.72	0.33	1.69
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	10	1.71	0.34	1.72
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	10	1.71	0.32	1.72
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	10	1.69	0.26	1.62
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	10	1.69	0.3	1.6
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	10	1.68	0.27	1.61
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	10	1.66	0.25	1.61
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	9	1.33	0.17	1.29
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	9	1.33	0.18	1.32
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	9	1.32	0.16	1.24
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	9	1.31	0.27	1.19
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	9	1.31	0.25	1.2
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	9	1.3	0.16	1.28
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	9	1.3	0.18	1.27
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	9	1.29	0.16	1.25
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	9	1.29	0.15	1.26
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	9	1.29	0.18	1.25
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	9	1.28	0.14	1.24
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	9	1.28	0.17	1.2
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	9	1.28	0.16	1.24
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	9	1.27	0.17	1.24
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	9	1.27	0.15	1.28
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	9	1.24	0.16	1.2
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	8	1.97	0.7	1.82
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	8	1.96	0.69	1.82
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	8	1.95	0.71	1.76
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	8	1.95	0.7	1.79
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	8	1.94	0.64	1.8
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	8	1.94	0.69	1.76
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	8	1.93	0.72	1.74
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	8	1.92	0.68	1.77
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	8	1.9	0.69	1.73
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	8	1.89	0.69	1.7
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	8	1.88	0.67	1.69
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	8	1.86	0.67	1.64
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	8	1.86	0.69	1.68
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	8	1.36	0.25	1.3
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	8	1.34	0.26	1.26
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	8	1.34	0.24	1.23
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	8	1.33	0.24	1.25
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	8	1.33	0.24	1.23
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	8	1.33	0.23	1.24
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	8	1.32	0.24	1.23
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	8	1.3	0.24	1.22
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	8	1.3	0.24	1.2
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	8	1.28	0.25	1.19
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	8	1.25	0.16	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	8	1.23	0.09	1.22
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	8	1.22	0.1	1.23
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	8	1.21	0.08	1.2
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	8	1.2	0.09	1.23
(1,903)	1:74:G:ARG:C	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	7	1.99	0.67	1.67
(1,1183)	1:74:I:ARG:C	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	7	1.94	0.65	1.71
(1,504)	1:18:D:ASP:N	1:18:D:ASP:CA	1:18:D:ASP:C	1:19:D:GLU:N	7	1.39	0.26	1.42
(1,458)	1:45:D:LEU:C	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	7	1.38	0.24	1.35
(1,1484)	1:18:K:ASP:N	1:18:K:ASP:CA	1:18:K:ASP:C	1:19:K:GLU:N	7	1.38	0.25	1.36
(1,364)	1:18:C:ASP:N	1:18:C:ASP:CA	1:18:C:ASP:C	1:19:C:GLU:N	7	1.37	0.24	1.41
(1,1344)	1:18:J:ASP:N	1:18:J:ASP:CA	1:18:J:ASP:C	1:19:J:GLU:N	7	1.37	0.25	1.36
(1,644)	1:18:E:ASP:N	1:18:E:ASP:CA	1:18:E:ASP:C	1:19:E:GLU:N	7	1.37	0.21	1.36
(1,611)	1:58:E:SER:C	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	7	1.36	0.25	1.45
(1,1904)	1:18:N:ASP:N	1:18:N:ASP:CA	1:18:N:ASP:C	1:19:N:GLU:N	7	1.36	0.24	1.31
(1,84)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:GLU:N	7	1.36	0.23	1.35
(1,224)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:GLU:N	7	1.36	0.22	1.33
(1,1998)	1:45:O:LEU:C	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	7	1.35	0.26	1.27
(1,1578)	1:45:L:LEU:C	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	7	1.35	0.23	1.33
(1,1064)	1:18:H:ASP:N	1:18:H:ASP:CA	1:18:H:ASP:C	1:19:H:GLU:N	7	1.35	0.24	1.26
(1,1204)	1:18:I:ASP:N	1:18:I:ASP:CA	1:18:I:ASP:C	1:19:I:GLU:N	7	1.34	0.21	1.33
(1,1624)	1:18:L:ASP:N	1:18:L:ASP:CA	1:18:L:ASP:C	1:19:L:GLU:N	7	1.34	0.22	1.31
(1,924)	1:18:G:ASP:N	1:18:G:ASP:CA	1:18:G:ASP:C	1:19:G:GLU:N	7	1.34	0.27	1.27
(1,784)	1:18:F:ASP:N	1:18:F:ASP:CA	1:18:F:ASP:C	1:19:F:GLU:N	7	1.33	0.24	1.33
(1,2044)	1:18:O:ASP:N	1:18:O:ASP:CA	1:18:O:ASP:C	1:19:O:GLU:N	7	1.32	0.21	1.28
(1,1764)	1:18:M:ASP:N	1:18:M:ASP:CA	1:18:M:ASP:C	1:19:M:GLU:N	7	1.31	0.23	1.27
(1,214)	1:7:B:ALA:N	1:7:B:ALA:CA	1:7:B:ALA:C	1:8:B:ILE:N	7	1.23	0.1	1.2
(1,914)	1:7:G:ALA:N	1:7:G:ALA:CA	1:7:G:ALA:C	1:8:G:ILE:N	7	1.21	0.1	1.19
(1,1054)	1:7:H:ALA:N	1:7:H:ALA:CA	1:7:H:ALA:C	1:8:H:ILE:N	7	1.19	0.08	1.18
(1,1334)	1:7:J:ALA:N	1:7:J:ALA:CA	1:7:J:ALA:C	1:8:J:ILE:N	7	1.18	0.06	1.18
(1,1754)	1:7:M:ALA:N	1:7:M:ALA:CA	1:7:M:ALA:C	1:8:M:ILE:N	7	1.17	0.09	1.16
(1,634)	1:7:E:ALA:N	1:7:E:ALA:CA	1:7:E:ALA:C	1:8:E:ILE:N	7	1.15	0.07	1.13
(1,494)	1:7:D:ALA:N	1:7:D:ALA:CA	1:7:D:ALA:C	1:8:D:ILE:N	7	1.14	0.06	1.11
(1,1614)	1:7:L:ALA:N	1:7:L:ALA:CA	1:7:L:ALA:C	1:8:L:ILE:N	7	1.14	0.06	1.13
(1,74)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	7	1.12	0.07	1.12
(1,1570)	1:37:L:GLY:C	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	6	1.64	0.78	1.16
(1,310)	1:37:C:GLY:C	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	6	1.61	0.77	1.1
(1,331)	1:58:C:SER:C	1:59:C:TYR:N	1:59:C:TYR:CA	1:59:C:TYR:C	6	1.41	0.24	1.5
(1,1976)	1:19:O:GLU:C	1:20:O:LEU:N	1:20:O:LEU:CA	1:20:O:LEU:C	6	1.37	0.23	1.34
(1,191)	1:58:B:SER:C	1:59:B:TYR:N	1:59:B:TYR:CA	1:59:B:TYR:C	6	1.37	0.22	1.46
(1,16)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	6	1.36	0.25	1.34
(1,1031)	1:58:H:SER:C	1:59:H:TYR:N	1:59:H:TYR:CA	1:59:H:TYR:C	6	1.35	0.21	1.44
(1,296)	1:19:C:GLU:C	1:20:C:LEU:N	1:20:C:LEU:CA	1:20:C:LEU:C	6	1.32	0.22	1.27
(1,436)	1:19:D:GLU:C	1:20:D:LEU:N	1:20:D:LEU:CA	1:20:D:LEU:C	6	1.32	0.22	1.27
(1,774)	1:7:F:ALA:N	1:7:F:ALA:CA	1:7:F:ALA:C	1:8:F:ILE:N	6	1.19	0.08	1.18
(1,2069)	1:47:O:MET:N	1:47:O:MET:CA	1:47:O:MET:C	1:48:O:ASP:N	6	1.18	0.1	1.18
(1,529)	1:47:D:MET:N	1:47:D:MET:CA	1:47:D:MET:C	1:48:D:ASP:N	6	1.17	0.11	1.14
(1,109)	1:47:A:MET:N	1:47:A:MET:CA	1:47:A:MET:C	1:48:A:ASP:N	6	1.17	0.11	1.17
(1,949)	1:47:G:MET:N	1:47:G:MET:CA	1:47:G:MET:C	1:48:G:ASP:N	6	1.17	0.09	1.16
(1,1369)	1:47:J:MET:N	1:47:J:MET:CA	1:47:J:MET:C	1:48:J:ASP:N	6	1.17	0.12	1.14
(1,1089)	1:47:H:MET:N	1:47:H:MET:CA	1:47:H:MET:C	1:48:H:ASP:N	6	1.15	0.11	1.12
(1,1649)	1:47:L:MET:N	1:47:L:MET:CA	1:47:L:MET:C	1:48:L:ASP:N	6	1.15	0.1	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,249)	1:47:B:MET:N	1:47:B:MET:CA	1:47:B:MET:C	1:48:B:ASP:N	6	1.15	0.12	1.15
(1,1229)	1:47:I:MET:N	1:47:I:MET:CA	1:47:I:MET:C	1:48:I:ASP:N	6	1.14	0.08	1.13
(1,2034)	1:7:O:ALA:N	1:7:O:ALA:CA	1:7:O:ALA:C	1:8:O:ILE:N	6	1.12	0.05	1.1
(1,1010)	1:37:H:GLY:C	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	5	1.78	0.79	1.23
(1,1150)	1:37:I:GLY:C	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	5	1.73	0.79	1.17
(1,470)	1:57:D:VAL:C	1:58:D:SER:N	1:58:D:SER:CA	1:58:D:SER:C	5	1.55	0.21	1.53
(1,190)	1:57:B:VAL:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	5	1.54	0.2	1.57
(1,1450)	1:57:K:VAL:C	1:58:K:SER:N	1:58:K:SER:CA	1:58:K:SER:C	5	1.53	0.18	1.52
(1,2010)	1:57:O:VAL:C	1:58:O:SER:N	1:58:O:SER:CA	1:58:O:SER:C	5	1.53	0.2	1.56
(1,1310)	1:57:J:VAL:C	1:58:J:SER:N	1:58:J:SER:CA	1:58:J:SER:C	5	1.53	0.21	1.5
(1,50)	1:57:A:VAL:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	5	1.52	0.2	1.52
(1,1730)	1:57:M:VAL:C	1:58:M:SER:N	1:58:M:SER:CA	1:58:M:SER:C	5	1.51	0.19	1.49
(1,890)	1:57:G:VAL:C	1:58:G:SER:N	1:58:G:SER:CA	1:58:G:SER:C	5	1.51	0.24	1.46
(1,1170)	1:57:I:VAL:C	1:58:I:SER:N	1:58:I:SER:CA	1:58:I:SER:C	5	1.5	0.18	1.49
(1,1030)	1:57:H:VAL:C	1:58:H:SER:N	1:58:H:SER:CA	1:58:H:SER:C	5	1.5	0.22	1.48
(1,1590)	1:57:L:VAL:C	1:58:L:SER:N	1:58:L:SER:CA	1:58:L:SER:C	5	1.5	0.22	1.61
(1,750)	1:57:F:VAL:C	1:58:F:SER:N	1:58:F:SER:CA	1:58:F:SER:C	5	1.48	0.18	1.5
(1,1871)	1:58:N:SER:C	1:59:N:TYR:N	1:59:N:TYR:CA	1:59:N:TYR:C	5	1.48	0.16	1.55
(1,1870)	1:57:N:VAL:C	1:58:N:SER:N	1:58:N:SER:CA	1:58:N:SER:C	5	1.46	0.2	1.47
(1,1311)	1:58:J:SER:C	1:59:J:TYR:N	1:59:J:TYR:CA	1:59:J:TYR:C	5	1.45	0.17	1.51
(1,610)	1:57:E:VAL:C	1:58:E:SER:N	1:58:E:SER:CA	1:58:E:SER:C	5	1.45	0.21	1.41
(1,1731)	1:58:M:SER:C	1:59:M:TYR:N	1:59:M:TYR:CA	1:59:M:TYR:C	5	1.44	0.14	1.53
(1,51)	1:58:A:SER:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	5	1.44	0.16	1.54
(1,330)	1:57:C:VAL:C	1:58:C:SER:N	1:58:C:SER:CA	1:58:C:SER:C	5	1.44	0.21	1.43
(1,471)	1:58:D:SER:C	1:59:D:TYR:N	1:59:D:TYR:CA	1:59:D:TYR:C	5	1.44	0.17	1.5
(1,751)	1:58:F:SER:C	1:59:F:TYR:N	1:59:F:TYR:CA	1:59:F:TYR:C	5	1.43	0.18	1.47
(1,1416)	1:19:K:GLU:C	1:20:K:LEU:N	1:20:K:LEU:CA	1:20:K:LEU:C	5	1.43	0.2	1.35
(1,891)	1:58:G:SER:C	1:59:G:TYR:N	1:59:G:TYR:CA	1:59:G:TYR:C	5	1.43	0.19	1.53
(1,1171)	1:58:I:SER:C	1:59:I:TYR:N	1:59:I:TYR:CA	1:59:I:TYR:C	5	1.43	0.18	1.48
(1,1451)	1:58:K:SER:C	1:59:K:TYR:N	1:59:K:TYR:CA	1:59:K:TYR:C	5	1.41	0.16	1.46
(1,716)	1:19:F:GLU:C	1:20:F:LEU:N	1:20:F:LEU:CA	1:20:F:LEU:C	5	1.41	0.21	1.32
(1,2011)	1:58:O:SER:C	1:59:O:TYR:N	1:59:O:TYR:CA	1:59:O:TYR:C	5	1.41	0.18	1.5
(1,1136)	1:19:I:GLU:C	1:20:I:LEU:N	1:20:I:LEU:CA	1:20:I:LEU:C	5	1.41	0.21	1.36
(1,1591)	1:58:L:SER:C	1:59:L:TYR:N	1:59:L:TYR:CA	1:59:L:TYR:C	5	1.4	0.15	1.47
(1,1836)	1:19:N:GLU:C	1:20:N:LEU:N	1:20:N:LEU:CA	1:20:N:LEU:C	5	1.4	0.21	1.4
(1,1696)	1:19:M:GLU:C	1:20:M:LEU:N	1:20:M:LEU:CA	1:20:M:LEU:C	5	1.39	0.21	1.25
(1,1276)	1:19:J:GLU:C	1:20:J:LEU:N	1:20:J:LEU:CA	1:20:J:LEU:C	5	1.39	0.2	1.33
(1,1556)	1:19:L:GLU:C	1:20:L:LEU:N	1:20:L:LEU:CA	1:20:L:LEU:C	5	1.37	0.17	1.31
(1,156)	1:19:B:GLU:C	1:20:B:LEU:N	1:20:B:LEU:CA	1:20:B:LEU:C	5	1.36	0.21	1.31
(1,576)	1:19:E:GLU:C	1:20:E:LEU:N	1:20:E:LEU:CA	1:20:E:LEU:C	5	1.36	0.19	1.29
(1,996)	1:19:H:GLU:C	1:20:H:LEU:N	1:20:H:LEU:CA	1:20:H:LEU:C	5	1.36	0.2	1.29
(1,856)	1:19:G:GLU:C	1:20:G:LEU:N	1:20:G:LEU:CA	1:20:G:LEU:C	5	1.31	0.19	1.27
(1,428)	1:10:D:ASP:C	1:11:D:ALA:N	1:11:D:ALA:CA	1:11:D:ALA:C	5	1.22	0.15	1.18
(1,288)	1:10:C:ASP:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	5	1.21	0.14	1.12
(1,1688)	1:10:M:ASP:C	1:11:M:ALA:N	1:11:M:ALA:CA	1:11:M:ALA:C	5	1.21	0.17	1.12
(1,1509)	1:47:K:MET:N	1:47:K:MET:CA	1:47:K:MET:C	1:48:K:ASP:N	5	1.19	0.11	1.19
(1,148)	1:10:B:ASP:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	5	1.19	0.12	1.15
(1,1929)	1:47:N:MET:N	1:47:N:MET:CA	1:47:N:MET:C	1:48:N:ASP:N	5	1.18	0.09	1.16
(1,669)	1:47:E:MET:N	1:47:E:MET:CA	1:47:E:MET:C	1:48:E:ASP:N	5	1.18	0.11	1.15
(1,389)	1:47:C:MET:N	1:47:C:MET:CA	1:47:C:MET:C	1:48:C:ASP:N	5	1.17	0.11	1.16
(1,8)	1:10:A:ASP:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	5	1.17	0.15	1.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,988)	1:10:H:ASP:C	1:11:H:ALA:N	1:11:H:ALA:CA	1:11:H:ALA:C	5	1.15	0.13	1.06
(1,1789)	1:47:M:MET:N	1:47:M:MET:CA	1:47:M:MET:C	1:48:M:ASP:N	5	1.15	0.1	1.16
(1,568)	1:10:E:ASP:C	1:11:E:ALA:N	1:11:E:ALA:CA	1:11:E:ALA:C	5	1.14	0.12	1.07
(1,2019)	1:70:O:MET:C	1:71:O:THR:N	1:71:O:THR:CA	1:71:O:THR:C	5	1.08	0.06	1.12
(1,170)	1:37:B:GLY:C	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	4	1.95	0.84	1.97
(1,30)	1:37:A:GLY:C	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	4	1.94	0.8	1.94
(1,450)	1:37:D:GLY:C	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	4	1.92	0.81	1.9
(1,730)	1:37:F:GLY:C	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	4	1.92	0.78	1.9
(1,1850)	1:37:N:GLY:C	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	4	1.92	0.81	1.92
(1,1290)	1:37:J:GLY:C	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	4	1.91	0.78	1.93
(1,1430)	1:37:K:GLY:C	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	4	1.9	0.8	1.88
(1,870)	1:37:G:GLY:C	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	4	1.88	0.78	1.9
(1,590)	1:37:E:GLY:C	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	4	1.88	0.8	1.86
(1,1710)	1:37:M:GLY:C	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	4	1.88	0.81	1.9
(1,1968)	1:10:O:ASP:C	1:11:O:ALA:N	1:11:O:ALA:CA	1:11:O:ALA:C	4	1.25	0.15	1.23
(1,1128)	1:10:I:ASP:C	1:11:I:ALA:N	1:11:I:ALA:CA	1:11:I:ALA:C	4	1.25	0.17	1.24
(1,1828)	1:10:N:ASP:C	1:11:N:ALA:N	1:11:N:ALA:CA	1:11:N:ALA:C	4	1.23	0.16	1.16
(1,708)	1:10:F:ASP:C	1:11:F:ALA:N	1:11:F:ALA:CA	1:11:F:ALA:C	4	1.17	0.16	1.12
(1,809)	1:47:F:MET:N	1:47:F:MET:CA	1:47:F:MET:C	1:48:F:ASP:N	4	1.16	0.07	1.13
(1,1268)	1:10:J:ASP:C	1:11:J:ALA:N	1:11:J:ALA:CA	1:11:J:ALA:C	4	1.16	0.14	1.12
(1,1599)	1:70:L:MET:C	1:71:L:THR:N	1:71:L:THR:CA	1:71:L:THR:C	4	1.1	0.01	1.11
(1,1739)	1:70:M:MET:C	1:71:M:THR:N	1:71:M:THR:CA	1:71:M:THR:C	4	1.05	0.03	1.04
(1,1350)	1:24:J:LYS:N	1:24:J:LYS:CA	1:24:J:LYS:C	1:25:J:MET:N	3	2.32	0.49	2.45
(1,90)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:MET:N	3	2.29	0.47	2.41
(1,790)	1:24:F:LYS:N	1:24:F:LYS:CA	1:24:F:LYS:C	1:25:F:MET:N	3	2.29	0.47	2.38
(1,1490)	1:24:K:LYS:N	1:24:K:LYS:CA	1:24:K:LYS:C	1:25:K:MET:N	3	2.29	0.49	2.43
(1,1910)	1:24:N:LYS:N	1:24:N:LYS:CA	1:24:N:LYS:C	1:25:N:MET:N	3	2.28	0.47	2.45
(1,370)	1:24:C:LYS:N	1:24:C:LYS:CA	1:24:C:LYS:C	1:25:C:MET:N	3	2.28	0.46	2.36
(1,930)	1:24:G:LYS:N	1:24:G:LYS:CA	1:24:G:LYS:C	1:25:G:MET:N	3	2.27	0.48	2.37
(1,230)	1:24:B:LYS:N	1:24:B:LYS:CA	1:24:B:LYS:C	1:25:B:MET:N	3	2.24	0.47	2.36
(1,1770)	1:24:M:LYS:N	1:24:M:LYS:CA	1:24:M:LYS:C	1:25:M:MET:N	3	2.24	0.5	2.32
(1,1210)	1:24:I:LYS:N	1:24:I:LYS:CA	1:24:I:LYS:C	1:25:I:MET:N	3	2.23	0.48	2.35
(1,2050)	1:24:O:LYS:N	1:24:O:LYS:CA	1:24:O:LYS:C	1:25:O:MET:N	3	2.23	0.48	2.34
(1,650)	1:24:E:LYS:N	1:24:E:LYS:CA	1:24:E:LYS:C	1:25:E:MET:N	3	2.22	0.48	2.38
(1,1070)	1:24:H:LYS:N	1:24:H:LYS:CA	1:24:H:LYS:C	1:25:H:MET:N	3	2.22	0.48	2.37
(1,510)	1:24:D:LYS:N	1:24:D:LYS:CA	1:24:D:LYS:C	1:25:D:MET:N	3	2.22	0.48	2.34
(1,1630)	1:24:L:LYS:N	1:24:L:LYS:CA	1:24:L:LYS:C	1:25:L:MET:N	3	2.21	0.43	2.37
(1,1990)	1:37:O:GLY:C	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	3	2.2	0.73	2.64
(1,848)	1:10:G:ASP:C	1:11:G:ALA:N	1:11:G:ALA:CA	1:11:G:ALA:C	3	1.27	0.17	1.24
(1,1408)	1:10:K:ASP:C	1:11:K:ALA:N	1:11:K:ALA:CA	1:11:K:ALA:C	3	1.26	0.1	1.27
(1,1548)	1:10:L:ASP:C	1:11:L:ALA:N	1:11:L:ALA:CA	1:11:L:ALA:C	3	1.23	0.15	1.28
(1,1879)	1:70:N:MET:C	1:71:N:THR:N	1:71:N:THR:CA	1:71:N:THR:C	3	1.1	0.02	1.11
(1,668)	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	1:47:E:MET:N	3	1.1	0.05	1.13
(1,1319)	1:70:J:MET:C	1:71:J:THR:N	1:71:J:THR:CA	1:71:J:THR:C	3	1.03	0.03	1.02
(1,1069)	1:23:H:PHE:N	1:23:H:PHE:CA	1:23:H:PHE:C	1:24:H:LYS:N	2	1.14	0.14	1.14
(1,929)	1:23:G:PHE:N	1:23:G:PHE:CA	1:23:G:PHE:C	1:24:G:LYS:N	2	1.13	0.09	1.13
(1,2049)	1:23:O:PHE:N	1:23:O:PHE:CA	1:23:O:PHE:C	1:24:O:LYS:N	2	1.12	0.07	1.12
(1,1629)	1:23:L:PHE:N	1:23:L:PHE:CA	1:23:L:PHE:C	1:24:L:LYS:N	2	1.12	0.12	1.12
(1,1909)	1:23:N:PHE:N	1:23:N:PHE:CA	1:23:N:PHE:C	1:24:N:LYS:N	2	1.1	0.09	1.1
(1,1088)	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	1:47:H:MET:N	2	1.08	0.04	1.08
(1,1648)	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	1:47:L:MET:N	2	1.08	0.02	1.08

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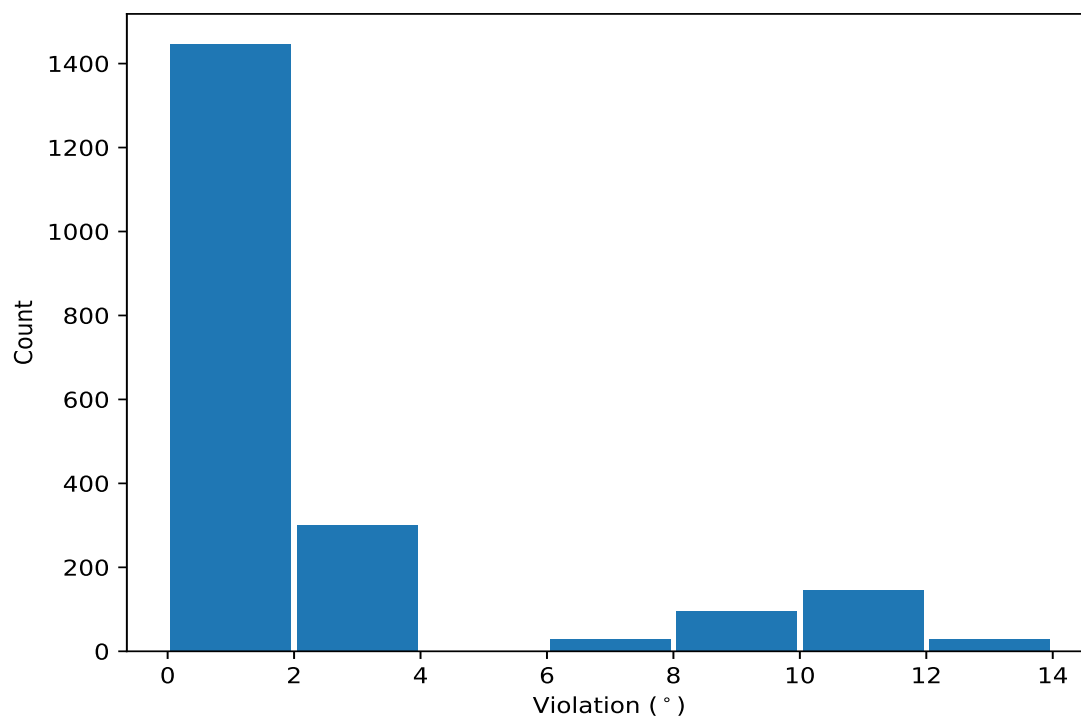
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,1788)	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	1:47:M:MET:N	2	1.08	0.02	1.08
(1,948)	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	1:47:G:MET:N	2	1.06	0.05	1.06
(1,1368)	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	1:47:J:MET:N	2	1.06	0.04	1.06
(1,388)	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	1:47:C:MET:N	2	1.06	0.01	1.06
(1,108)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:MET:N	2	1.05	0.02	1.05
(1,528)	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	1:47:D:MET:N	2	1.05	0.01	1.05
(1,199)	1:70:B:MET:C	1:71:B:THR:N	1:71:B:THR:CA	1:71:B:THR:C	2	1.04	0.02	1.04
(1,1508)	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	1:47:K:MET:N	2	1.04	0.03	1.04
(1,1228)	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	1:47:I:MET:N	2	1.04	0.02	1.04
(1,1928)	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	1:47:N:MET:N	2	1.04	0.02	1.04
(1,59)	1:70:A:MET:C	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	2	1.02	0.02	1.02
(1,339)	1:70:C:MET:C	1:71:C:THR:N	1:71:C:THR:CA	1:71:C:THR:C	2	1.02	0.02	1.02
(1,759)	1:70:F:MET:C	1:71:F:THR:N	1:71:F:THR:CA	1:71:F:THR:C	2	1.01	0.01	1.01

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 (°)
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	10	13.95
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	10	13.91
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	10	13.91
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	10	13.91
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	10	13.9
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	10	13.89
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	10	13.87
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	10	13.86
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	10	13.86
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	10	13.85
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	10	13.85
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	10	13.85
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	10	13.85
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	10	13.83
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	10	13.8
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	7	13.11
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	7	13.08
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	7	13.07
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	7	13.06
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	7	13.06
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	7	13.06
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	7	13.06
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	7	13.06
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	7	13.06
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	7	13.04
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	7	13.04
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	7	13.04
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	7	13.04
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	7	13.03
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	7	12.96
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	3	10.5
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	3	10.5
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	3	10.5
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	3	10.49
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	3	10.49
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	3	10.49
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	3	10.49
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	3	10.49
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	3	10.48
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	3	10.48
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	3	10.47
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	3	10.47
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	3	10.47
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	3	10.47
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	3	10.46
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	8	10.4
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	8	10.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	8	10.36
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	9	10.36
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	8	10.36
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	9	10.35
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	8	10.34
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	9	10.34
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	1	10.34
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	8	10.34
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	9	10.34
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	8	10.34
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	9	10.34
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	9	10.33
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	8	10.33
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	8	10.33
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	9	10.33
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	8	10.33
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	8	10.32
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	1	10.32
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	9	10.32
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	8	10.32
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	9	10.31
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	8	10.31
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	1	10.31
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	9	10.31
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	9	10.31
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	9	10.31
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	1	10.3
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	1	10.3
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	1	10.3
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	8	10.29
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	9	10.29
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	8	10.29
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	9	10.29
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	1	10.28
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	9	10.28
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	1	10.28
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	1	10.27
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	1	10.27
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	1	10.26
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	1	10.25
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	5	10.24
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	1	10.24
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	1	10.23
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	5	10.23
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	1	10.22
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	5	10.22
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	5	10.22
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	5	10.21
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	5	10.21
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	5	10.2
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	5	10.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	5	10.2
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	5	10.2
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	5	10.19
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	5	10.19
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	5	10.19
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	5	10.16
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	5	10.16
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	3	10.16
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	2	10.14
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	2	10.13
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	2	10.13
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	2	10.13
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	1	10.12
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	2	10.12
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	6	10.12
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	2	10.11
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	4	10.11
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	1	10.11
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	4	10.11
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	3	10.1
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	4	10.1
(1,240)	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1:39:B:ILE:N	6	10.1
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	2	10.09
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	6	10.09
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	4	10.08
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	4	10.08
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	2	10.08
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	3	10.08
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	3	10.08
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	2	10.07
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	6	10.07
(1,1220)	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1:39:I:ILE:N	4	10.07
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	2	10.07
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	1	10.07
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	2	10.07
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	1	10.07
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	1	10.07
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	2	10.07
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	3	10.06
(1,1780)	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1:39:M:ILE:N	4	10.06
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	1	10.06
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	6	10.06
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	3	10.06
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	6	10.06
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	6	10.06
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	3	10.06
(1,520)	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1:39:D:ILE:N	4	10.05
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	6	10.05
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	1	10.05
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	3	10.05
(1,100)	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1:39:A:ILE:N	4	10.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	1	10.04
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	3	10.04
(1,940)	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1:39:G:ILE:N	6	10.04
(1,380)	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1:39:C:ILE:N	4	10.04
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	6	10.03
(1,1920)	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1:39:N:ILE:N	6	10.03
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	2	10.03
(1,660)	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1:39:E:ILE:N	6	10.03
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	3	10.03
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	1	10.03
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	2	10.02
(1,2060)	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	1:39:O:ILE:N	4	10.02
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	3	10.02
(1,1360)	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1:39:J:ILE:N	4	10.02
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	2	10.02
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	6	10.02
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	1	10.02
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	1	10.01
(1,1640)	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1:39:L:ILE:N	6	10.01
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	4	10.01
(1,1500)	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1:39:K:ILE:N	6	10.01
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	3	10.01
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	3	10.01
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	3	10.01
(1,800)	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1:39:F:ILE:N	4	10.01
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	3	10.0
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	1	9.99
(1,1080)	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1:39:H:ILE:N	4	9.99
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	1	9.97
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	1	9.97
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	1	9.96
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	9	9.85
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	9	9.85
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	9	9.85
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	9	9.83
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	9	9.82
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	9	9.8
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	9	9.79
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	9	9.78
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	9	9.78
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	9	9.78
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	9	9.77
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	9	9.77
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	9	9.77
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	9	9.76
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	9	9.73
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	4	9.65
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	6	9.64
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	4	9.64
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	4	9.63
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	4	9.62

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	6	9.62
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	6	9.61
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	6	9.61
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	4	9.59
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	6	9.58
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	4	9.57
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	8	9.57
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	6	9.56
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	4	9.56
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	4	9.55
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	6	9.55
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	4	9.55
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	8	9.55
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	4	9.55
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	8	9.55
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	6	9.55
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	6	9.54
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	6	9.54
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	4	9.53
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	6	9.53
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	8	9.53
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	8	9.53
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	6	9.53
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	6	9.53
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	4	9.53
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	4	9.52
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	8	9.52
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	6	9.52
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	4	9.52
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	6	9.51
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	5	9.51
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	5	9.51
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	4	9.51
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	5	9.5
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	5	9.5
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	5	9.5
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	5	9.49
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	5	9.49
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	8	9.48
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	8	9.48
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	5	9.48
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	2	9.48
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	8	9.48
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	8	9.47
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	8	9.47
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	2	9.47
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	2	9.47
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	5	9.47
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	5	9.47
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	5	9.46
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	2	9.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	8	9.46
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	5	9.45
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	5	9.45
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	8	9.44
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	8	9.44
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	8	9.44
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	5	9.43
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	2	9.42
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	5	9.42
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	2	9.41
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	2	9.41
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	2	9.4
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	2	9.4
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	2	9.37
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	2	9.37
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	2	9.36
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	2	9.35
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	2	9.34
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	2	9.34
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	7	8.0
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	7	7.98
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	7	7.96
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	7	7.95
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	7	7.94
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	7	7.94
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	7	7.93
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	7	7.92
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	7	7.92
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	7	7.92
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	7	7.91
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	7	7.91
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	7	7.9
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	7	7.9
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	7	7.89
(1,1291)	1:38:J:ARG:C	1:39:J:ILE:N	1:39:J:ILE:CA	1:39:J:ILE:C	10	7.81
(1,311)	1:38:C:ARG:C	1:39:C:ILE:N	1:39:C:ILE:CA	1:39:C:ILE:C	10	7.81
(1,451)	1:38:D:ARG:C	1:39:D:ILE:N	1:39:D:ILE:CA	1:39:D:ILE:C	10	7.8
(1,1851)	1:38:N:ARG:C	1:39:N:ILE:N	1:39:N:ILE:CA	1:39:N:ILE:C	10	7.78
(1,731)	1:38:F:ARG:C	1:39:F:ILE:N	1:39:F:ILE:CA	1:39:F:ILE:C	10	7.77
(1,871)	1:38:G:ARG:C	1:39:G:ILE:N	1:39:G:ILE:CA	1:39:G:ILE:C	10	7.76
(1,1011)	1:38:H:ARG:C	1:39:H:ILE:N	1:39:H:ILE:CA	1:39:H:ILE:C	10	7.75
(1,591)	1:38:E:ARG:C	1:39:E:ILE:N	1:39:E:ILE:CA	1:39:E:ILE:C	10	7.75
(1,31)	1:38:A:ARG:C	1:39:A:ILE:N	1:39:A:ILE:CA	1:39:A:ILE:C	10	7.74
(1,1991)	1:38:O:ARG:C	1:39:O:ILE:N	1:39:O:ILE:CA	1:39:O:ILE:C	10	7.72
(1,1711)	1:38:M:ARG:C	1:39:M:ILE:N	1:39:M:ILE:CA	1:39:M:ILE:C	10	7.71
(1,1571)	1:38:L:ARG:C	1:39:L:ILE:N	1:39:L:ILE:CA	1:39:L:ILE:C	10	7.7
(1,1431)	1:38:K:ARG:C	1:39:K:ILE:N	1:39:K:ILE:CA	1:39:K:ILE:C	10	7.7
(1,1151)	1:38:I:ARG:C	1:39:I:ILE:N	1:39:I:ILE:CA	1:39:I:ILE:C	10	7.65
(1,171)	1:38:B:ARG:C	1:39:B:ILE:N	1:39:B:ILE:CA	1:39:B:ILE:C	10	7.64
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	8	3.38
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	8	3.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	8	3.37
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	8	3.35
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	8	3.33
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	8	3.31
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	8	3.29
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	8	3.29
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	8	3.27
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	8	3.26
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	8	3.25
(1,903)	1:74:G:ARG:C	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	8	3.25
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	8	3.23
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	8	3.23
(1,1183)	1:74:I:ARG:C	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	8	3.21
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	9	2.93
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	9	2.92
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	9	2.91
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	9	2.91
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	9	2.91
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	9	2.91
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	9	2.9
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	9	2.88
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	9	2.88
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	9	2.88
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	9	2.88
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	9	2.88
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	9	2.87
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	9	2.85
(1,1350)	1:24:J:LYS:N	1:24:J:LYS:CA	1:24:J:LYS:C	1:25:J:MET:N	10	2.85
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	9	2.85
(1,170)	1:37:B:GLY:C	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	10	2.82
(1,790)	1:24:F:LYS:N	1:24:F:LYS:CA	1:24:F:LYS:C	1:25:F:MET:N	10	2.81
(1,1770)	1:24:M:LYS:N	1:24:M:LYS:CA	1:24:M:LYS:C	1:25:M:MET:N	10	2.8
(1,1490)	1:24:K:LYS:N	1:24:K:LYS:CA	1:24:K:LYS:C	1:25:K:MET:N	10	2.8
(1,930)	1:24:G:LYS:N	1:24:G:LYS:CA	1:24:G:LYS:C	1:25:G:MET:N	10	2.8
(1,450)	1:37:D:GLY:C	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	10	2.8
(1,90)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:MET:N	10	2.8
(1,1010)	1:37:H:GLY:C	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	10	2.79
(1,370)	1:24:C:LYS:N	1:24:C:LYS:CA	1:24:C:LYS:C	1:25:C:MET:N	10	2.79
(1,30)	1:37:A:GLY:C	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	10	2.79
(1,1990)	1:37:O:GLY:C	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	10	2.78
(1,730)	1:37:F:GLY:C	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	10	2.78
(1,1850)	1:37:N:GLY:C	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	10	2.77
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	4	2.77
(1,1910)	1:24:N:LYS:N	1:24:N:LYS:CA	1:24:N:LYS:C	1:25:N:MET:N	10	2.76
(1,1570)	1:37:L:GLY:C	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	10	2.76
(1,170)	1:37:B:GLY:C	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	7	2.76
(1,2050)	1:24:O:LYS:N	1:24:O:LYS:CA	1:24:O:LYS:C	1:25:O:MET:N	10	2.75
(1,1290)	1:37:J:GLY:C	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	10	2.75
(1,1210)	1:24:I:LYS:N	1:24:I:LYS:CA	1:24:I:LYS:C	1:25:I:MET:N	10	2.75
(1,230)	1:24:B:LYS:N	1:24:B:LYS:CA	1:24:B:LYS:C	1:25:B:MET:N	10	2.75
(1,1430)	1:37:K:GLY:C	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	10	2.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,590)	1:37:E:GLY:C	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	10	2.73
(1,510)	1:24:D:LYS:N	1:24:D:LYS:CA	1:24:D:LYS:C	1:25:D:MET:N	10	2.73
(1,310)	1:37:C:GLY:C	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	10	2.73
(1,1070)	1:24:H:LYS:N	1:24:H:LYS:CA	1:24:H:LYS:C	1:25:H:MET:N	10	2.72
(1,650)	1:24:E:LYS:N	1:24:E:LYS:CA	1:24:E:LYS:C	1:25:E:MET:N	10	2.72
(1,1570)	1:37:L:GLY:C	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	7	2.71
(1,1150)	1:37:I:GLY:C	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	10	2.71
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	4	2.71
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	4	2.71
(1,1710)	1:37:M:GLY:C	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	10	2.7
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	4	2.7
(1,1010)	1:37:H:GLY:C	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	7	2.7
(1,1850)	1:37:N:GLY:C	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	7	2.69
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	4	2.69
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	4	2.69
(1,1150)	1:37:I:GLY:C	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	7	2.68
(1,30)	1:37:A:GLY:C	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	7	2.68
(1,1710)	1:37:M:GLY:C	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	7	2.67
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	4	2.67
(1,870)	1:37:G:GLY:C	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	7	2.67
(1,450)	1:37:D:GLY:C	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	7	2.67
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	3	2.66
(1,1430)	1:37:K:GLY:C	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	7	2.66
(1,903)	1:74:G:ARG:C	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	4	2.66
(1,870)	1:37:G:GLY:C	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	10	2.66
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	3	2.65
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	3	2.65
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	3	2.65
(1,310)	1:37:C:GLY:C	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	7	2.65
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	4	2.64
(1,1990)	1:37:O:GLY:C	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	7	2.64
(1,1630)	1:24:L:LYS:N	1:24:L:LYS:CA	1:24:L:LYS:C	1:25:L:MET:N	10	2.64
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	3	2.63
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	7	2.63
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	3	2.63
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	3	2.63
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	3	2.63
(1,590)	1:37:E:GLY:C	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	7	2.63
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	7	2.62
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	4	2.62
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	3	2.62
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	3	2.62
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	7	2.62
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	7	2.61
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	4	2.61
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	3	2.61
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	7	2.61
(1,1290)	1:37:J:GLY:C	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	7	2.61
(1,730)	1:37:F:GLY:C	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	7	2.61
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	7	2.61
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	4	2.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	7	2.6
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	3	2.6
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	4	2.6
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	7	2.59
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	3	2.59
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	7	2.59
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	7	2.59
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	3	2.58
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	7	2.58
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	3	2.57
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	7	2.56
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	7	2.56
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	4	2.56
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	7	2.56
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	8	2.55
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	5	2.55
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	5	2.54
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	8	2.54
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	5	2.53
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	5	2.53
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	7	2.53
(1,1183)	1:74:I:ARG:C	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	4	2.53
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	8	2.53
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	5	2.52
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	2	2.52
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	2	2.52
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	8	2.52
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	5	2.51
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	8	2.51
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	5	2.5
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	8	2.5
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	2	2.5
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	5	2.5
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	2	2.49
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	2	2.49
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	5	2.49
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	5	2.49
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	5	2.49
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	5	2.49
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	8	2.48
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	5	2.48
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	2	2.48
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	5	2.48
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	2	2.47
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	2	2.47
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	8	2.47
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	8	2.46
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	2	2.46
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	8	2.46
(1,1910)	1:24:N:LYS:N	1:24:N:LYS:CA	1:24:N:LYS:C	1:25:N:MET:N	8	2.45
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	2	2.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1350)	1:24:J:LYS:N	1:24:J:LYS:CA	1:24:J:LYS:C	1:25:J:MET:N	8	2.45
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	8	2.45
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	2	2.45
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	8	2.45
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	5	2.45
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	2	2.45
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	2	2.44
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	2	2.43
(1,1490)	1:24:K:LYS:N	1:24:K:LYS:CA	1:24:K:LYS:C	1:25:K:MET:N	8	2.43
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	8	2.43
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	8	2.42
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	2	2.42
(1,90)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:MET:N	8	2.41
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	8	2.4
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	1	2.39
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	1	2.38
(1,790)	1:24:F:LYS:N	1:24:F:LYS:CA	1:24:F:LYS:C	1:25:F:MET:N	8	2.38
(1,650)	1:24:E:LYS:N	1:24:E:LYS:CA	1:24:E:LYS:C	1:25:E:MET:N	8	2.38
(1,1630)	1:24:L:LYS:N	1:24:L:LYS:CA	1:24:L:LYS:C	1:25:L:MET:N	8	2.37
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	1	2.37
(1,1070)	1:24:H:LYS:N	1:24:H:LYS:CA	1:24:H:LYS:C	1:25:H:MET:N	8	2.37
(1,930)	1:24:G:LYS:N	1:24:G:LYS:CA	1:24:G:LYS:C	1:25:G:MET:N	8	2.37
(1,370)	1:24:C:LYS:N	1:24:C:LYS:CA	1:24:C:LYS:C	1:25:C:MET:N	8	2.36
(1,230)	1:24:B:LYS:N	1:24:B:LYS:CA	1:24:B:LYS:C	1:25:B:MET:N	8	2.36
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	1	2.35
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	1	2.35
(1,1210)	1:24:I:LYS:N	1:24:I:LYS:CA	1:24:I:LYS:C	1:25:I:MET:N	8	2.35
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	1	2.35
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	1	2.35
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	1	2.34
(1,2050)	1:24:O:LYS:N	1:24:O:LYS:CA	1:24:O:LYS:C	1:25:O:MET:N	8	2.34
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	1	2.34
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	1	2.34
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	1	2.34
(1,510)	1:24:D:LYS:N	1:24:D:LYS:CA	1:24:D:LYS:C	1:25:D:MET:N	8	2.34
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	1	2.33
(1,1770)	1:24:M:LYS:N	1:24:M:LYS:CA	1:24:M:LYS:C	1:25:M:MET:N	8	2.32
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	1	2.3
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	1	2.3
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	10	2.29
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	1	2.29
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	6	2.28
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	10	2.28
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	6	2.28
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	10	2.27
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	10	2.27
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	6	2.27
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	10	2.26
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	6	2.26
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	6	2.26
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	10	2.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	4	2.26
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	10	2.26
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	1	2.26
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	6	2.25
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	6	2.25
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	1	2.25
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	4	2.25
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	6	2.25
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	10	2.25
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	4	2.25
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	10	2.25
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	10	2.24
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	10	2.24
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	4	2.24
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	4	2.24
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	6	2.24
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	4	2.24
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	10	2.24
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	10	2.24
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	4	2.23
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	6	2.23
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	1	2.23
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	10	2.23
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	6	2.23
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	6	2.23
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	1	2.22
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	1	2.22
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	4	2.22
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	6	2.22
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	10	2.22
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	1	2.22
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	4	2.21
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	1	2.21
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	1	2.21
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	6	2.21
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	8	2.21
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	9	2.21
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	6	2.21
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	1	2.2
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	1	2.2
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	8	2.2
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	4	2.2
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	4	2.2
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	4	2.19
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	1	2.19
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	9	2.18
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	4	2.18
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	4	2.17
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	9	2.17
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	8	2.16
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	4	2.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	8	2.15
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	9	2.15
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	1	2.15
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	8	2.14
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	9	2.14
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	9	2.12
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	1	2.12
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	1	2.12
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	8	2.12
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	1	2.11
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	8	2.11
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	4	2.11
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	8	2.11
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	8	2.11
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	8	2.08
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	9	2.08
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	8	2.08
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	9	2.08
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	9	2.07
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	9	2.07
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	9	2.06
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	9	2.06
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	4	2.06
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	9	2.06
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	8	2.06
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	4	2.06
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	8	2.06
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	4	2.05
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	8	2.05
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	9	2.03
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	4	2.03
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	4	2.03
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	4	2.03
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	6	2.02
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	6	2.02
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	6	2.02
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	4	2.02
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	4	2.01
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	4	2.01
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	6	2.01
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	6	2.01
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	9	2.0
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	6	2.0
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	6	2.0
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	4	1.98
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	6	1.98
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	4	1.98
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	8	1.97
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	6	1.97
(1,903)	1:74:G:ARG:C	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	6	1.97
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	4	1.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	4	1.95
(1,1183)	1:74:I:ARG:C	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	6	1.94
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	6	1.92
(1,504)	1:18:D:ASP:N	1:18:D:ASP:CA	1:18:D:ASP:C	1:19:D:GLU:N	8	1.92
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	6	1.92
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	5	1.92
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	6	1.91
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	4	1.91
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	5	1.91
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	4	1.9
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	6	1.9
(1,1344)	1:18:J:ASP:N	1:18:J:ASP:CA	1:18:J:ASP:C	1:19:J:GLU:N	8	1.89
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	5	1.89
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	5	1.89
(1,1904)	1:18:N:ASP:N	1:18:N:ASP:CA	1:18:N:ASP:C	1:19:N:GLU:N	8	1.88
(1,1484)	1:18:K:ASP:N	1:18:K:ASP:CA	1:18:K:ASP:C	1:19:K:GLU:N	8	1.88
(1,924)	1:18:G:ASP:N	1:18:G:ASP:CA	1:18:G:ASP:C	1:19:G:GLU:N	8	1.88
(1,798)	1:32:F:LEU:N	1:32:F:LEU:CA	1:32:F:LEU:C	1:33:F:ARG:N	8	1.88
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	10	1.88
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	5	1.87
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	5	1.87
(1,1064)	1:18:H:ASP:N	1:18:H:ASP:CA	1:18:H:ASP:C	1:19:H:GLU:N	8	1.86
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	9	1.85
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	5	1.85
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	3	1.85
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	10	1.85
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	4	1.85
(1,658)	1:32:E:LEU:N	1:32:E:LEU:CA	1:32:E:LEU:C	1:33:E:ARG:N	8	1.85
(1,84)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:GLU:N	8	1.85
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	4	1.85
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	5	1.84
(1,1358)	1:32:J:LEU:N	1:32:J:LEU:CA	1:32:J:LEU:C	1:33:J:ARG:N	8	1.84
(1,364)	1:18:C:ASP:N	1:18:C:ASP:CA	1:18:C:ASP:C	1:19:C:GLU:N	8	1.84
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	3	1.84
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	10	1.84
(1,224)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:GLU:N	8	1.84
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	5	1.83
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	4	1.83
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	4	1.83
(1,1078)	1:32:H:LEU:N	1:32:H:LEU:CA	1:32:H:LEU:C	1:33:H:ARG:N	8	1.83
(1,890)	1:57:G:VAL:C	1:58:G:SER:N	1:58:G:SER:CA	1:58:G:SER:C	6	1.83
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	5	1.83
(1,784)	1:18:F:ASP:N	1:18:F:ASP:CA	1:18:F:ASP:C	1:19:F:GLU:N	8	1.83
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	6	1.83
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	5	1.83
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	5	1.82
(1,1624)	1:18:L:ASP:N	1:18:L:ASP:CA	1:18:L:ASP:C	1:19:L:GLU:N	8	1.82
(1,1498)	1:32:K:LEU:N	1:32:K:LEU:CA	1:32:K:LEU:C	1:33:K:ARG:N	8	1.82
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	9	1.82
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	3	1.82
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	6	1.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	9	1.82
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	9	1.81
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	6	1.81
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	5	1.81
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	5	1.81
(1,644)	1:18:E:ASP:N	1:18:E:ASP:CA	1:18:E:ASP:C	1:19:E:GLU:N	8	1.81
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	9	1.81
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	5	1.81
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	6	1.81
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	10	1.81
(1,1638)	1:32:L:LEU:N	1:32:L:LEU:CA	1:32:L:LEU:C	1:33:L:ARG:N	8	1.8
(1,1310)	1:57:J:VAL:C	1:58:J:SER:N	1:58:J:SER:CA	1:58:J:SER:C	5	1.8
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	4	1.8
(1,470)	1:57:D:VAL:C	1:58:D:SER:N	1:58:D:SER:CA	1:58:D:SER:C	6	1.8
(1,2010)	1:57:O:VAL:C	1:58:O:SER:N	1:58:O:SER:CA	1:58:O:SER:C	6	1.79
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	4	1.79
(1,1778)	1:32:M:LEU:N	1:32:M:LEU:CA	1:32:M:LEU:C	1:33:M:ARG:N	8	1.79
(1,1204)	1:18:I:ASP:N	1:18:I:ASP:CA	1:18:I:ASP:C	1:19:I:GLU:N	8	1.79
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	9	1.79
(1,518)	1:32:D:LEU:N	1:32:D:LEU:CA	1:32:D:LEU:C	1:33:D:ARG:N	8	1.79
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	3	1.79
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	10	1.79
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	5	1.79
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	3	1.79
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	4	1.79
(1,1918)	1:32:N:LEU:N	1:32:N:LEU:CA	1:32:N:LEU:C	1:33:N:ARG:N	8	1.78
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	1	1.78
(1,1764)	1:18:M:ASP:N	1:18:M:ASP:CA	1:18:M:ASP:C	1:19:M:GLU:N	8	1.78
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	5	1.78
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	5	1.78
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	9	1.78
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	9	1.78
(1,938)	1:32:G:LEU:N	1:32:G:LEU:CA	1:32:G:LEU:C	1:33:G:ARG:N	8	1.78
(1,2058)	1:32:O:LEU:N	1:32:O:LEU:CA	1:32:O:LEU:C	1:33:O:ARG:N	8	1.77
(1,1730)	1:57:M:VAL:C	1:58:M:SER:N	1:58:M:SER:CA	1:58:M:SER:C	5	1.77
(1,1136)	1:19:I:GLU:C	1:20:I:LEU:N	1:20:I:LEU:CA	1:20:I:LEU:C	2	1.77
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	3	1.77
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	6	1.77
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	5	1.77
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	1	1.77
(1,470)	1:57:D:VAL:C	1:58:D:SER:N	1:58:D:SER:CA	1:58:D:SER:C	5	1.77
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	4	1.77
(1,190)	1:57:B:VAL:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	6	1.77
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	9	1.77
(1,98)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ARG:N	8	1.77
(1,2044)	1:18:O:ASP:N	1:18:O:ASP:CA	1:18:O:ASP:C	1:19:O:GLU:N	8	1.76
(1,1976)	1:19:O:GLU:C	1:20:O:LEU:N	1:20:O:LEU:CA	1:20:O:LEU:C	2	1.76
(1,1590)	1:57:L:VAL:C	1:58:L:SER:N	1:58:L:SER:CA	1:58:L:SER:C	5	1.76
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	9	1.76
(1,1450)	1:57:K:VAL:C	1:58:K:SER:N	1:58:K:SER:CA	1:58:K:SER:C	6	1.76
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	3	1.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	4	1.76
(1,1218)	1:32:I:LEU:N	1:32:I:LEU:CA	1:32:I:LEU:C	1:33:I:ARG:N	8	1.76
(1,1170)	1:57:I:VAL:C	1:58:I:SER:N	1:58:I:SER:CA	1:58:I:SER:C	5	1.76
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	3	1.76
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	5	1.76
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	5	1.75
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	3	1.75
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	10	1.75
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	4	1.75
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	10	1.75
(1,1030)	1:57:H:VAL:C	1:58:H:SER:N	1:58:H:SER:CA	1:58:H:SER:C	6	1.75
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	4	1.75
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	5	1.75
(1,378)	1:32:C:LEU:N	1:32:C:LEU:CA	1:32:C:LEU:C	1:33:C:ARG:N	8	1.75
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	3	1.75
(1,238)	1:32:B:LEU:N	1:32:B:LEU:CA	1:32:B:LEU:C	1:33:B:ARG:N	8	1.75
(1,190)	1:57:B:VAL:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	5	1.75
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	6	1.75
(1,50)	1:57:A:VAL:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	6	1.75
(1,16)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	2	1.75
(1,1998)	1:45:O:LEU:C	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	1	1.74
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	10	1.74
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	3	1.74
(1,1310)	1:57:J:VAL:C	1:58:J:SER:N	1:58:J:SER:CA	1:58:J:SER:C	6	1.74
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	1	1.74
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	3	1.74
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	6	1.74
(1,50)	1:57:A:VAL:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	5	1.74
(1,1870)	1:57:N:VAL:C	1:58:N:SER:N	1:58:N:SER:CA	1:58:N:SER:C	6	1.73
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	2	1.73
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	6	1.73
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	4	1.73
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	6	1.73
(1,1416)	1:19:K:GLU:C	1:20:K:LEU:N	1:20:K:LEU:CA	1:20:K:LEU:C	2	1.73
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	3	1.73
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	1	1.73
(1,1030)	1:57:H:VAL:C	1:58:H:SER:N	1:58:H:SER:CA	1:58:H:SER:C	5	1.73
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	2	1.73
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	10	1.73
(1,458)	1:45:D:LEU:C	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	2	1.73
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	5	1.73
(1,156)	1:19:B:GLU:C	1:20:B:LEU:N	1:20:B:LEU:CA	1:20:B:LEU:C	2	1.73
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	4	1.72
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	5	1.72
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	9	1.72
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	1	1.72
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	1	1.72
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	10	1.72
(1,890)	1:57:G:VAL:C	1:58:G:SER:N	1:58:G:SER:CA	1:58:G:SER:C	5	1.72
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	10	1.72
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	3	1.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,716)	1:19:F:GLU:C	1:20:F:LEU:N	1:20:F:LEU:CA	1:20:F:LEU:C	2	1.72
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	5	1.72
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	9	1.72
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	1	1.72
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	5	1.71
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	1	1.71
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	2	1.71
(1,1450)	1:57:K:VAL:C	1:58:K:SER:N	1:58:K:SER:CA	1:58:K:SER:C	5	1.71
(1,1183)	1:74:I:ARG:C	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	3	1.71
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	4	1.71
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	1	1.71
(1,296)	1:19:C:GLU:C	1:20:C:LEU:N	1:20:C:LEU:CA	1:20:C:LEU:C	2	1.71
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	2	1.71
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	10	1.71
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	3	1.7
(1,2010)	1:57:O:VAL:C	1:58:O:SER:N	1:58:O:SER:CA	1:58:O:SER:C	5	1.7
(1,1836)	1:19:N:GLU:C	1:20:N:LEU:N	1:20:N:LEU:CA	1:20:N:LEU:C	2	1.7
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	10	1.7
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	10	1.7
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	6	1.7
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	10	1.7
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	2	1.7
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	2	1.7
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	1	1.7
(1,750)	1:57:F:VAL:C	1:58:F:SER:N	1:58:F:SER:CA	1:58:F:SER:C	6	1.7
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	9	1.7
(1,610)	1:57:E:VAL:C	1:58:E:SER:N	1:58:E:SER:CA	1:58:E:SER:C	5	1.7
(1,458)	1:45:D:LEU:C	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	1	1.7
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	1	1.7
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	3	1.69
(1,1998)	1:45:O:LEU:C	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	2	1.69
(1,1696)	1:19:M:GLU:C	1:20:M:LEU:N	1:20:M:LEU:CA	1:20:M:LEU:C	2	1.69
(1,1578)	1:45:L:LEU:C	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	1	1.69
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	5	1.69
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	3	1.69
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	10	1.69
(1,330)	1:57:C:VAL:C	1:58:C:SER:N	1:58:C:SER:CA	1:58:C:SER:C	5	1.69
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	10	1.69
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	5	1.69
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	9	1.69
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	6	1.68
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	5	1.68
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	9	1.68
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	3	1.68
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	3	1.68
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	6	1.68
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	10	1.68
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	2	1.68
(1,611)	1:58:E:SER:C	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	6	1.68
(1,610)	1:57:E:VAL:C	1:58:E:SER:N	1:58:E:SER:CA	1:58:E:SER:C	6	1.68
(1,370)	1:24:C:LYS:N	1:24:C:LYS:CA	1:24:C:LYS:C	1:25:C:MET:N	4	1.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	3	1.68
(1,1730)	1:57:M:VAL:C	1:58:M:SER:N	1:58:M:SER:CA	1:58:M:SER:C	6	1.67
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	10	1.67
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	6	1.67
(1,996)	1:19:H:GLU:C	1:20:H:LEU:N	1:20:H:LEU:CA	1:20:H:LEU:C	2	1.67
(1,903)	1:74:G:ARG:C	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	3	1.67
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	6	1.67
(1,790)	1:24:F:LYS:N	1:24:F:LYS:CA	1:24:F:LYS:C	1:25:F:MET:N	4	1.67
(1,330)	1:57:C:VAL:C	1:58:C:SER:N	1:58:C:SER:CA	1:58:C:SER:C	6	1.67
(1,90)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:MET:N	4	1.67
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1	1.67
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	5	1.66
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	3	1.66
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	3	1.66
(1,1578)	1:45:L:LEU:C	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	2	1.66
(1,1350)	1:24:J:LYS:N	1:24:J:LYS:CA	1:24:J:LYS:C	1:25:J:MET:N	4	1.66
(1,903)	1:74:G:ARG:C	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	5	1.66
(1,750)	1:57:F:VAL:C	1:58:F:SER:N	1:58:F:SER:CA	1:58:F:SER:C	5	1.66
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	6	1.66
(1,436)	1:19:D:GLU:C	1:20:D:LEU:N	1:20:D:LEU:CA	1:20:D:LEU:C	2	1.66
(1,331)	1:58:C:SER:C	1:59:C:TYR:N	1:59:C:TYR:CA	1:59:C:TYR:C	4	1.66
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	3	1.66
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	5	1.66
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	10	1.65
(1,1590)	1:57:L:VAL:C	1:58:L:SER:N	1:58:L:SER:CA	1:58:L:SER:C	6	1.65
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	10	1.65
(1,1276)	1:19:J:GLU:C	1:20:J:LEU:N	1:20:J:LEU:CA	1:20:J:LEU:C	2	1.65
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	6	1.65
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	2	1.65
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	10	1.65
(1,576)	1:19:E:GLU:C	1:20:E:LEU:N	1:20:E:LEU:CA	1:20:E:LEU:C	2	1.65
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	10	1.65
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	3	1.65
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	2	1.65
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	6	1.65
(1,1910)	1:24:N:LYS:N	1:24:N:LYS:CA	1:24:N:LYS:C	1:25:N:MET:N	4	1.64
(1,1870)	1:57:N:VAL:C	1:58:N:SER:N	1:58:N:SER:CA	1:58:N:SER:C	5	1.64
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	10	1.64
(1,1170)	1:57:I:VAL:C	1:58:I:SER:N	1:58:I:SER:CA	1:58:I:SER:C	6	1.64
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	5	1.64
(1,930)	1:24:G:LYS:N	1:24:G:LYS:CA	1:24:G:LYS:C	1:25:G:MET:N	4	1.64
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	10	1.64
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	5	1.64
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	2	1.64
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	6	1.64
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	10	1.64
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	10	1.63
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	5	1.63
(1,1556)	1:19:L:GLU:C	1:20:L:LEU:N	1:20:L:LEU:CA	1:20:L:LEU:C	2	1.63
(1,1490)	1:24:K:LYS:N	1:24:K:LYS:CA	1:24:K:LYS:C	1:25:K:MET:N	4	1.63
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	10	1.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	3	1.63
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	3	1.63
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	10	1.63
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	10	1.63
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	2	1.63
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	10	1.62
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	6	1.62
(1,1630)	1:24:L:LYS:N	1:24:L:LYS:CA	1:24:L:LYS:C	1:25:L:MET:N	4	1.62
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	7	1.62
(1,1183)	1:74:I:ARG:C	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	5	1.62
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	5	1.62
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	5	1.62
(1,331)	1:58:C:SER:C	1:59:C:TYR:N	1:59:C:TYR:CA	1:59:C:TYR:C	6	1.62
(1,230)	1:24:B:LYS:N	1:24:B:LYS:CA	1:24:B:LYS:C	1:25:B:MET:N	4	1.62
(1,1590)	1:57:L:VAL:C	1:58:L:SER:N	1:58:L:SER:CA	1:58:L:SER:C	3	1.61
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	5	1.61
(1,1311)	1:58:J:SER:C	1:59:J:TYR:N	1:59:J:TYR:CA	1:59:J:TYR:C	4	1.61
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	2	1.61
(1,1171)	1:58:I:SER:C	1:59:I:TYR:N	1:59:I:TYR:CA	1:59:I:TYR:C	6	1.61
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	5	1.61
(1,856)	1:19:G:GLU:C	1:20:G:LEU:N	1:20:G:LEU:CA	1:20:G:LEU:C	2	1.61
(1,751)	1:58:F:SER:C	1:59:F:TYR:N	1:59:F:TYR:CA	1:59:F:TYR:C	10	1.61
(1,611)	1:58:E:SER:C	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	10	1.61
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	3	1.61
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	5	1.61
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	3	1.61
(1,2050)	1:24:O:LYS:N	1:24:O:LYS:CA	1:24:O:LYS:C	1:25:O:MET:N	4	1.6
(1,1871)	1:58:N:SER:C	1:59:N:TYR:N	1:59:N:TYR:CA	1:59:N:TYR:C	10	1.6
(1,1416)	1:19:K:GLU:C	1:20:K:LEU:N	1:20:K:LEU:CA	1:20:K:LEU:C	9	1.6
(1,1210)	1:24:I:LYS:N	1:24:I:LYS:CA	1:24:I:LYS:C	1:25:I:MET:N	4	1.6
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	6	1.6
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	3	1.6
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	3	1.6
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	10	1.6
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	3	1.6
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	3	1.59
(1,1770)	1:24:M:LYS:N	1:24:M:LYS:CA	1:24:M:LYS:C	1:25:M:MET:N	4	1.59
(1,1696)	1:19:M:GLU:C	1:20:M:LEU:N	1:20:M:LEU:CA	1:20:M:LEU:C	9	1.59
(1,1311)	1:58:J:SER:C	1:59:J:TYR:N	1:59:J:TYR:CA	1:59:J:TYR:C	6	1.59
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	10	1.59
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	6	1.59
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	6	1.59
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	3	1.59
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	7	1.59
(1,471)	1:58:D:SER:C	1:59:D:TYR:N	1:59:D:TYR:CA	1:59:D:TYR:C	6	1.59
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	5	1.58
(1,1070)	1:24:H:LYS:N	1:24:H:LYS:CA	1:24:H:LYS:C	1:25:H:MET:N	4	1.58
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	5	1.58
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	6	1.58
(1,716)	1:19:F:GLU:C	1:20:F:LEU:N	1:20:F:LEU:CA	1:20:F:LEU:C	9	1.58
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	3	1.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,510)	1:24:D:LYS:N	1:24:D:LYS:CA	1:24:D:LYS:C	1:25:D:MET:N	4	1.58
(1,331)	1:58:C:SER:C	1:59:C:TYR:N	1:59:C:TYR:CA	1:59:C:TYR:C	10	1.58
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	7	1.58
(1,191)	1:58:B:SER:C	1:59:B:TYR:N	1:59:B:TYR:CA	1:59:B:TYR:C	10	1.58
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	5	1.58
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	10	1.58
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	10	1.57
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	10	1.57
(1,1031)	1:58:H:SER:C	1:59:H:TYR:N	1:59:H:TYR:CA	1:59:H:TYR:C	6	1.57
(1,650)	1:24:E:LYS:N	1:24:E:LYS:CA	1:24:E:LYS:C	1:25:E:MET:N	4	1.57
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	6	1.57
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	10	1.57
(1,191)	1:58:B:SER:C	1:59:B:TYR:N	1:59:B:TYR:CA	1:59:B:TYR:C	6	1.57
(1,190)	1:57:B:VAL:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	3	1.57
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	6	1.57
(1,51)	1:58:A:SER:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	6	1.57
(1,16)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	9	1.57
(1,2011)	1:58:O:SER:C	1:59:O:TYR:N	1:59:O:TYR:CA	1:59:O:TYR:C	4	1.56
(1,2010)	1:57:O:VAL:C	1:58:O:SER:N	1:58:O:SER:CA	1:58:O:SER:C	3	1.56
(1,1871)	1:58:N:SER:C	1:59:N:TYR:N	1:59:N:TYR:CA	1:59:N:TYR:C	4	1.56
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	5	1.56
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	7	1.56
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	6	1.56
(1,1276)	1:19:J:GLU:C	1:20:J:LEU:N	1:20:J:LEU:CA	1:20:J:LEU:C	9	1.56
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	7	1.56
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	10	1.56
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	6	1.56
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	7	1.56
(1,751)	1:58:F:SER:C	1:59:F:TYR:N	1:59:F:TYR:CA	1:59:F:TYR:C	6	1.56
(1,1871)	1:58:N:SER:C	1:59:N:TYR:N	1:59:N:TYR:CA	1:59:N:TYR:C	6	1.55
(1,1591)	1:58:L:SER:C	1:59:L:TYR:N	1:59:L:TYR:CA	1:59:L:TYR:C	10	1.55
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	6	1.55
(1,1171)	1:58:I:SER:C	1:59:I:TYR:N	1:59:I:TYR:CA	1:59:I:TYR:C	10	1.55
(1,891)	1:58:G:SER:C	1:59:G:TYR:N	1:59:G:TYR:CA	1:59:G:TYR:C	10	1.55
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	6	1.55
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	7	1.55
(1,51)	1:58:A:SER:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	10	1.55
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	10	1.54
(1,1731)	1:58:M:SER:C	1:59:M:TYR:N	1:59:M:TYR:CA	1:59:M:TYR:C	4	1.54
(1,1451)	1:58:K:SER:C	1:59:K:TYR:N	1:59:K:TYR:CA	1:59:K:TYR:C	6	1.54
(1,1031)	1:58:H:SER:C	1:59:H:TYR:N	1:59:H:TYR:CA	1:59:H:TYR:C	10	1.54
(1,891)	1:58:G:SER:C	1:59:G:TYR:N	1:59:G:TYR:CA	1:59:G:TYR:C	4	1.54
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	7	1.54
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	10	1.54
(1,611)	1:58:E:SER:C	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	4	1.54
(1,471)	1:58:D:SER:C	1:59:D:TYR:N	1:59:D:TYR:CA	1:59:D:TYR:C	4	1.54
(1,436)	1:19:D:GLU:C	1:20:D:LEU:N	1:20:D:LEU:CA	1:20:D:LEU:C	9	1.54
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	6	1.54
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	7	1.54
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	7	1.54
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	10	1.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,51)	1:58:A:SER:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	4	1.54
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	7	1.54
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	6	1.53
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	7	1.53
(1,1976)	1:19:O:GLU:C	1:20:O:LEU:N	1:20:O:LEU:CA	1:20:O:LEU:C	9	1.53
(1,1836)	1:19:N:GLU:C	1:20:N:LEU:N	1:20:N:LEU:CA	1:20:N:LEU:C	9	1.53
(1,1731)	1:58:M:SER:C	1:59:M:TYR:N	1:59:M:TYR:CA	1:59:M:TYR:C	6	1.53
(1,1731)	1:58:M:SER:C	1:59:M:TYR:N	1:59:M:TYR:CA	1:59:M:TYR:C	10	1.53
(1,1451)	1:58:K:SER:C	1:59:K:TYR:N	1:59:K:TYR:CA	1:59:K:TYR:C	10	1.53
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	10	1.53
(1,891)	1:58:G:SER:C	1:59:G:TYR:N	1:59:G:TYR:CA	1:59:G:TYR:C	6	1.53
(1,470)	1:57:D:VAL:C	1:58:D:SER:N	1:58:D:SER:CA	1:58:D:SER:C	3	1.53
(1,2011)	1:58:O:SER:C	1:59:O:TYR:N	1:59:O:TYR:CA	1:59:O:TYR:C	6	1.52
(1,1450)	1:57:K:VAL:C	1:58:K:SER:N	1:58:K:SER:CA	1:58:K:SER:C	3	1.52
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	3	1.52
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	10	1.52
(1,903)	1:74:G:ARG:C	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	10	1.52
(1,50)	1:57:A:VAL:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	3	1.52
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	6	1.51
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	3	1.51
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	3	1.51
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	6	1.51
(1,1311)	1:58:J:SER:C	1:59:J:TYR:N	1:59:J:TYR:CA	1:59:J:TYR:C	10	1.51
(1,1031)	1:58:H:SER:C	1:59:H:TYR:N	1:59:H:TYR:CA	1:59:H:TYR:C	4	1.51
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	6	1.51
(1,576)	1:19:E:GLU:C	1:20:E:LEU:N	1:20:E:LEU:CA	1:20:E:LEU:C	9	1.51
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	3	1.51
(1,296)	1:19:C:GLU:C	1:20:C:LEU:N	1:20:C:LEU:CA	1:20:C:LEU:C	9	1.51
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	1	1.51
(1,2011)	1:58:O:SER:C	1:59:O:TYR:N	1:59:O:TYR:CA	1:59:O:TYR:C	10	1.5
(1,1871)	1:58:N:SER:C	1:59:N:TYR:N	1:59:N:TYR:CA	1:59:N:TYR:C	9	1.5
(1,1591)	1:58:L:SER:C	1:59:L:TYR:N	1:59:L:TYR:CA	1:59:L:TYR:C	6	1.5
(1,1484)	1:18:K:ASP:N	1:18:K:ASP:CA	1:18:K:ASP:C	1:19:K:GLU:N	2	1.5
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	6	1.5
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	7	1.5
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	7	1.5
(1,1344)	1:18:J:ASP:N	1:18:J:ASP:CA	1:18:J:ASP:C	1:19:J:GLU:N	2	1.5
(1,1310)	1:57:J:VAL:C	1:58:J:SER:N	1:58:J:SER:CA	1:58:J:SER:C	3	1.5
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	6	1.5
(1,1136)	1:19:I:GLU:C	1:20:I:LEU:N	1:20:I:LEU:CA	1:20:I:LEU:C	9	1.5
(1,996)	1:19:H:GLU:C	1:20:H:LEU:N	1:20:H:LEU:CA	1:20:H:LEU:C	9	1.5
(1,750)	1:57:F:VAL:C	1:58:F:SER:N	1:58:F:SER:CA	1:58:F:SER:C	3	1.5
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	3	1.5
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	1	1.5
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	2	1.5
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	3	1.5
(1,471)	1:58:D:SER:C	1:59:D:TYR:N	1:59:D:TYR:CA	1:59:D:TYR:C	10	1.5
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	1	1.5
(1,191)	1:58:B:SER:C	1:59:B:TYR:N	1:59:B:TYR:CA	1:59:B:TYR:C	4	1.5
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	6	1.5
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	3	1.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1828)	1:10:N:ASP:C	1:11:N:ALA:N	1:11:N:ALA:CA	1:11:N:ALA:C	7	1.49
(1,1730)	1:57:M:VAL:C	1:58:M:SER:N	1:58:M:SER:CA	1:58:M:SER:C	3	1.49
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	6	1.49
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	7	1.49
(1,1556)	1:19:L:GLU:C	1:20:L:LEU:N	1:20:L:LEU:CA	1:20:L:LEU:C	9	1.49
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	7	1.49
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	6	1.49
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	3	1.49
(1,1170)	1:57:I:VAL:C	1:58:I:SER:N	1:58:I:SER:CA	1:58:I:SER:C	3	1.49
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	6	1.49
(1,924)	1:18:G:ASP:N	1:18:G:ASP:CA	1:18:G:ASP:C	1:19:G:GLU:N	2	1.49
(1,848)	1:10:G:ASP:C	1:11:G:ALA:N	1:11:G:ALA:CA	1:11:G:ALA:C	7	1.49
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	6	1.49
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	7	1.49
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	3	1.49
(1,1968)	1:10:O:ASP:C	1:11:O:ALA:N	1:11:O:ALA:CA	1:11:O:ALA:C	7	1.48
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	6	1.48
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	1	1.48
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	6	1.48
(1,1688)	1:10:M:ASP:C	1:11:M:ALA:N	1:11:M:ALA:CA	1:11:M:ALA:C	7	1.48
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	2	1.48
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	3	1.48
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	3	1.48
(1,1171)	1:58:I:SER:C	1:59:I:TYR:N	1:59:I:TYR:CA	1:59:I:TYR:C	4	1.48
(1,1164)	1:51:I:ASP:C	1:52:I:LEU:N	1:52:I:LEU:CA	1:52:I:LEU:C	2	1.48
(1,1128)	1:10:I:ASP:C	1:11:I:ALA:N	1:11:I:ALA:CA	1:11:I:ALA:C	7	1.48
(1,1030)	1:57:H:VAL:C	1:58:H:SER:N	1:58:H:SER:CA	1:58:H:SER:C	3	1.48
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	3	1.48
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	5	1.48
(1,428)	1:10:D:ASP:C	1:11:D:ALA:N	1:11:D:ALA:CA	1:11:D:ALA:C	7	1.48
(1,324)	1:51:C:ASP:C	1:52:C:LEU:N	1:52:C:LEU:CA	1:52:C:LEU:C	2	1.48
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	1	1.47
(1,1870)	1:57:N:VAL:C	1:58:N:SER:N	1:58:N:SER:CA	1:58:N:SER:C	3	1.47
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	3	1.47
(1,1591)	1:58:L:SER:C	1:59:L:TYR:N	1:59:L:TYR:CA	1:59:L:TYR:C	4	1.47
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	5	1.47
(1,1484)	1:18:K:ASP:N	1:18:K:ASP:CA	1:18:K:ASP:C	1:19:K:GLU:N	5	1.47
(1,1064)	1:18:H:ASP:N	1:18:H:ASP:CA	1:18:H:ASP:C	1:19:H:GLU:N	2	1.47
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	3	1.47
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	7	1.47
(1,751)	1:58:F:SER:C	1:59:F:TYR:N	1:59:F:TYR:CA	1:59:F:TYR:C	4	1.47
(1,644)	1:18:E:ASP:N	1:18:E:ASP:CA	1:18:E:ASP:C	1:19:E:GLU:N	2	1.47
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	6	1.47
(1,604)	1:51:E:ASP:C	1:52:E:LEU:N	1:52:E:LEU:CA	1:52:E:LEU:C	7	1.47
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	3	1.47
(1,504)	1:18:D:ASP:N	1:18:D:ASP:CA	1:18:D:ASP:C	1:19:D:GLU:N	5	1.47
(1,471)	1:58:D:SER:C	1:59:D:TYR:N	1:59:D:TYR:CA	1:59:D:TYR:C	9	1.47
(1,364)	1:18:C:ASP:N	1:18:C:ASP:CA	1:18:C:ASP:C	1:19:C:GLU:N	2	1.47
(1,288)	1:10:C:ASP:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	7	1.47
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	3	1.47
(1,1904)	1:18:N:ASP:N	1:18:N:ASP:CA	1:18:N:ASP:C	1:19:N:GLU:N	2	1.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1731)	1:58:M:SER:C	1:59:M:TYR:N	1:59:M:TYR:CA	1:59:M:TYR:C	9	1.46
(1,1451)	1:58:K:SER:C	1:59:K:TYR:N	1:59:K:TYR:CA	1:59:K:TYR:C	4	1.46
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	1	1.46
(1,1183)	1:74:I:ARG:C	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	10	1.46
(1,890)	1:57:G:VAL:C	1:58:G:SER:N	1:58:G:SER:CA	1:58:G:SER:C	3	1.46
(1,884)	1:51:G:ASP:C	1:52:G:LEU:N	1:52:G:LEU:CA	1:52:G:LEU:C	2	1.46
(1,458)	1:45:D:LEU:C	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	6	1.46
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	3	1.46
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	1	1.46
(1,84)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:GLU:N	2	1.46
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	3	1.45
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	3	1.45
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	7	1.45
(1,1584)	1:51:L:ASP:C	1:52:L:LEU:N	1:52:L:LEU:CA	1:52:L:LEU:C	6	1.45
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	7	1.45
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	3	1.45
(1,891)	1:58:G:SER:C	1:59:G:TYR:N	1:59:G:TYR:CA	1:59:G:TYR:C	9	1.45
(1,744)	1:51:F:ASP:C	1:52:F:LEU:N	1:52:F:LEU:CA	1:52:F:LEU:C	2	1.45
(1,611)	1:58:E:SER:C	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	9	1.45
(1,504)	1:18:D:ASP:N	1:18:D:ASP:CA	1:18:D:ASP:C	1:19:D:GLU:N	2	1.45
(1,184)	1:51:B:ASP:C	1:52:B:LEU:N	1:52:B:LEU:CA	1:52:B:LEU:C	2	1.45
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	7	1.45
(1,2044)	1:18:O:ASP:N	1:18:O:ASP:CA	1:18:O:ASP:C	1:19:O:GLU:N	2	1.44
(1,1998)	1:45:O:LEU:C	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	6	1.44
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	6	1.44
(1,1764)	1:18:M:ASP:N	1:18:M:ASP:CA	1:18:M:ASP:C	1:19:M:GLU:N	2	1.44
(1,1724)	1:51:M:ASP:C	1:52:M:LEU:N	1:52:M:LEU:CA	1:52:M:LEU:C	2	1.44
(1,1451)	1:58:K:SER:C	1:59:K:TYR:N	1:59:K:TYR:CA	1:59:K:TYR:C	9	1.44
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	6	1.44
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	6	1.44
(1,1204)	1:18:I:ASP:N	1:18:I:ASP:CA	1:18:I:ASP:C	1:19:I:GLU:N	2	1.44
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	5	1.44
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	7	1.44
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	7	1.44
(1,156)	1:19:B:GLU:C	1:20:B:LEU:N	1:20:B:LEU:CA	1:20:B:LEU:C	9	1.44
(1,1444)	1:51:K:ASP:C	1:52:K:LEU:N	1:52:K:LEU:CA	1:52:K:LEU:C	2	1.43
(1,1304)	1:51:J:ASP:C	1:52:J:LEU:N	1:52:J:LEU:CA	1:52:J:LEU:C	2	1.43
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	1	1.43
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	7	1.43
(1,706)	1:8:F:ILE:C	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	2	1.43
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	7	1.43
(1,331)	1:58:C:SER:C	1:59:C:TYR:N	1:59:C:TYR:CA	1:59:C:TYR:C	9	1.43
(1,330)	1:57:C:VAL:C	1:58:C:SER:N	1:58:C:SER:CA	1:58:C:SER:C	3	1.43
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	6	1.43
(1,214)	1:7:B:ALA:N	1:7:B:ALA:CA	1:7:B:ALA:C	1:8:B:ILE:N	8	1.43
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	6	1.43
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	6	1.43
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	5	1.43
(1,8)	1:10:A:ASP:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	7	1.43
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	7	1.42
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	1	1.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	1	1.42
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	3	1.42
(1,708)	1:10:F:ASP:C	1:11:F:ALA:N	1:11:F:ALA:CA	1:11:F:ALA:C	7	1.42
(1,504)	1:18:D:ASP:N	1:18:D:ASP:CA	1:18:D:ASP:C	1:19:D:GLU:N	9	1.42
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	7	1.42
(1,364)	1:18:C:ASP:N	1:18:C:ASP:CA	1:18:C:ASP:C	1:19:C:GLU:N	9	1.42
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	7	1.42
(1,51)	1:58:A:SER:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	9	1.42
(1,2011)	1:58:O:SER:C	1:59:O:TYR:N	1:59:O:TYR:CA	1:59:O:TYR:C	9	1.41
(1,1904)	1:18:N:ASP:N	1:18:N:ASP:CA	1:18:N:ASP:C	1:19:N:GLU:N	5	1.41
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	7	1.41
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	3	1.41
(1,1624)	1:18:L:ASP:N	1:18:L:ASP:CA	1:18:L:ASP:C	1:19:L:GLU:N	2	1.41
(1,1406)	1:8:K:ILE:C	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	2	1.41
(1,1311)	1:58:J:SER:C	1:59:J:TYR:N	1:59:J:TYR:CA	1:59:J:TYR:C	9	1.41
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	1	1.41
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	7	1.41
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	6	1.41
(1,924)	1:18:G:ASP:N	1:18:G:ASP:CA	1:18:G:ASP:C	1:19:G:GLU:N	5	1.41
(1,751)	1:58:F:SER:C	1:59:F:TYR:N	1:59:F:TYR:CA	1:59:F:TYR:C	9	1.41
(1,610)	1:57:E:VAL:C	1:58:E:SER:N	1:58:E:SER:CA	1:58:E:SER:C	3	1.41
(1,364)	1:18:C:ASP:N	1:18:C:ASP:CA	1:18:C:ASP:C	1:19:C:GLU:N	5	1.41
(1,191)	1:58:B:SER:C	1:59:B:TYR:N	1:59:B:TYR:CA	1:59:B:TYR:C	9	1.41
(1,6)	1:8:A:ILE:C	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	2	1.41
(1,2004)	1:51:O:ASP:C	1:52:O:LEU:N	1:52:O:LEU:CA	1:52:O:LEU:C	2	1.4
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	7	1.4
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	7	1.4
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	5	1.4
(1,1836)	1:19:N:GLU:C	1:20:N:LEU:N	1:20:N:LEU:CA	1:20:N:LEU:C	8	1.4
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	6	1.4
(1,784)	1:18:F:ASP:N	1:18:F:ASP:CA	1:18:F:ASP:C	1:19:F:GLU:N	5	1.4
(1,644)	1:18:E:ASP:N	1:18:E:ASP:CA	1:18:E:ASP:C	1:19:E:GLU:N	9	1.4
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	1	1.4
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	5	1.4
(1,224)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:GLU:N	2	1.4
(1,224)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:GLU:N	5	1.4
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	6	1.4
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	7	1.4
(1,1369)	1:47:J:MET:N	1:47:J:MET:CA	1:47:J:MET:C	1:48:J:ASP:N	6	1.39
(1,1344)	1:18:J:ASP:N	1:18:J:ASP:CA	1:18:J:ASP:C	1:19:J:GLU:N	5	1.39
(1,1171)	1:58:I:SER:C	1:59:I:TYR:N	1:59:I:TYR:CA	1:59:I:TYR:C	9	1.39
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	7	1.39
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	5	1.39
(1,856)	1:19:G:GLU:C	1:20:G:LEU:N	1:20:G:LEU:CA	1:20:G:LEU:C	9	1.39
(1,784)	1:18:F:ASP:N	1:18:F:ASP:CA	1:18:F:ASP:C	1:19:F:GLU:N	2	1.39
(1,669)	1:47:E:MET:N	1:47:E:MET:CA	1:47:E:MET:C	1:48:E:ASP:N	6	1.39
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	6	1.39
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	5	1.39
(1,286)	1:8:C:ILE:C	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	2	1.39
(1,84)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:GLU:N	5	1.39
(1,1624)	1:18:L:ASP:N	1:18:L:ASP:CA	1:18:L:ASP:C	1:19:L:GLU:N	5	1.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1548)	1:10:L:ASP:C	1:11:L:ALA:N	1:11:L:ALA:CA	1:11:L:ALA:C	7	1.38
(1,1450)	1:57:K:VAL:C	1:58:K:SER:N	1:58:K:SER:CA	1:58:K:SER:C	9	1.38
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	3	1.38
(1,1408)	1:10:K:ASP:C	1:11:K:ALA:N	1:11:K:ALA:CA	1:11:K:ALA:C	7	1.38
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	5	1.38
(1,1268)	1:10:J:ASP:C	1:11:J:ALA:N	1:11:J:ALA:CA	1:11:J:ALA:C	7	1.38
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	7	1.38
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	1	1.38
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	1	1.38
(1,529)	1:47:D:MET:N	1:47:D:MET:CA	1:47:D:MET:C	1:48:D:ASP:N	6	1.38
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	7	1.38
(1,148)	1:10:B:ASP:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	7	1.38
(1,44)	1:51:A:ASP:C	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	2	1.38
(1,1976)	1:19:O:GLU:C	1:20:O:LEU:N	1:20:O:LEU:CA	1:20:O:LEU:C	8	1.37
(1,1764)	1:18:M:ASP:N	1:18:M:ASP:CA	1:18:M:ASP:C	1:19:M:GLU:N	5	1.37
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	7	1.37
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	8	1.37
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	3	1.37
(1,988)	1:10:H:ASP:C	1:11:H:ALA:N	1:11:H:ALA:CA	1:11:H:ALA:C	7	1.37
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	7	1.37
(1,846)	1:8:G:ILE:C	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	2	1.37
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	8	1.37
(1,2069)	1:47:O:MET:N	1:47:O:MET:CA	1:47:O:MET:C	1:48:O:ASP:N	6	1.36
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	7	1.36
(1,1509)	1:47:K:MET:N	1:47:K:MET:CA	1:47:K:MET:C	1:48:K:ASP:N	6	1.36
(1,1484)	1:18:K:ASP:N	1:18:K:ASP:CA	1:18:K:ASP:C	1:19:K:GLU:N	9	1.36
(1,1344)	1:18:J:ASP:N	1:18:J:ASP:CA	1:18:J:ASP:C	1:19:J:GLU:N	9	1.36
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	4	1.36
(1,1136)	1:19:I:GLU:C	1:20:I:LEU:N	1:20:I:LEU:CA	1:20:I:LEU:C	8	1.36
(1,1031)	1:58:H:SER:C	1:59:H:TYR:N	1:59:H:TYR:CA	1:59:H:TYR:C	9	1.36
(1,914)	1:7:G:ALA:N	1:7:G:ALA:CA	1:7:G:ALA:C	1:8:G:ILE:N	4	1.36
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	6	1.36
(1,644)	1:18:E:ASP:N	1:18:E:ASP:CA	1:18:E:ASP:C	1:19:E:GLU:N	5	1.36
(1,554)	1:76:D:MET:N	1:76:D:MET:CA	1:76:D:MET:C	1:77:D:GLY:N	3	1.36
(1,470)	1:57:D:VAL:C	1:58:D:SER:N	1:58:D:SER:CA	1:58:D:SER:C	9	1.36
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	2	1.36
(1,464)	1:51:D:ASP:C	1:52:D:LEU:N	1:52:D:LEU:CA	1:52:D:LEU:C	6	1.36
(1,389)	1:47:C:MET:N	1:47:C:MET:CA	1:47:C:MET:C	1:48:C:ASP:N	6	1.36
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	1	1.36
(1,109)	1:47:A:MET:N	1:47:A:MET:CA	1:47:A:MET:C	1:48:A:ASP:N	6	1.36
(1,16)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	8	1.36
(1,2010)	1:57:O:VAL:C	1:58:O:SER:N	1:58:O:SER:CA	1:58:O:SER:C	9	1.35
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	5	1.35
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	8	1.35
(1,1416)	1:19:K:GLU:C	1:20:K:LEU:N	1:20:K:LEU:CA	1:20:K:LEU:C	5	1.35
(1,1204)	1:18:I:ASP:N	1:18:I:ASP:CA	1:18:I:ASP:C	1:19:I:GLU:N	5	1.35
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	5	1.35
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	5	1.35
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	7	1.35
(1,568)	1:10:E:ASP:C	1:11:E:ALA:N	1:11:E:ALA:CA	1:11:E:ALA:C	7	1.35
(1,458)	1:45:D:LEU:C	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	8	1.35

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,249)	1:47:B:MET:N	1:47:B:MET:CA	1:47:B:MET:C	1:48:B:ASP:N	6	1.35
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	5	1.35
(1,84)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:GLU:N	9	1.35
(1,2044)	1:18:O:ASP:N	1:18:O:ASP:CA	1:18:O:ASP:C	1:19:O:GLU:N	5	1.34
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	5	1.34
(1,1929)	1:47:N:MET:N	1:47:N:MET:CA	1:47:N:MET:C	1:48:N:ASP:N	6	1.34
(1,1826)	1:8:N:ILE:C	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	2	1.34
(1,1730)	1:57:M:VAL:C	1:58:M:SER:N	1:58:M:SER:CA	1:58:M:SER:C	9	1.34
(1,1688)	1:10:M:ASP:C	1:11:M:ALA:N	1:11:M:ALA:CA	1:11:M:ALA:C	4	1.34
(1,1591)	1:58:L:SER:C	1:59:L:TYR:N	1:59:L:TYR:CA	1:59:L:TYR:C	9	1.34
(1,1578)	1:45:L:LEU:C	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	8	1.34
(1,1519)	1:57:K:VAL:N	1:57:K:VAL:CA	1:57:K:VAL:C	1:58:K:SER:N	5	1.34
(1,1254)	1:76:I:MET:N	1:76:I:MET:CA	1:76:I:MET:C	1:77:I:GLY:N	3	1.34
(1,1089)	1:47:H:MET:N	1:47:H:MET:CA	1:47:H:MET:C	1:48:H:ASP:N	6	1.34
(1,1064)	1:18:H:ASP:N	1:18:H:ASP:CA	1:18:H:ASP:C	1:19:H:GLU:N	5	1.34
(1,914)	1:7:G:ALA:N	1:7:G:ALA:CA	1:7:G:ALA:C	1:8:G:ILE:N	8	1.34
(1,890)	1:57:G:VAL:C	1:58:G:SER:N	1:58:G:SER:CA	1:58:G:SER:C	9	1.34
(1,426)	1:8:D:ILE:C	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	2	1.34
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	8	1.33
(1,1864)	1:51:N:ASP:C	1:52:N:LEU:N	1:52:N:LEU:CA	1:52:N:LEU:C	2	1.33
(1,1649)	1:47:L:MET:N	1:47:L:MET:CA	1:47:L:MET:C	1:48:L:ASP:N	6	1.33
(1,1578)	1:45:L:LEU:C	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	6	1.33
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	7	1.33
(1,1276)	1:19:J:GLU:C	1:20:J:LEU:N	1:20:J:LEU:CA	1:20:J:LEU:C	8	1.33
(1,1204)	1:18:I:ASP:N	1:18:I:ASP:CA	1:18:I:ASP:C	1:19:I:GLU:N	9	1.33
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	8	1.33
(1,1030)	1:57:H:VAL:C	1:58:H:SER:N	1:58:H:SER:CA	1:58:H:SER:C	9	1.33
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	8	1.33
(1,986)	1:8:H:ILE:C	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	2	1.33
(1,784)	1:18:F:ASP:N	1:18:F:ASP:CA	1:18:F:ASP:C	1:19:F:GLU:N	9	1.33
(1,566)	1:8:E:ILE:C	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	2	1.33
(1,224)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:GLU:N	9	1.33
(1,146)	1:8:B:ILE:C	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	2	1.33
(1,50)	1:57:A:VAL:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	9	1.33
(1,1954)	1:76:N:MET:N	1:76:N:MET:CA	1:76:N:MET:C	1:77:N:GLY:N	3	1.32
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	7	1.32
(1,1534)	1:76:K:MET:N	1:76:K:MET:CA	1:76:K:MET:C	1:77:K:GLY:N	3	1.32
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	8	1.32
(1,1310)	1:57:J:VAL:C	1:58:J:SER:N	1:58:J:SER:CA	1:58:J:SER:C	2	1.32
(1,1276)	1:19:J:GLU:C	1:20:J:LEU:N	1:20:J:LEU:CA	1:20:J:LEU:C	5	1.32
(1,1126)	1:8:I:ILE:C	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	2	1.32
(1,949)	1:47:G:MET:N	1:47:G:MET:CA	1:47:G:MET:C	1:48:G:ASP:N	6	1.32
(1,750)	1:57:F:VAL:C	1:58:F:SER:N	1:58:F:SER:CA	1:58:F:SER:C	9	1.32
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	8	1.32
(1,716)	1:19:F:GLU:C	1:20:F:LEU:N	1:20:F:LEU:CA	1:20:F:LEU:C	5	1.32
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	8	1.32
(1,190)	1:57:B:VAL:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	2	1.32
(1,1976)	1:19:O:GLU:C	1:20:O:LEU:N	1:20:O:LEU:CA	1:20:O:LEU:C	5	1.31
(1,1904)	1:18:N:ASP:N	1:18:N:ASP:CA	1:18:N:ASP:C	1:19:N:GLU:N	9	1.31
(1,1789)	1:47:M:MET:N	1:47:M:MET:CA	1:47:M:MET:C	1:48:M:ASP:N	6	1.31
(1,1624)	1:18:L:ASP:N	1:18:L:ASP:CA	1:18:L:ASP:C	1:19:L:GLU:N	9	1.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	7	1.31
(1,1556)	1:19:L:GLU:C	1:20:L:LEU:N	1:20:L:LEU:CA	1:20:L:LEU:C	8	1.31
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	5	1.31
(1,1394)	1:76:J:MET:N	1:76:J:MET:CA	1:76:J:MET:C	1:77:J:GLY:N	3	1.31
(1,1266)	1:8:J:ILE:C	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	2	1.31
(1,1170)	1:57:I:VAL:C	1:58:I:SER:N	1:58:I:SER:CA	1:58:I:SER:C	9	1.31
(1,1054)	1:7:H:ALA:N	1:7:H:ALA:CA	1:7:H:ALA:C	1:8:H:ILE:N	8	1.31
(1,774)	1:7:F:ALA:N	1:7:F:ALA:CA	1:7:F:ALA:C	1:8:F:ILE:N	8	1.31
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	4	1.31
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	8	1.31
(1,190)	1:57:B:VAL:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	9	1.31
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	7	1.31
(1,156)	1:19:B:GLU:C	1:20:B:LEU:N	1:20:B:LEU:CA	1:20:B:LEU:C	8	1.31
(1,16)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	5	1.31
(1,2094)	1:76:O:MET:N	1:76:O:MET:CA	1:76:O:MET:C	1:77:O:GLY:N	3	1.3
(1,1754)	1:7:M:ALA:N	1:7:M:ALA:CA	1:7:M:ALA:C	1:8:M:ILE:N	8	1.3
(1,1674)	1:76:L:MET:N	1:76:L:MET:CA	1:76:L:MET:C	1:77:L:GLY:N	3	1.3
(1,1416)	1:19:K:GLU:C	1:20:K:LEU:N	1:20:K:LEU:CA	1:20:K:LEU:C	8	1.3
(1,1170)	1:57:I:VAL:C	1:58:I:SER:N	1:58:I:SER:CA	1:58:I:SER:C	2	1.3
(1,819)	1:57:F:VAL:N	1:57:F:VAL:CA	1:57:F:VAL:C	1:58:F:SER:N	5	1.3
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	8	1.3
(1,436)	1:19:D:GLU:C	1:20:D:LEU:N	1:20:D:LEU:CA	1:20:D:LEU:C	8	1.3
(1,414)	1:76:C:MET:N	1:76:C:MET:CA	1:76:C:MET:C	1:77:C:GLY:N	3	1.3
(1,214)	1:7:B:ALA:N	1:7:B:ALA:CA	1:7:B:ALA:C	1:8:B:ILE:N	4	1.3
(1,134)	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	1:77:A:GLY:N	3	1.3
(1,2079)	1:57:O:VAL:N	1:57:O:VAL:CA	1:57:O:VAL:C	1:58:O:SER:N	5	1.29
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	7	1.29
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	4	1.29
(1,1450)	1:57:K:VAL:C	1:58:K:SER:N	1:58:K:SER:CA	1:58:K:SER:C	2	1.29
(1,1128)	1:10:I:ASP:C	1:11:I:ALA:N	1:11:I:ALA:CA	1:11:I:ALA:C	4	1.29
(1,996)	1:19:H:GLU:C	1:20:H:LEU:N	1:20:H:LEU:CA	1:20:H:LEU:C	5	1.29
(1,809)	1:47:F:MET:N	1:47:F:MET:CA	1:47:F:MET:C	1:48:F:ASP:N	6	1.29
(1,694)	1:76:E:MET:N	1:76:E:MET:CA	1:76:E:MET:C	1:77:E:GLY:N	3	1.29
(1,576)	1:19:E:GLU:C	1:20:E:LEU:N	1:20:E:LEU:CA	1:20:E:LEU:C	8	1.29
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	8	1.29
(1,2044)	1:18:O:ASP:N	1:18:O:ASP:CA	1:18:O:ASP:C	1:19:O:GLU:N	9	1.28
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	8	1.28
(1,1870)	1:57:N:VAL:C	1:58:N:SER:N	1:58:N:SER:CA	1:58:N:SER:C	9	1.28
(1,1730)	1:57:M:VAL:C	1:58:M:SER:N	1:58:M:SER:CA	1:58:M:SER:C	2	1.28
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	1	1.28
(1,1548)	1:10:L:ASP:C	1:11:L:ALA:N	1:11:L:ALA:CA	1:11:L:ALA:C	4	1.28
(1,1310)	1:57:J:VAL:C	1:58:J:SER:N	1:58:J:SER:CA	1:58:J:SER:C	9	1.28
(1,1229)	1:47:I:MET:N	1:47:I:MET:CA	1:47:I:MET:C	1:48:I:ASP:N	6	1.28
(1,1136)	1:19:I:GLU:C	1:20:I:LEU:N	1:20:I:LEU:CA	1:20:I:LEU:C	5	1.28
(1,1069)	1:23:H:PHE:N	1:23:H:PHE:CA	1:23:H:PHE:C	1:24:H:LYS:N	9	1.28
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	8	1.28
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	8	1.28
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	1	1.28
(1,748)	1:55:F:LYS:C	1:56:F:LEU:N	1:56:F:LEU:CA	1:56:F:LEU:C	2	1.28
(1,470)	1:57:D:VAL:C	1:58:D:SER:N	1:58:D:SER:CA	1:58:D:SER:C	2	1.28
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	7	1.28

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:57:A:VAL:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	2	1.28
(1,1998)	1:45:O:LEU:C	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	8	1.27
(1,1868)	1:55:N:LYS:C	1:56:N:LEU:N	1:56:N:LEU:CA	1:56:N:LEU:C	2	1.27
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	8	1.27
(1,1764)	1:18:M:ASP:N	1:18:M:ASP:CA	1:18:M:ASP:C	1:19:M:GLU:N	9	1.27
(1,1686)	1:8:M:ILE:C	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	2	1.27
(1,1590)	1:57:L:VAL:C	1:58:L:SER:N	1:58:L:SER:CA	1:58:L:SER:C	9	1.27
(1,1588)	1:55:L:LYS:C	1:56:L:LEU:N	1:56:L:LEU:CA	1:56:L:LEU:C	2	1.27
(1,1408)	1:10:K:ASP:C	1:11:K:ALA:N	1:11:K:ALA:CA	1:11:K:ALA:C	4	1.27
(1,1334)	1:7:J:ALA:N	1:7:J:ALA:CA	1:7:J:ALA:C	1:8:J:ILE:N	4	1.27
(1,1114)	1:76:H:MET:N	1:76:H:MET:CA	1:76:H:MET:C	1:77:H:GLY:N	3	1.27
(1,1024)	1:51:H:ASP:C	1:52:H:LEU:N	1:52:H:LEU:CA	1:52:H:LEU:C	2	1.27
(1,924)	1:18:G:ASP:N	1:18:G:ASP:CA	1:18:G:ASP:C	1:19:G:GLU:N	9	1.27
(1,914)	1:7:G:ALA:N	1:7:G:ALA:CA	1:7:G:ALA:C	1:8:G:ILE:N	7	1.27
(1,856)	1:19:G:GLU:C	1:20:G:LEU:N	1:20:G:LEU:CA	1:20:G:LEU:C	8	1.27
(1,716)	1:19:F:GLU:C	1:20:F:LEU:N	1:20:F:LEU:CA	1:20:F:LEU:C	8	1.27
(1,610)	1:57:E:VAL:C	1:58:E:SER:N	1:58:E:SER:CA	1:58:E:SER:C	9	1.27
(1,539)	1:57:D:VAL:N	1:57:D:VAL:CA	1:57:D:VAL:C	1:58:D:SER:N	5	1.27
(1,428)	1:10:D:ASP:C	1:11:D:ALA:N	1:11:D:ALA:CA	1:11:D:ALA:C	4	1.27
(1,296)	1:19:C:GLU:C	1:20:C:LEU:N	1:20:C:LEU:CA	1:20:C:LEU:C	8	1.27
(1,288)	1:10:C:ASP:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	4	1.27
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	8	1.27
(1,148)	1:10:B:ASP:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	4	1.27
(1,1968)	1:10:O:ASP:C	1:11:O:ALA:N	1:11:O:ALA:CA	1:11:O:ALA:C	4	1.26
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	8	1.26
(1,1836)	1:19:N:GLU:C	1:20:N:LEU:N	1:20:N:LEU:CA	1:20:N:LEU:C	5	1.26
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	8	1.26
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	7	1.26
(1,1371)	1:49:J:ALA:N	1:49:J:ALA:CA	1:49:J:ALA:C	1:50:J:ILE:N	4	1.26
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	8	1.26
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	2	1.26
(1,1064)	1:18:H:ASP:N	1:18:H:ASP:CA	1:18:H:ASP:C	1:19:H:GLU:N	9	1.26
(1,1054)	1:7:H:ALA:N	1:7:H:ALA:CA	1:7:H:ALA:C	1:8:H:ILE:N	4	1.26
(1,974)	1:76:G:MET:N	1:76:G:MET:CA	1:76:G:MET:C	1:77:G:GLY:N	3	1.26
(1,774)	1:7:F:ALA:N	1:7:F:ALA:CA	1:7:F:ALA:C	1:8:F:ILE:N	4	1.26
(1,671)	1:49:E:ALA:N	1:49:E:ALA:CA	1:49:E:ALA:C	1:50:E:ILE:N	4	1.26
(1,356)	1:9:C:LEU:N	1:9:C:LEU:CA	1:9:C:LEU:C	1:10:C:ASP:N	9	1.26
(1,296)	1:19:C:GLU:C	1:20:C:LEU:N	1:20:C:LEU:CA	1:20:C:LEU:C	5	1.26
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	1	1.26
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	8	1.26
(1,111)	1:49:A:ALA:N	1:49:A:ALA:CA	1:49:A:ALA:C	1:50:A:ILE:N	4	1.26
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	8	1.26
(1,2010)	1:57:O:VAL:C	1:58:O:SER:N	1:58:O:SER:CA	1:58:O:SER:C	2	1.25
(1,1966)	1:8:O:ILE:C	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	2	1.25
(1,1814)	1:76:M:MET:N	1:76:M:MET:CA	1:76:M:MET:C	1:77:M:GLY:N	3	1.25
(1,1754)	1:7:M:ALA:N	1:7:M:ALA:CA	1:7:M:ALA:C	1:8:M:ILE:N	4	1.25
(1,1696)	1:19:M:GLU:C	1:20:M:LEU:N	1:20:M:LEU:CA	1:20:M:LEU:C	8	1.25
(1,1578)	1:45:L:LEU:C	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	9	1.25
(1,1546)	1:8:L:ILE:C	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	2	1.25
(1,1290)	1:37:J:GLY:C	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	8	1.25
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	1	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,951)	1:49:G:ALA:N	1:49:G:ALA:CA	1:49:G:ALA:C	1:50:G:ILE:N	4	1.25
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	1	1.25
(1,634)	1:7:E:ALA:N	1:7:E:ALA:CA	1:7:E:ALA:C	1:8:E:ILE:N	8	1.25
(1,504)	1:18:D:ASP:N	1:18:D:ASP:CA	1:18:D:ASP:C	1:19:D:GLU:N	4	1.25
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	8	1.25
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	8	1.25
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1	1.25
(1,8)	1:10:A:ASP:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	4	1.25
(1,1696)	1:19:M:GLU:C	1:20:M:LEU:N	1:20:M:LEU:CA	1:20:M:LEU:C	5	1.24
(1,1509)	1:47:K:MET:N	1:47:K:MET:CA	1:47:K:MET:C	1:48:K:ASP:N	4	1.24
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	5	1.24
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	1	1.24
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	1	1.24
(1,1204)	1:18:I:ASP:N	1:18:I:ASP:CA	1:18:I:ASP:C	1:19:I:GLU:N	4	1.24
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	9	1.24
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	8	1.24
(1,1064)	1:18:H:ASP:N	1:18:H:ASP:CA	1:18:H:ASP:C	1:19:H:GLU:N	4	1.24
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	8	1.24
(1,996)	1:19:H:GLU:C	1:20:H:LEU:N	1:20:H:LEU:CA	1:20:H:LEU:C	8	1.24
(1,988)	1:10:H:ASP:C	1:11:H:ALA:N	1:11:H:ALA:CA	1:11:H:ALA:C	4	1.24
(1,848)	1:10:G:ASP:C	1:11:G:ALA:N	1:11:G:ALA:CA	1:11:G:ALA:C	4	1.24
(1,834)	1:76:F:MET:N	1:76:F:MET:CA	1:76:F:MET:C	1:77:F:GLY:N	3	1.24
(1,784)	1:18:F:ASP:N	1:18:F:ASP:CA	1:18:F:ASP:C	1:19:F:GLU:N	4	1.24
(1,750)	1:57:F:VAL:C	1:58:F:SER:N	1:58:F:SER:CA	1:58:F:SER:C	2	1.24
(1,649)	1:23:E:PHE:N	1:23:E:PHE:CA	1:23:E:PHE:C	1:24:E:LYS:N	9	1.24
(1,634)	1:7:E:ALA:N	1:7:E:ALA:CA	1:7:E:ALA:C	1:8:E:ILE:N	4	1.24
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	8	1.24
(1,529)	1:47:D:MET:N	1:47:D:MET:CA	1:47:D:MET:C	1:48:D:ASP:N	4	1.24
(1,494)	1:7:D:ALA:N	1:7:D:ALA:CA	1:7:D:ALA:C	1:8:D:ILE:N	8	1.24
(1,330)	1:57:C:VAL:C	1:58:C:SER:N	1:58:C:SER:CA	1:58:C:SER:C	9	1.24
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	1	1.24
(1,224)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:GLU:N	4	1.24
(1,214)	1:7:B:ALA:N	1:7:B:ALA:CA	1:7:B:ALA:C	1:8:B:ILE:N	7	1.24
(1,2071)	1:49:O:ALA:N	1:49:O:ALA:CA	1:49:O:ALA:C	1:50:O:ILE:N	4	1.23
(1,2069)	1:47:O:MET:N	1:47:O:MET:CA	1:47:O:MET:C	1:48:O:ASP:N	4	1.23
(1,1939)	1:57:N:VAL:N	1:57:N:VAL:CA	1:57:N:VAL:C	1:58:N:SER:N	5	1.23
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	4	1.23
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	9	1.23
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	1	1.23
(1,1728)	1:55:M:LYS:C	1:56:M:LEU:N	1:56:M:LEU:CA	1:56:M:LEU:C	2	1.23
(1,1649)	1:47:L:MET:N	1:47:L:MET:CA	1:47:L:MET:C	1:48:L:ASP:N	4	1.23
(1,1629)	1:23:L:PHE:N	1:23:L:PHE:CA	1:23:L:PHE:C	1:24:L:LYS:N	9	1.23
(1,1614)	1:7:L:ALA:N	1:7:L:ALA:CA	1:7:L:ALA:C	1:8:L:ILE:N	8	1.23
(1,1556)	1:19:L:GLU:C	1:20:L:LEU:N	1:20:L:LEU:CA	1:20:L:LEU:C	5	1.23
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	1	1.23
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	8	1.23
(1,1369)	1:47:J:MET:N	1:47:J:MET:CA	1:47:J:MET:C	1:48:J:ASP:N	4	1.23
(1,1334)	1:7:J:ALA:N	1:7:J:ALA:CA	1:7:J:ALA:C	1:8:J:ILE:N	8	1.23
(1,1231)	1:49:I:ALA:N	1:49:I:ALA:CA	1:49:I:ALA:C	1:50:I:ILE:N	4	1.23
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	1	1.23
(1,1089)	1:47:H:MET:N	1:47:H:MET:CA	1:47:H:MET:C	1:48:H:ASP:N	4	1.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1010)	1:37:H:GLY:C	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	8	1.23
(1,949)	1:47:G:MET:N	1:47:G:MET:CA	1:47:G:MET:C	1:48:G:ASP:N	4	1.23
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	10	1.23
(1,774)	1:7:F:ALA:N	1:7:F:ALA:CA	1:7:F:ALA:C	1:8:F:ILE:N	7	1.23
(1,468)	1:55:D:LYS:C	1:56:D:LEU:N	1:56:D:LEU:CA	1:56:D:LEU:C	2	1.23
(1,436)	1:19:D:GLU:C	1:20:D:LEU:N	1:20:D:LEU:CA	1:20:D:LEU:C	5	1.23
(1,399)	1:57:C:VAL:N	1:57:C:VAL:CA	1:57:C:VAL:C	1:58:C:SER:N	5	1.23
(1,259)	1:57:B:VAL:N	1:57:B:VAL:CA	1:57:B:VAL:C	1:58:B:SER:N	5	1.23
(1,251)	1:49:B:ALA:N	1:49:B:ALA:CA	1:49:B:ALA:C	1:50:B:ILE:N	4	1.23
(1,74)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	8	1.23
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	10	1.23
(1,2036)	1:9:O:LEU:N	1:9:O:LEU:CA	1:9:O:LEU:C	1:10:O:ASP:N	9	1.22
(1,2008)	1:55:O:LYS:C	1:56:O:LEU:N	1:56:O:LEU:CA	1:56:O:LEU:C	2	1.22
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	2	1.22
(1,1799)	1:57:M:VAL:N	1:57:M:VAL:CA	1:57:M:VAL:C	1:58:M:SER:N	5	1.22
(1,1754)	1:7:M:ALA:N	1:7:M:ALA:CA	1:7:M:ALA:C	1:8:M:ILE:N	2	1.22
(1,1570)	1:37:L:GLY:C	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	8	1.22
(1,1448)	1:55:K:LYS:C	1:56:K:LEU:N	1:56:K:LEU:CA	1:56:K:LEU:C	2	1.22
(1,1239)	1:57:I:VAL:N	1:57:I:VAL:CA	1:57:I:VAL:C	1:58:I:SER:N	5	1.22
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	5	1.22
(1,1054)	1:7:H:ALA:N	1:7:H:ALA:CA	1:7:H:ALA:C	1:8:H:ILE:N	2	1.22
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	10	1.22
(1,929)	1:23:G:PHE:N	1:23:G:PHE:CA	1:23:G:PHE:C	1:24:G:LYS:N	9	1.22
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	9	1.22
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	1	1.22
(1,364)	1:18:C:ASP:N	1:18:C:ASP:CA	1:18:C:ASP:C	1:19:C:GLU:N	4	1.22
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	2	1.22
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	1	1.22
(1,249)	1:47:B:MET:N	1:47:B:MET:CA	1:47:B:MET:C	1:48:B:ASP:N	4	1.22
(1,229)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:LYS:N	9	1.22
(1,156)	1:19:B:GLU:C	1:20:B:LEU:N	1:20:B:LEU:CA	1:20:B:LEU:C	5	1.22
(1,84)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:GLU:N	4	1.22
(1,1931)	1:49:N:ALA:N	1:49:N:ALA:CA	1:49:N:ALA:C	1:50:N:ILE:N	4	1.21
(1,1929)	1:47:N:MET:N	1:47:N:MET:CA	1:47:N:MET:C	1:48:N:ASP:N	4	1.21
(1,1828)	1:10:N:ASP:C	1:11:N:ALA:N	1:11:N:ALA:CA	1:11:N:ALA:C	4	1.21
(1,1511)	1:49:K:ALA:N	1:49:K:ALA:CA	1:49:K:ALA:C	1:50:K:ILE:N	4	1.21
(1,1209)	1:23:I:PHE:N	1:23:I:PHE:CA	1:23:I:PHE:C	1:24:I:LYS:N	9	1.21
(1,1113)	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	1:76:H:MET:N	6	1.21
(1,1099)	1:57:H:VAL:N	1:57:H:VAL:CA	1:57:H:VAL:C	1:58:H:SER:N	5	1.21
(1,811)	1:49:F:ALA:N	1:49:F:ALA:CA	1:49:F:ALA:C	1:50:F:ILE:N	4	1.21
(1,644)	1:18:E:ASP:N	1:18:E:ASP:CA	1:18:E:ASP:C	1:19:E:GLU:N	4	1.21
(1,494)	1:7:D:ALA:N	1:7:D:ALA:CA	1:7:D:ALA:C	1:8:D:ILE:N	4	1.21
(1,389)	1:47:C:MET:N	1:47:C:MET:CA	1:47:C:MET:C	1:48:C:ASP:N	4	1.21
(1,109)	1:47:A:MET:N	1:47:A:MET:CA	1:47:A:MET:C	1:48:A:ASP:N	4	1.21
(1,76)	1:9:A:LEU:N	1:9:A:LEU:CA	1:9:A:LEU:C	1:10:A:ASP:N	9	1.21
(1,2069)	1:47:O:MET:N	1:47:O:MET:CA	1:47:O:MET:C	1:48:O:ASP:N	9	1.2
(1,2049)	1:23:O:PHE:N	1:23:O:PHE:CA	1:23:O:PHE:C	1:24:O:LYS:N	9	1.2
(1,2044)	1:18:O:ASP:N	1:18:O:ASP:CA	1:18:O:ASP:C	1:19:O:GLU:N	4	1.2
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	1	1.2
(1,1909)	1:23:N:PHE:N	1:23:N:PHE:CA	1:23:N:PHE:C	1:24:N:LYS:N	9	1.2
(1,1904)	1:18:N:ASP:N	1:18:N:ASP:CA	1:18:N:ASP:C	1:19:N:GLU:N	4	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1870)	1:57:N:VAL:C	1:58:N:SER:N	1:58:N:SER:CA	1:58:N:SER:C	2	1.2
(1,1706)	1:29:M:THR:C	1:30:M:VAL:N	1:30:M:VAL:CA	1:30:M:VAL:C	8	1.2
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	8	1.2
(1,1624)	1:18:L:ASP:N	1:18:L:ASP:CA	1:18:L:ASP:C	1:19:L:GLU:N	4	1.2
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	8	1.2
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	2	1.2
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	9	1.2
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	3	1.2
(1,1334)	1:7:J:ALA:N	1:7:J:ALA:CA	1:7:J:ALA:C	1:8:J:ILE:N	7	1.2
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	7	1.2
(1,1030)	1:57:H:VAL:C	1:58:H:SER:N	1:58:H:SER:CA	1:58:H:SER:C	2	1.2
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	1	1.2
(1,856)	1:19:G:GLU:C	1:20:G:LEU:N	1:20:G:LEU:CA	1:20:G:LEU:C	5	1.2
(1,776)	1:9:F:LEU:N	1:9:F:LEU:CA	1:9:F:LEU:C	1:10:F:ASP:N	9	1.2
(1,730)	1:37:F:GLY:C	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	8	1.2
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	10	1.2
(1,708)	1:10:F:ASP:C	1:11:F:ALA:N	1:11:F:ALA:CA	1:11:F:ALA:C	4	1.2
(1,576)	1:19:E:GLU:C	1:20:E:LEU:N	1:20:E:LEU:CA	1:20:E:LEU:C	5	1.2
(1,496)	1:9:D:LEU:N	1:9:D:LEU:CA	1:9:D:LEU:C	1:10:D:ASP:N	9	1.2
(1,391)	1:49:C:ALA:N	1:49:C:ALA:CA	1:49:C:ALA:C	1:50:C:ILE:N	4	1.2
(1,274)	1:76:B:MET:N	1:76:B:MET:CA	1:76:B:MET:C	1:77:B:GLY:N	3	1.2
(1,249)	1:47:B:MET:N	1:47:B:MET:CA	1:47:B:MET:C	1:48:B:ASP:N	9	1.2
(1,214)	1:7:B:ALA:N	1:7:B:ALA:CA	1:7:B:ALA:C	1:8:B:ILE:N	9	1.2
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	10	1.2
(1,89)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:LYS:N	9	1.2
(1,74)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	4	1.2
(1,30)	1:37:A:GLY:C	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	8	1.2
(1,2034)	1:7:O:ALA:N	1:7:O:ALA:CA	1:7:O:ALA:C	1:8:O:ILE:N	8	1.19
(1,1968)	1:10:O:ASP:C	1:11:O:ALA:N	1:11:O:ALA:CA	1:11:O:ALA:C	1	1.19
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	5	1.19
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	9	1.19
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	1	1.19
(1,1791)	1:49:M:ALA:N	1:49:M:ALA:CA	1:49:M:ALA:C	1:50:M:ILE:N	4	1.19
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	9	1.19
(1,1696)	1:19:M:GLU:C	1:20:M:LEU:N	1:20:M:LEU:CA	1:20:M:LEU:C	1	1.19
(1,1614)	1:7:L:ALA:N	1:7:L:ALA:CA	1:7:L:ALA:C	1:8:L:ILE:N	4	1.19
(1,1590)	1:57:L:VAL:C	1:58:L:SER:N	1:58:L:SER:CA	1:58:L:SER:C	2	1.19
(1,1556)	1:19:L:GLU:C	1:20:L:LEU:N	1:20:L:LEU:CA	1:20:L:LEU:C	1	1.19
(1,1533)	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	1:76:K:MET:N	6	1.19
(1,1509)	1:47:K:MET:N	1:47:K:MET:CA	1:47:K:MET:C	1:48:K:ASP:N	9	1.19
(1,1379)	1:57:J:VAL:N	1:57:J:VAL:CA	1:57:J:VAL:C	1:58:J:SER:N	5	1.19
(1,1344)	1:18:J:ASP:N	1:18:J:ASP:CA	1:18:J:ASP:C	1:19:J:GLU:N	4	1.19
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	8	1.19
(1,1229)	1:47:I:MET:N	1:47:I:MET:CA	1:47:I:MET:C	1:48:I:ASP:N	4	1.19
(1,1128)	1:10:I:ASP:C	1:11:I:ALA:N	1:11:I:ALA:CA	1:11:I:ALA:C	1	1.19
(1,1028)	1:55:H:LYS:C	1:56:H:LEU:N	1:56:H:LEU:CA	1:56:H:LEU:C	2	1.19
(1,959)	1:57:G:VAL:N	1:57:G:VAL:CA	1:57:G:VAL:C	1:58:G:SER:N	5	1.19
(1,914)	1:7:G:ALA:N	1:7:G:ALA:CA	1:7:G:ALA:C	1:8:G:ILE:N	9	1.19
(1,890)	1:57:G:VAL:C	1:58:G:SER:N	1:58:G:SER:CA	1:58:G:SER:C	2	1.19
(1,763)	1:74:F:ARG:C	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	7	1.19
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	9	1.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,644)	1:18:E:ASP:N	1:18:E:ASP:CA	1:18:E:ASP:C	1:19:E:GLU:N	7	1.19
(1,568)	1:10:E:ASP:C	1:11:E:ALA:N	1:11:E:ALA:CA	1:11:E:ALA:C	4	1.19
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	5	1.19
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	9	1.19
(1,331)	1:58:C:SER:C	1:59:C:TYR:N	1:59:C:TYR:CA	1:59:C:TYR:C	5	1.19
(1,224)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:GLU:N	7	1.19
(1,214)	1:7:B:ALA:N	1:7:B:ALA:CA	1:7:B:ALA:C	1:8:B:ILE:N	10	1.19
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	9	1.19
(1,119)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:SER:N	5	1.19
(1,1976)	1:19:O:GLU:C	1:20:O:LEU:N	1:20:O:LEU:CA	1:20:O:LEU:C	1	1.18
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	3	1.18
(1,1846)	1:29:N:THR:C	1:30:N:VAL:N	1:30:N:VAL:CA	1:30:N:VAL:C	8	1.18
(1,1789)	1:47:M:MET:N	1:47:M:MET:CA	1:47:M:MET:C	1:48:M:ASP:N	9	1.18
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	10	1.18
(1,1484)	1:18:K:ASP:N	1:18:K:ASP:CA	1:18:K:ASP:C	1:19:K:GLU:N	4	1.18
(1,1476)	1:9:K:LEU:N	1:9:K:LEU:CA	1:9:K:LEU:C	1:10:K:ASP:N	9	1.18
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	4	1.18
(1,1416)	1:19:K:GLU:C	1:20:K:LEU:N	1:20:K:LEU:CA	1:20:K:LEU:C	1	1.18
(1,1334)	1:7:J:ALA:N	1:7:J:ALA:CA	1:7:J:ALA:C	1:8:J:ILE:N	5	1.18
(1,1204)	1:18:I:ASP:N	1:18:I:ASP:CA	1:18:I:ASP:C	1:19:I:GLU:N	7	1.18
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	9	1.18
(1,1054)	1:7:H:ALA:N	1:7:H:ALA:CA	1:7:H:ALA:C	1:8:H:ILE:N	5	1.18
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	1	1.18
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	1	1.18
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	10	1.18
(1,428)	1:10:D:ASP:C	1:11:D:ALA:N	1:11:D:ALA:CA	1:11:D:ALA:C	1	1.18
(1,330)	1:57:C:VAL:C	1:58:C:SER:N	1:58:C:SER:CA	1:58:C:SER:C	2	1.18
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	10	1.18
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	1	1.18
(1,170)	1:37:B:GLY:C	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	8	1.18
(1,109)	1:47:A:MET:N	1:47:A:MET:CA	1:47:A:MET:C	1:48:A:ASP:N	9	1.18
(1,2034)	1:7:O:ALA:N	1:7:O:ALA:CA	1:7:O:ALA:C	1:8:O:ILE:N	4	1.17
(1,1990)	1:37:O:GLY:C	1:38:O:ARG:N	1:38:O:ARG:CA	1:38:O:ARG:C	8	1.17
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	1	1.17
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	10	1.17
(1,1871)	1:58:N:SER:C	1:59:N:TYR:N	1:59:N:TYR:CA	1:59:N:TYR:C	5	1.17
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	10	1.17
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	3	1.17
(1,1334)	1:7:J:ALA:N	1:7:J:ALA:CA	1:7:J:ALA:C	1:8:J:ILE:N	9	1.17
(1,1150)	1:37:I:GLY:C	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	8	1.17
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	10	1.17
(1,1054)	1:7:H:ALA:N	1:7:H:ALA:CA	1:7:H:ALA:C	1:8:H:ILE:N	7	1.17
(1,916)	1:9:G:LEU:N	1:9:G:LEU:CA	1:9:G:LEU:C	1:10:G:ASP:N	9	1.17
(1,903)	1:74:G:ARG:C	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	1	1.17
(1,789)	1:23:F:PHE:N	1:23:F:PHE:CA	1:23:F:PHE:C	1:24:F:LYS:N	9	1.17
(1,716)	1:19:F:GLU:C	1:20:F:LEU:N	1:20:F:LEU:CA	1:20:F:LEU:C	1	1.17
(1,669)	1:47:E:MET:N	1:47:E:MET:CA	1:47:E:MET:C	1:48:E:ASP:N	4	1.17
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	1	1.17
(1,611)	1:58:E:SER:C	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	5	1.17
(1,610)	1:57:E:VAL:C	1:58:E:SER:N	1:58:E:SER:CA	1:58:E:SER:C	2	1.17
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	10	1.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	1	1.17
(1,436)	1:19:D:GLU:C	1:20:D:LEU:N	1:20:D:LEU:CA	1:20:D:LEU:C	1	1.17
(1,413)	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	1:76:C:MET:N	6	1.17
(1,369)	1:23:C:PHE:N	1:23:C:PHE:CA	1:23:C:PHE:C	1:24:C:LYS:N	9	1.17
(1,364)	1:18:C:ASP:N	1:18:C:ASP:CA	1:18:C:ASP:C	1:19:C:GLU:N	7	1.17
(1,296)	1:19:C:GLU:C	1:20:C:LEU:N	1:20:C:LEU:CA	1:20:C:LEU:C	1	1.17
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	3	1.17
(1,166)	1:29:B:THR:C	1:30:B:VAL:N	1:30:B:VAL:CA	1:30:B:VAL:C	8	1.17
(1,48)	1:55:A:LYS:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	2	1.17
(1,16)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1	1.17
(1,2069)	1:47:O:MET:N	1:47:O:MET:CA	1:47:O:MET:C	1:48:O:ASP:N	2	1.16
(1,1929)	1:47:N:MET:N	1:47:N:MET:CA	1:47:N:MET:C	1:48:N:ASP:N	2	1.16
(1,1904)	1:18:N:ASP:N	1:18:N:ASP:CA	1:18:N:ASP:C	1:19:N:GLU:N	7	1.16
(1,1850)	1:37:N:GLY:C	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	8	1.16
(1,1789)	1:47:M:MET:N	1:47:M:MET:CA	1:47:M:MET:C	1:48:M:ASP:N	4	1.16
(1,1754)	1:7:M:ALA:N	1:7:M:ALA:CA	1:7:M:ALA:C	1:8:M:ILE:N	7	1.16
(1,1731)	1:58:M:SER:C	1:59:M:TYR:N	1:59:M:TYR:CA	1:59:M:TYR:C	5	1.16
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	1	1.16
(1,1616)	1:9:L:LEU:N	1:9:L:LEU:CA	1:9:L:LEU:C	1:10:L:ASP:N	9	1.16
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	1	1.16
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	10	1.16
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	10	1.16
(1,1268)	1:10:J:ASP:C	1:11:J:ALA:N	1:11:J:ALA:CA	1:11:J:ALA:C	4	1.16
(1,1196)	1:9:I:LEU:N	1:9:I:LEU:CA	1:9:I:LEU:C	1:10:I:ASP:N	9	1.16
(1,1143)	1:26:I:LYS:C	1:27:I:LEU:N	1:27:I:LEU:CA	1:27:I:LEU:C	2	1.16
(1,1056)	1:9:H:LEU:N	1:9:H:LEU:CA	1:9:H:LEU:C	1:10:H:ASP:N	9	1.16
(1,949)	1:47:G:MET:N	1:47:G:MET:CA	1:47:G:MET:C	1:48:G:ASP:N	2	1.16
(1,949)	1:47:G:MET:N	1:47:G:MET:CA	1:47:G:MET:C	1:48:G:ASP:N	9	1.16
(1,924)	1:18:G:ASP:N	1:18:G:ASP:CA	1:18:G:ASP:C	1:19:G:GLU:N	4	1.16
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	9	1.16
(1,636)	1:9:E:LEU:N	1:9:E:LEU:CA	1:9:E:LEU:C	1:10:E:ASP:N	9	1.16
(1,634)	1:7:E:ALA:N	1:7:E:ALA:CA	1:7:E:ALA:C	1:8:E:ILE:N	9	1.16
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	3	1.16
(1,458)	1:45:D:LEU:C	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	9	1.16
(1,389)	1:47:C:MET:N	1:47:C:MET:CA	1:47:C:MET:C	1:48:C:ASP:N	9	1.16
(1,109)	1:47:A:MET:N	1:47:A:MET:CA	1:47:A:MET:C	1:48:A:ASP:N	2	1.16
(1,84)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:GLU:N	7	1.16
(1,2044)	1:18:O:ASP:N	1:18:O:ASP:CA	1:18:O:ASP:C	1:19:O:GLU:N	6	1.15
(1,1998)	1:45:O:LEU:C	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	3	1.15
(1,1929)	1:47:N:MET:N	1:47:N:MET:CA	1:47:N:MET:C	1:48:N:ASP:N	9	1.15
(1,1659)	1:57:L:VAL:N	1:57:L:VAL:CA	1:57:L:VAL:C	1:58:L:SER:N	5	1.15
(1,1614)	1:7:L:ALA:N	1:7:L:ALA:CA	1:7:L:ALA:C	1:8:L:ILE:N	9	1.15
(1,1369)	1:47:J:MET:N	1:47:J:MET:CA	1:47:J:MET:C	1:48:J:ASP:N	9	1.15
(1,1349)	1:23:J:PHE:N	1:23:J:PHE:CA	1:23:J:PHE:C	1:24:J:LYS:N	9	1.15
(1,1336)	1:9:J:LEU:N	1:9:J:LEU:CA	1:9:J:LEU:C	1:10:J:ASP:N	9	1.15
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	10	1.15
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	9	1.15
(1,1089)	1:47:H:MET:N	1:47:H:MET:CA	1:47:H:MET:C	1:48:H:ASP:N	9	1.15
(1,1054)	1:7:H:ALA:N	1:7:H:ALA:CA	1:7:H:ALA:C	1:8:H:ILE:N	9	1.15
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	4	1.15
(1,1010)	1:37:H:GLY:C	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	1	1.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1006)	1:29:H:THR:C	1:30:H:VAL:N	1:30:H:VAL:CA	1:30:H:VAL:C	8	1.15
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	4	1.15
(1,870)	1:37:G:GLY:C	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	8	1.15
(1,726)	1:29:F:THR:C	1:30:F:VAL:N	1:30:F:VAL:CA	1:30:F:VAL:C	8	1.15
(1,669)	1:47:E:MET:N	1:47:E:MET:CA	1:47:E:MET:C	1:48:E:ASP:N	9	1.15
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	4	1.15
(1,576)	1:19:E:GLU:C	1:20:E:LEU:N	1:20:E:LEU:CA	1:20:E:LEU:C	1	1.15
(1,553)	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	1:76:D:MET:N	6	1.15
(1,509)	1:23:D:PHE:N	1:23:D:PHE:CA	1:23:D:PHE:C	1:24:D:LYS:N	9	1.15
(1,494)	1:7:D:ALA:N	1:7:D:ALA:CA	1:7:D:ALA:C	1:8:D:ILE:N	7	1.15
(1,343)	1:74:C:ARG:C	1:75:C:ASP:N	1:75:C:ASP:CA	1:75:C:ASP:C	7	1.15
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	3	1.15
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	9	1.15
(1,310)	1:37:C:GLY:C	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	8	1.15
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	2	1.15
(1,148)	1:10:B:ASP:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	1	1.15
(1,26)	1:29:A:THR:C	1:30:A:VAL:N	1:30:A:VAL:CA	1:30:A:VAL:C	8	1.15
(1,2019)	1:70:O:MET:C	1:71:O:THR:N	1:71:O:THR:CA	1:71:O:THR:C	5	1.14
(1,1998)	1:45:O:LEU:C	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	9	1.14
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	10	1.14
(1,1624)	1:18:L:ASP:N	1:18:L:ASP:CA	1:18:L:ASP:C	1:19:L:GLU:N	6	1.14
(1,1591)	1:58:L:SER:C	1:59:L:TYR:N	1:59:L:TYR:CA	1:59:L:TYR:C	5	1.14
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	2	1.14
(1,1509)	1:47:K:MET:N	1:47:K:MET:CA	1:47:K:MET:C	1:48:K:ASP:N	2	1.14
(1,1489)	1:23:K:PHE:N	1:23:K:PHE:CA	1:23:K:PHE:C	1:24:K:LYS:N	9	1.14
(1,1484)	1:18:K:ASP:N	1:18:K:ASP:CA	1:18:K:ASP:C	1:19:K:GLU:N	7	1.14
(1,1426)	1:29:K:THR:C	1:30:K:VAL:N	1:30:K:VAL:CA	1:30:K:VAL:C	8	1.14
(1,1408)	1:10:K:ASP:C	1:11:K:ALA:N	1:11:K:ALA:CA	1:11:K:ALA:C	1	1.14
(1,1308)	1:55:J:LYS:C	1:56:J:LEU:N	1:56:J:LEU:CA	1:56:J:LEU:C	2	1.14
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	9	1.14
(1,1229)	1:47:I:MET:N	1:47:I:MET:CA	1:47:I:MET:C	1:48:I:ASP:N	9	1.14
(1,1168)	1:55:I:LYS:C	1:56:I:LEU:N	1:56:I:LEU:CA	1:56:I:LEU:C	2	1.14
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	3	1.14
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	4	1.14
(1,1136)	1:19:I:GLU:C	1:20:I:LEU:N	1:20:I:LEU:CA	1:20:I:LEU:C	1	1.14
(1,1091)	1:49:H:ALA:N	1:49:H:ALA:CA	1:49:H:ALA:C	1:50:H:ILE:N	4	1.14
(1,1064)	1:18:H:ASP:N	1:18:H:ASP:CA	1:18:H:ASP:C	1:19:H:GLU:N	7	1.14
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	3	1.14
(1,914)	1:7:G:ALA:N	1:7:G:ALA:CA	1:7:G:ALA:C	1:8:G:ILE:N	2	1.14
(1,833)	1:75:F:ASP:N	1:75:F:ASP:CA	1:75:F:ASP:C	1:76:F:MET:N	6	1.14
(1,809)	1:47:F:MET:N	1:47:F:MET:CA	1:47:F:MET:C	1:48:F:ASP:N	4	1.14
(1,774)	1:7:F:ALA:N	1:7:F:ALA:CA	1:7:F:ALA:C	1:8:F:ILE:N	9	1.14
(1,669)	1:47:E:MET:N	1:47:E:MET:CA	1:47:E:MET:C	1:48:E:ASP:N	2	1.14
(1,668)	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	1:47:E:MET:N	2	1.14
(1,623)	1:74:E:ARG:C	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	7	1.14
(1,529)	1:47:D:MET:N	1:47:D:MET:CA	1:47:D:MET:C	1:48:D:ASP:N	2	1.14
(1,529)	1:47:D:MET:N	1:47:D:MET:CA	1:47:D:MET:C	1:48:D:ASP:N	9	1.14
(1,446)	1:29:D:THR:C	1:30:D:VAL:N	1:30:D:VAL:CA	1:30:D:VAL:C	8	1.14
(1,216)	1:9:B:LEU:N	1:9:B:LEU:CA	1:9:B:LEU:C	1:10:B:ASP:N	9	1.14
(1,214)	1:7:B:ALA:N	1:7:B:ALA:CA	1:7:B:ALA:C	1:8:B:ILE:N	2	1.14
(1,74)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	7	1.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	1	1.14
(1,51)	1:58:A:SER:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	5	1.14
(1,1986)	1:29:O:THR:C	1:30:O:VAL:N	1:30:O:VAL:CA	1:30:O:VAL:C	8	1.13
(1,1896)	1:9:N:LEU:N	1:9:N:LEU:CA	1:9:N:LEU:C	1:10:N:ASP:N	9	1.13
(1,1813)	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	1:76:M:MET:N	6	1.13
(1,1764)	1:18:M:ASP:N	1:18:M:ASP:CA	1:18:M:ASP:C	1:19:M:GLU:N	4	1.13
(1,1764)	1:18:M:ASP:N	1:18:M:ASP:CA	1:18:M:ASP:C	1:19:M:GLU:N	7	1.13
(1,1754)	1:7:M:ALA:N	1:7:M:ALA:CA	1:7:M:ALA:C	1:8:M:ILE:N	9	1.13
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	1	1.13
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	4	1.13
(1,1651)	1:49:L:ALA:N	1:49:L:ALA:CA	1:49:L:ALA:C	1:50:L:ILE:N	4	1.13
(1,1649)	1:47:L:MET:N	1:47:L:MET:CA	1:47:L:MET:C	1:48:L:ASP:N	9	1.13
(1,1614)	1:7:L:ALA:N	1:7:L:ALA:CA	1:7:L:ALA:C	1:8:L:ILE:N	7	1.13
(1,1566)	1:29:L:THR:C	1:30:L:VAL:N	1:30:L:VAL:CA	1:30:L:VAL:C	8	1.13
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	9	1.13
(1,1369)	1:47:J:MET:N	1:47:J:MET:CA	1:47:J:MET:C	1:48:J:ASP:N	2	1.13
(1,1344)	1:18:J:ASP:N	1:18:J:ASP:CA	1:18:J:ASP:C	1:19:J:GLU:N	6	1.13
(1,1344)	1:18:J:ASP:N	1:18:J:ASP:CA	1:18:J:ASP:C	1:19:J:GLU:N	7	1.13
(1,1323)	1:74:J:ARG:C	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	7	1.13
(1,1311)	1:58:J:SER:C	1:59:J:TYR:N	1:59:J:TYR:CA	1:59:J:TYR:C	5	1.13
(1,1253)	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	1:76:I:MET:N	6	1.13
(1,1183)	1:74:I:ARG:C	1:75:I:ASP:N	1:75:I:ASP:CA	1:75:I:ASP:C	1	1.13
(1,1031)	1:58:H:SER:C	1:59:H:TYR:N	1:59:H:TYR:CA	1:59:H:TYR:C	5	1.13
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	9	1.13
(1,679)	1:57:E:VAL:N	1:57:E:VAL:CA	1:57:E:VAL:C	1:58:E:SER:N	5	1.13
(1,668)	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	1:47:E:MET:N	9	1.13
(1,644)	1:18:E:ASP:N	1:18:E:ASP:CA	1:18:E:ASP:C	1:19:E:GLU:N	6	1.13
(1,634)	1:7:E:ALA:N	1:7:E:ALA:CA	1:7:E:ALA:C	1:8:E:ILE:N	7	1.13
(1,619)	1:70:E:MET:C	1:71:E:THR:N	1:71:E:THR:CA	1:71:E:THR:C	5	1.13
(1,504)	1:18:D:ASP:N	1:18:D:ASP:CA	1:18:D:ASP:C	1:19:D:GLU:N	7	1.13
(1,458)	1:45:D:LEU:C	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	3	1.13
(1,450)	1:37:D:GLY:C	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	8	1.13
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	10	1.13
(1,328)	1:55:C:LYS:C	1:56:C:LEU:N	1:56:C:LEU:CA	1:56:C:LEU:C	2	1.13
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	4	1.13
(1,191)	1:58:B:SER:C	1:59:B:TYR:N	1:59:B:TYR:CA	1:59:B:TYR:C	5	1.13
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	2	1.13
(1,2019)	1:70:O:MET:C	1:71:O:THR:N	1:71:O:THR:CA	1:71:O:THR:C	1	1.12
(1,2019)	1:70:O:MET:C	1:71:O:THR:N	1:71:O:THR:CA	1:71:O:THR:C	3	1.12
(1,1879)	1:70:N:MET:C	1:71:N:THR:N	1:71:N:THR:CA	1:71:N:THR:C	7	1.12
(1,1710)	1:37:M:GLY:C	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	8	1.12
(1,1688)	1:10:M:ASP:C	1:11:M:ALA:N	1:11:M:ALA:CA	1:11:M:ALA:C	1	1.12
(1,1649)	1:47:L:MET:N	1:47:L:MET:CA	1:47:L:MET:C	1:48:L:ASP:N	2	1.12
(1,1614)	1:7:L:ALA:N	1:7:L:ALA:CA	1:7:L:ALA:C	1:8:L:ILE:N	2	1.12
(1,1614)	1:7:L:ALA:N	1:7:L:ALA:CA	1:7:L:ALA:C	1:8:L:ILE:N	5	1.12
(1,1484)	1:18:K:ASP:N	1:18:K:ASP:CA	1:18:K:ASP:C	1:19:K:GLU:N	6	1.12
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	1	1.12
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	3	1.12
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	4	1.12
(1,1229)	1:47:I:MET:N	1:47:I:MET:CA	1:47:I:MET:C	1:48:I:ASP:N	2	1.12
(1,1064)	1:18:H:ASP:N	1:18:H:ASP:CA	1:18:H:ASP:C	1:19:H:GLU:N	6	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1043)	1:74:H:ARG:C	1:75:H:ASP:N	1:75:H:ASP:CA	1:75:H:ASP:C	7	1.12
(1,973)	1:75:G:ASP:N	1:75:G:ASP:CA	1:75:G:ASP:C	1:76:G:MET:N	6	1.12
(1,924)	1:18:G:ASP:N	1:18:G:ASP:CA	1:18:G:ASP:C	1:19:G:GLU:N	7	1.12
(1,914)	1:7:G:ALA:N	1:7:G:ALA:CA	1:7:G:ALA:C	1:8:G:ILE:N	5	1.12
(1,809)	1:47:F:MET:N	1:47:F:MET:CA	1:47:F:MET:C	1:48:F:ASP:N	2	1.12
(1,774)	1:7:F:ALA:N	1:7:F:ALA:CA	1:7:F:ALA:C	1:8:F:ILE:N	2	1.12
(1,634)	1:7:E:ALA:N	1:7:E:ALA:CA	1:7:E:ALA:C	1:8:E:ILE:N	2	1.12
(1,458)	1:45:D:LEU:C	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	4	1.12
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	2	1.12
(1,306)	1:29:C:THR:C	1:30:C:VAL:N	1:30:C:VAL:CA	1:30:C:VAL:C	8	1.12
(1,288)	1:10:C:ASP:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	1	1.12
(1,224)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:GLU:N	6	1.12
(1,203)	1:74:B:ARG:C	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	7	1.12
(1,188)	1:55:B:LYS:C	1:56:B:LEU:N	1:56:B:LEU:CA	1:56:B:LEU:C	2	1.12
(1,156)	1:19:B:GLU:C	1:20:B:LEU:N	1:20:B:LEU:CA	1:20:B:LEU:C	1	1.12
(1,74)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	9	1.12
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	9	1.12
(1,1904)	1:18:N:ASP:N	1:18:N:ASP:CA	1:18:N:ASP:C	1:19:N:GLU:N	6	1.11
(1,1879)	1:70:N:MET:C	1:71:N:THR:N	1:71:N:THR:CA	1:71:N:THR:C	5	1.11
(1,1828)	1:10:N:ASP:C	1:11:N:ALA:N	1:11:N:ALA:CA	1:11:N:ALA:C	1	1.11
(1,1743)	1:74:M:ARG:C	1:75:M:ASP:N	1:75:M:ASP:CA	1:75:M:ASP:C	7	1.11
(1,1624)	1:18:L:ASP:N	1:18:L:ASP:CA	1:18:L:ASP:C	1:19:L:GLU:N	7	1.11
(1,1603)	1:74:L:ARG:C	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	7	1.11
(1,1599)	1:70:L:MET:C	1:71:L:THR:N	1:71:L:THR:CA	1:71:L:THR:C	3	1.11
(1,1599)	1:70:L:MET:C	1:71:L:THR:N	1:71:L:THR:CA	1:71:L:THR:C	5	1.11
(1,1599)	1:70:L:MET:C	1:71:L:THR:N	1:71:L:THR:CA	1:71:L:THR:C	7	1.11
(1,1578)	1:45:L:LEU:C	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	3	1.11
(1,1393)	1:75:J:ASP:N	1:75:J:ASP:CA	1:75:J:ASP:C	1:76:J:MET:N	6	1.11
(1,1334)	1:7:J:ALA:N	1:7:J:ALA:CA	1:7:J:ALA:C	1:8:J:ILE:N	2	1.11
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	9	1.11
(1,1146)	1:29:I:THR:C	1:30:I:VAL:N	1:30:I:VAL:CA	1:30:I:VAL:C	8	1.11
(1,1088)	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	1:47:H:MET:N	2	1.11
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	9	1.11
(1,948)	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	1:47:G:MET:N	2	1.11
(1,888)	1:55:G:LYS:C	1:56:G:LEU:N	1:56:G:LEU:CA	1:56:G:LEU:C	2	1.11
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	3	1.11
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	2	1.11
(1,809)	1:47:F:MET:N	1:47:F:MET:CA	1:47:F:MET:C	1:48:F:ASP:N	9	1.11
(1,751)	1:58:F:SER:C	1:59:F:TYR:N	1:59:F:TYR:CA	1:59:F:TYR:C	5	1.11
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	4	1.11
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	9	1.11
(1,634)	1:7:E:ALA:N	1:7:E:ALA:CA	1:7:E:ALA:C	1:8:E:ILE:N	5	1.11
(1,531)	1:49:D:ALA:N	1:49:D:ALA:CA	1:49:D:ALA:C	1:50:D:ILE:N	4	1.11
(1,494)	1:7:D:ALA:N	1:7:D:ALA:CA	1:7:D:ALA:C	1:8:D:ILE:N	2	1.11
(1,494)	1:7:D:ALA:N	1:7:D:ALA:CA	1:7:D:ALA:C	1:8:D:ILE:N	5	1.11
(1,483)	1:74:D:ARG:C	1:75:D:ASP:N	1:75:D:ASP:CA	1:75:D:ASP:C	7	1.11
(1,471)	1:58:D:SER:C	1:59:D:TYR:N	1:59:D:TYR:CA	1:59:D:TYR:C	5	1.11
(1,389)	1:47:C:MET:N	1:47:C:MET:CA	1:47:C:MET:C	1:48:C:ASP:N	2	1.11
(1,288)	1:10:C:ASP:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	8	1.11
(1,23)	1:26:A:LYS:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	9	1.11
(1,2093)	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	1:76:O:MET:N	6	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2044)	1:18:O:ASP:N	1:18:O:ASP:CA	1:18:O:ASP:C	1:19:O:GLU:N	7	1.1
(1,2034)	1:7:O:ALA:N	1:7:O:ALA:CA	1:7:O:ALA:C	1:8:O:ILE:N	2	1.1
(1,2034)	1:7:O:ALA:N	1:7:O:ALA:CA	1:7:O:ALA:C	1:8:O:ILE:N	7	1.1
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	2	1.1
(1,1883)	1:74:N:ARG:C	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	7	1.1
(1,1789)	1:47:M:MET:N	1:47:M:MET:CA	1:47:M:MET:C	1:48:M:ASP:N	2	1.1
(1,1754)	1:7:M:ALA:N	1:7:M:ALA:CA	1:7:M:ALA:C	1:8:M:ILE:N	5	1.1
(1,1739)	1:70:M:MET:C	1:71:M:THR:N	1:71:M:THR:CA	1:71:M:THR:C	5	1.1
(1,1570)	1:37:L:GLY:C	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	1	1.1
(1,1451)	1:58:K:SER:C	1:59:K:TYR:N	1:59:K:TYR:CA	1:59:K:TYR:C	5	1.1
(1,1430)	1:37:K:GLY:C	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	8	1.1
(1,1368)	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	1:47:J:MET:N	2	1.1
(1,1171)	1:58:I:SER:C	1:59:I:TYR:N	1:59:I:TYR:CA	1:59:I:TYR:C	5	1.1
(1,1089)	1:47:H:MET:N	1:47:H:MET:CA	1:47:H:MET:C	1:48:H:ASP:N	2	1.1
(1,1003)	1:26:H:LYS:C	1:27:H:LEU:N	1:27:H:LEU:CA	1:27:H:LEU:C	2	1.1
(1,949)	1:47:G:MET:N	1:47:G:MET:CA	1:47:G:MET:C	1:48:G:ASP:N	8	1.1
(1,863)	1:26:G:LYS:C	1:27:G:LEU:N	1:27:G:LEU:CA	1:27:G:LEU:C	9	1.1
(1,784)	1:18:F:ASP:N	1:18:F:ASP:CA	1:18:F:ASP:C	1:19:F:GLU:N	7	1.1
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	3	1.1
(1,494)	1:7:D:ALA:N	1:7:D:ALA:CA	1:7:D:ALA:C	1:8:D:ILE:N	9	1.1
(1,450)	1:37:D:GLY:C	1:38:D:ARG:N	1:38:D:ARG:CA	1:38:D:ARG:C	1	1.1
(1,249)	1:47:B:MET:N	1:47:B:MET:CA	1:47:B:MET:C	1:48:B:ASP:N	2	1.1
(1,248)	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	1:47:B:MET:N	2	1.1
(1,214)	1:7:B:ALA:N	1:7:B:ALA:CA	1:7:B:ALA:C	1:8:B:ILE:N	5	1.1
(1,133)	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	1:76:A:MET:N	6	1.1
(1,84)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:GLU:N	6	1.1
(1,2069)	1:47:O:MET:N	1:47:O:MET:CA	1:47:O:MET:C	1:48:O:ASP:N	8	1.09
(1,1975)	1:18:O:ASP:C	1:19:O:GLU:N	1:19:O:GLU:CA	1:19:O:GLU:C	10	1.09
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	10	1.09
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	9	1.09
(1,1836)	1:19:N:GLU:C	1:20:N:LEU:N	1:20:N:LEU:CA	1:20:N:LEU:C	1	1.09
(1,1828)	1:10:N:ASP:C	1:11:N:ALA:N	1:11:N:ALA:CA	1:11:N:ALA:C	10	1.09
(1,1788)	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	1:47:M:MET:N	2	1.09
(1,1673)	1:75:L:ASP:N	1:75:L:ASP:CA	1:75:L:ASP:C	1:76:L:MET:N	6	1.09
(1,1648)	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	1:47:L:MET:N	2	1.09
(1,1430)	1:37:K:GLY:C	1:38:K:ARG:N	1:38:K:ARG:CA	1:38:K:ARG:C	1	1.09
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	10	1.09
(1,1286)	1:29:J:THR:C	1:30:J:VAL:N	1:30:J:VAL:CA	1:30:J:VAL:C	8	1.09
(1,1283)	1:26:J:LYS:C	1:27:J:LEU:N	1:27:J:LEU:CA	1:27:J:LEU:C	2	1.09
(1,1276)	1:19:J:GLU:C	1:20:J:LEU:N	1:20:J:LEU:CA	1:20:J:LEU:C	1	1.09
(1,1268)	1:10:J:ASP:C	1:11:J:ALA:N	1:11:J:ALA:CA	1:11:J:ALA:C	1	1.09
(1,1150)	1:37:I:GLY:C	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	1	1.09
(1,996)	1:19:H:GLU:C	1:20:H:LEU:N	1:20:H:LEU:CA	1:20:H:LEU:C	1	1.09
(1,866)	1:29:G:THR:C	1:30:G:VAL:N	1:30:G:VAL:CA	1:30:G:VAL:C	8	1.09
(1,730)	1:37:F:GLY:C	1:38:F:ARG:N	1:38:F:ARG:CA	1:38:F:ARG:C	1	1.09
(1,608)	1:55:E:LYS:C	1:56:E:LEU:N	1:56:E:LEU:CA	1:56:E:LEU:C	2	1.09
(1,590)	1:37:E:GLY:C	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	8	1.09
(1,529)	1:47:D:MET:N	1:47:D:MET:CA	1:47:D:MET:C	1:48:D:ASP:N	8	1.09
(1,428)	1:10:D:ASP:C	1:11:D:ALA:N	1:11:D:ALA:CA	1:11:D:ALA:C	10	1.09
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	9	1.09
(1,288)	1:10:C:ASP:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	10	1.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,273)	1:75:B:ASP:N	1:75:B:ASP:CA	1:75:B:ASP:C	1:76:B:MET:N	6	1.09
(1,74)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	2	1.09
(1,74)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	5	1.09
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	3	1.09
(1,30)	1:37:A:GLY:C	1:38:A:ARG:N	1:38:A:ARG:CA	1:38:A:ARG:C	1	1.09
(1,2034)	1:7:O:ALA:N	1:7:O:ALA:CA	1:7:O:ALA:C	1:8:O:ILE:N	9	1.08
(1,2023)	1:74:O:ARG:C	1:75:O:ASP:N	1:75:O:ASP:CA	1:75:O:ASP:C	7	1.08
(1,1879)	1:70:N:MET:C	1:71:N:THR:N	1:71:N:THR:CA	1:71:N:THR:C	3	1.08
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	4	1.08
(1,1843)	1:26:N:LYS:C	1:27:N:LEU:N	1:27:N:LEU:CA	1:27:N:LEU:C	2	1.08
(1,1769)	1:23:M:PHE:N	1:23:M:PHE:CA	1:23:M:PHE:C	1:24:M:LYS:N	9	1.08
(1,1756)	1:9:M:LEU:N	1:9:M:LEU:CA	1:9:M:LEU:C	1:10:M:ASP:N	9	1.08
(1,1599)	1:70:L:MET:C	1:71:L:THR:N	1:71:L:THR:CA	1:71:L:THR:C	1	1.08
(1,1555)	1:18:L:ASP:C	1:19:L:GLU:N	1:19:L:GLU:CA	1:19:L:GLU:C	10	1.08
(1,1204)	1:18:I:ASP:N	1:18:I:ASP:CA	1:18:I:ASP:C	1:19:I:GLU:N	6	1.08
(1,1089)	1:47:H:MET:N	1:47:H:MET:CA	1:47:H:MET:C	1:48:H:ASP:N	8	1.08
(1,1018)	1:45:H:LEU:C	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	5	1.08
(1,774)	1:7:F:ALA:N	1:7:F:ALA:CA	1:7:F:ALA:C	1:8:F:ILE:N	5	1.08
(1,494)	1:7:D:ALA:N	1:7:D:ALA:CA	1:7:D:ALA:C	1:8:D:ILE:N	10	1.08
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	4	1.08
(1,178)	1:45:B:LEU:C	1:46:B:GLN:N	1:46:B:GLN:CA	1:46:B:GLN:C	5	1.08
(1,2034)	1:7:O:ALA:N	1:7:O:ALA:CA	1:7:O:ALA:C	1:8:O:ILE:N	10	1.07
(1,2011)	1:58:O:SER:C	1:59:O:TYR:N	1:59:O:TYR:CA	1:59:O:TYR:C	5	1.07
(1,1968)	1:10:O:ASP:C	1:11:O:ALA:N	1:11:O:ALA:CA	1:11:O:ALA:C	10	1.07
(1,1953)	1:75:N:ASP:N	1:75:N:ASP:CA	1:75:N:ASP:C	1:76:N:MET:N	6	1.07
(1,1688)	1:10:M:ASP:C	1:11:M:ALA:N	1:11:M:ALA:CA	1:11:M:ALA:C	8	1.07
(1,1649)	1:47:L:MET:N	1:47:L:MET:CA	1:47:L:MET:C	1:48:L:ASP:N	3	1.07
(1,1508)	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	1:47:K:MET:N	9	1.07
(1,1474)	1:7:K:ALA:N	1:7:K:ALA:CA	1:7:K:ALA:C	1:8:K:ILE:N	6	1.07
(1,1463)	1:74:K:ARG:C	1:75:K:ASP:N	1:75:K:ASP:CA	1:75:K:ASP:C	7	1.07
(1,1334)	1:7:J:ALA:N	1:7:J:ALA:CA	1:7:J:ALA:C	1:8:J:ILE:N	10	1.07
(1,1319)	1:70:J:MET:C	1:71:J:THR:N	1:71:J:THR:CA	1:71:J:THR:C	5	1.07
(1,1229)	1:47:I:MET:N	1:47:I:MET:CA	1:47:I:MET:C	1:48:I:ASP:N	8	1.07
(1,914)	1:7:G:ALA:N	1:7:G:ALA:CA	1:7:G:ALA:C	1:8:G:ILE:N	10	1.07
(1,848)	1:10:G:ASP:C	1:11:G:ALA:N	1:11:G:ALA:CA	1:11:G:ALA:C	1	1.07
(1,822)	1:64:F:TYR:N	1:64:F:TYR:CA	1:64:F:TYR:C	1:65:F:GLY:N	6	1.07
(1,738)	1:45:F:LEU:C	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	5	1.07
(1,590)	1:37:E:GLY:C	1:38:E:ARG:N	1:38:E:ARG:CA	1:38:E:ARG:C	1	1.07
(1,568)	1:10:E:ASP:C	1:11:E:ALA:N	1:11:E:ALA:CA	1:11:E:ALA:C	1	1.07
(1,568)	1:10:E:ASP:C	1:11:E:ALA:N	1:11:E:ALA:CA	1:11:E:ALA:C	8	1.07
(1,504)	1:18:D:ASP:N	1:18:D:ASP:CA	1:18:D:ASP:C	1:19:D:GLU:N	6	1.07
(1,148)	1:10:B:ASP:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	8	1.07
(1,148)	1:10:B:ASP:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	10	1.07
(1,108)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:MET:N	2	1.07
(1,8)	1:10:A:ASP:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1	1.07
(1,8)	1:10:A:ASP:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	8	1.07
(1,2069)	1:47:O:MET:N	1:47:O:MET:CA	1:47:O:MET:C	1:48:O:ASP:N	3	1.06
(1,1976)	1:19:O:GLU:C	1:20:O:LEU:N	1:20:O:LEU:CA	1:20:O:LEU:C	4	1.06
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	5	1.06
(1,1858)	1:45:N:LEU:C	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	7	1.06
(1,1788)	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	1:47:M:MET:N	9	1.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1764)	1:18:M:ASP:N	1:18:M:ASP:CA	1:18:M:ASP:C	1:19:M:GLU:N	6	1.06
(1,1718)	1:45:M:LEU:C	1:46:M:GLN:N	1:46:M:GLN:CA	1:46:M:GLN:C	5	1.06
(1,1648)	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	1:47:L:MET:N	9	1.06
(1,1578)	1:45:L:LEU:C	1:46:L:GLN:N	1:46:L:GLN:CA	1:46:L:GLN:C	4	1.06
(1,1563)	1:26:L:LYS:C	1:27:L:LEU:N	1:27:L:LEU:CA	1:27:L:LEU:C	9	1.06
(1,1369)	1:47:J:MET:N	1:47:J:MET:CA	1:47:J:MET:C	1:48:J:ASP:N	3	1.06
(1,1267)	1:9:J:LEU:C	1:10:J:ASP:N	1:10:J:ASP:CA	1:10:J:ASP:C	1	1.06
(1,988)	1:10:H:ASP:C	1:11:H:ALA:N	1:11:H:ALA:CA	1:11:H:ALA:C	1	1.06
(1,988)	1:10:H:ASP:C	1:11:H:ALA:N	1:11:H:ALA:CA	1:11:H:ALA:C	8	1.06
(1,891)	1:58:G:SER:C	1:59:G:TYR:N	1:59:G:TYR:CA	1:59:G:TYR:C	5	1.06
(1,856)	1:19:G:GLU:C	1:20:G:LEU:N	1:20:G:LEU:CA	1:20:G:LEU:C	1	1.06
(1,723)	1:26:F:LYS:C	1:27:F:LEU:N	1:27:F:LEU:CA	1:27:F:LEU:C	2	1.06
(1,693)	1:75:E:ASP:N	1:75:E:ASP:CA	1:75:E:ASP:C	1:76:E:MET:N	6	1.06
(1,611)	1:58:E:SER:C	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	7	1.06
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	2	1.06
(1,528)	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	1:47:D:MET:N	2	1.06
(1,479)	1:70:D:MET:C	1:71:D:THR:N	1:71:D:THR:CA	1:71:D:THR:C	5	1.06
(1,428)	1:10:D:ASP:C	1:11:D:ALA:N	1:11:D:ALA:CA	1:11:D:ALA:C	8	1.06
(1,402)	1:64:C:TYR:N	1:64:C:TYR:CA	1:64:C:TYR:C	1:65:C:GLY:N	6	1.06
(1,388)	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	1:47:C:MET:N	9	1.06
(1,364)	1:18:C:ASP:N	1:18:C:ASP:CA	1:18:C:ASP:C	1:19:C:GLU:N	6	1.06
(1,354)	1:7:C:ALA:N	1:7:C:ALA:CA	1:7:C:ALA:C	1:8:C:ILE:N	6	1.06
(1,199)	1:70:B:MET:C	1:71:B:THR:N	1:71:B:THR:CA	1:71:B:THR:C	3	1.06
(1,163)	1:26:B:LYS:C	1:27:B:LEU:N	1:27:B:LEU:CA	1:27:B:LEU:C	9	1.06
(1,109)	1:47:A:MET:N	1:47:A:MET:CA	1:47:A:MET:C	1:48:A:ASP:N	8	1.06
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	4	1.06
(1,15)	1:18:A:ASP:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	10	1.06
(1,2049)	1:23:O:PHE:N	1:23:O:PHE:CA	1:23:O:PHE:C	1:24:O:LYS:N	7	1.05
(1,1929)	1:47:N:MET:N	1:47:N:MET:CA	1:47:N:MET:C	1:48:N:ASP:N	8	1.05
(1,1928)	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	1:47:N:MET:N	2	1.05
(1,1894)	1:7:N:ALA:N	1:7:N:ALA:CA	1:7:N:ALA:C	1:8:N:ILE:N	6	1.05
(1,1850)	1:37:N:GLY:C	1:38:N:ARG:N	1:38:N:ARG:CA	1:38:N:ARG:C	1	1.05
(1,1739)	1:70:M:MET:C	1:71:M:THR:N	1:71:M:THR:CA	1:71:M:THR:C	1	1.05
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	2	1.05
(1,1688)	1:10:M:ASP:C	1:11:M:ALA:N	1:11:M:ALA:CA	1:11:M:ALA:C	10	1.05
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	5	1.05
(1,1275)	1:18:J:ASP:C	1:19:J:GLU:N	1:19:J:GLU:CA	1:19:J:GLU:C	10	1.05
(1,1228)	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	1:47:I:MET:N	2	1.05
(1,1135)	1:18:I:ASP:C	1:19:I:GLU:N	1:19:I:GLU:CA	1:19:I:GLU:C	10	1.05
(1,962)	1:64:G:TYR:N	1:64:G:TYR:CA	1:64:G:TYR:C	1:65:G:GLY:N	6	1.05
(1,870)	1:37:G:GLY:C	1:38:G:ARG:N	1:38:G:ARG:CA	1:38:G:ARG:C	1	1.05
(1,784)	1:18:F:ASP:N	1:18:F:ASP:CA	1:18:F:ASP:C	1:19:F:GLU:N	6	1.05
(1,669)	1:47:E:MET:N	1:47:E:MET:CA	1:47:E:MET:C	1:48:E:ASP:N	8	1.05
(1,655)	1:29:E:THR:N	1:29:E:THR:CA	1:29:E:THR:C	1:30:E:VAL:N	8	1.05
(1,634)	1:7:E:ALA:N	1:7:E:ALA:CA	1:7:E:ALA:C	1:8:E:ILE:N	10	1.05
(1,598)	1:45:E:LEU:C	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	5	1.05
(1,583)	1:26:E:LYS:C	1:27:E:LEU:N	1:27:E:LEU:CA	1:27:E:LEU:C	9	1.05
(1,421)	1:3:D:ARG:C	1:4:D:ALA:N	1:4:D:ALA:CA	1:4:D:ALA:C	6	1.05
(1,388)	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	1:47:C:MET:N	2	1.05
(1,310)	1:37:C:GLY:C	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	1	1.05
(1,310)	1:37:C:GLY:C	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	5	1.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,303)	1:26:C:LYS:C	1:27:C:LEU:N	1:27:C:LEU:CA	1:27:C:LEU:C	2	1.05
(1,155)	1:18:B:ASP:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	10	1.05
(1,1998)	1:45:O:LEU:C	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	4	1.04
(1,1983)	1:26:O:LYS:C	1:27:O:LEU:N	1:27:O:LEU:CA	1:27:O:LEU:C	9	1.04
(1,1739)	1:70:M:MET:C	1:71:M:THR:N	1:71:M:THR:CA	1:71:M:THR:C	3	1.04
(1,1649)	1:47:L:MET:N	1:47:L:MET:CA	1:47:L:MET:C	1:48:L:ASP:N	8	1.04
(1,1423)	1:26:K:LYS:C	1:27:K:LEU:N	1:27:K:LEU:CA	1:27:K:LEU:C	9	1.04
(1,1369)	1:47:J:MET:N	1:47:J:MET:CA	1:47:J:MET:C	1:48:J:ASP:N	8	1.04
(1,1121)	1:3:I:ARG:C	1:4:I:ALA:N	1:4:I:ALA:CA	1:4:I:ALA:C	6	1.04
(1,1088)	1:46:H:GLN:N	1:46:H:GLN:CA	1:46:H:GLN:C	1:47:H:MET:N	9	1.04
(1,1039)	1:70:H:MET:C	1:71:H:THR:N	1:71:H:THR:CA	1:71:H:THR:C	5	1.04
(1,949)	1:47:G:MET:N	1:47:G:MET:CA	1:47:G:MET:C	1:48:G:ASP:N	3	1.04
(1,929)	1:23:G:PHE:N	1:23:G:PHE:CA	1:23:G:PHE:C	1:24:G:LYS:N	7	1.04
(1,715)	1:18:F:ASP:C	1:19:F:GLU:N	1:19:F:GLU:CA	1:19:F:GLU:C	10	1.04
(1,708)	1:10:F:ASP:C	1:11:F:ALA:N	1:11:F:ALA:CA	1:11:F:ALA:C	1	1.04
(1,681)	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	1:60:E:TYR:N	4	1.04
(1,568)	1:10:E:ASP:C	1:11:E:ALA:N	1:11:E:ALA:CA	1:11:E:ALA:C	10	1.04
(1,528)	1:46:D:GLN:N	1:46:D:GLN:CA	1:46:D:GLN:C	1:47:D:MET:N	9	1.04
(1,339)	1:70:C:MET:C	1:71:C:THR:N	1:71:C:THR:CA	1:71:C:THR:C	5	1.04
(1,235)	1:29:B:THR:N	1:29:B:THR:CA	1:29:B:THR:C	1:30:B:VAL:N	8	1.04
(1,170)	1:37:B:GLY:C	1:38:B:ARG:N	1:38:B:ARG:CA	1:38:B:ARG:C	1	1.04
(1,122)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:GLY:N	6	1.04
(1,109)	1:47:A:MET:N	1:47:A:MET:CA	1:47:A:MET:C	1:48:A:ASP:N	3	1.04
(1,63)	1:74:A:ARG:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	7	1.04
(1,59)	1:70:A:MET:C	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	5	1.04
(1,2068)	1:46:O:GLN:N	1:46:O:GLN:CA	1:46:O:GLN:C	1:47:O:MET:N	2	1.03
(1,2055)	1:29:O:THR:N	1:29:O:THR:CA	1:29:O:THR:C	1:30:O:VAL:N	8	1.03
(1,1835)	1:18:N:ASP:C	1:19:N:GLU:N	1:19:N:GLU:CA	1:19:N:GLU:C	10	1.03
(1,1802)	1:64:M:TYR:N	1:64:M:TYR:CA	1:64:M:TYR:C	1:65:M:GLY:N	6	1.03
(1,1570)	1:37:L:GLY:C	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	5	1.03
(1,1509)	1:47:K:MET:N	1:47:K:MET:CA	1:47:K:MET:C	1:48:K:ASP:N	8	1.03
(1,1382)	1:64:J:TYR:N	1:64:J:TYR:CA	1:64:J:TYR:C	1:65:J:GLY:N	6	1.03
(1,1368)	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	1:47:J:MET:N	9	1.03
(1,1194)	1:7:I:ALA:N	1:7:I:ALA:CA	1:7:I:ALA:C	1:8:I:ILE:N	6	1.03
(1,1179)	1:70:I:MET:C	1:71:I:THR:N	1:71:I:THR:CA	1:71:I:THR:C	5	1.03
(1,1054)	1:7:H:ALA:N	1:7:H:ALA:CA	1:7:H:ALA:C	1:8:H:ILE:N	10	1.03
(1,988)	1:10:H:ASP:C	1:11:H:ALA:N	1:11:H:ALA:CA	1:11:H:ALA:C	10	1.03
(1,611)	1:58:E:SER:C	1:59:E:TYR:N	1:59:E:TYR:CA	1:59:E:TYR:C	2	1.03
(1,586)	1:29:E:THR:C	1:30:E:VAL:N	1:30:E:VAL:CA	1:30:E:VAL:C	8	1.03
(1,529)	1:47:D:MET:N	1:47:D:MET:CA	1:47:D:MET:C	1:48:D:ASP:N	3	1.03
(1,389)	1:47:C:MET:N	1:47:C:MET:CA	1:47:C:MET:C	1:48:C:ASP:N	8	1.03
(1,296)	1:19:C:GLU:C	1:20:C:LEU:N	1:20:C:LEU:CA	1:20:C:LEU:C	4	1.03
(1,108)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:MET:N	9	1.03
(1,2082)	1:64:O:TYR:N	1:64:O:TYR:CA	1:64:O:TYR:C	1:65:O:GLY:N	6	1.02
(1,2019)	1:70:O:MET:C	1:71:O:THR:N	1:71:O:THR:CA	1:71:O:THR:C	7	1.02
(1,1928)	1:46:N:GLN:N	1:46:N:GLN:CA	1:46:N:GLN:C	1:47:N:MET:N	9	1.02
(1,1710)	1:37:M:GLY:C	1:38:M:ARG:N	1:38:M:ARG:CA	1:38:M:ARG:C	1	1.02
(1,1703)	1:26:M:LYS:C	1:27:M:LEU:N	1:27:M:LEU:CA	1:27:M:LEU:C	9	1.02
(1,1548)	1:10:L:ASP:C	1:11:L:ALA:N	1:11:L:ALA:CA	1:11:L:ALA:C	1	1.02
(1,1415)	1:18:K:ASP:C	1:19:K:GLU:N	1:19:K:GLU:CA	1:19:K:GLU:C	10	1.02
(1,1319)	1:70:J:MET:C	1:71:J:THR:N	1:71:J:THR:CA	1:71:J:THR:C	3	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1290)	1:37:J:GLY:C	1:38:J:ARG:N	1:38:J:ARG:CA	1:38:J:ARG:C	1	1.02
(1,1229)	1:47:I:MET:N	1:47:I:MET:CA	1:47:I:MET:C	1:48:I:ASP:N	3	1.02
(1,1228)	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	1:47:I:MET:N	9	1.02
(1,1150)	1:37:I:GLY:C	1:38:I:ARG:N	1:38:I:ARG:CA	1:38:I:ARG:C	4	1.02
(1,1128)	1:10:I:ASP:C	1:11:I:ALA:N	1:11:I:ALA:CA	1:11:I:ALA:C	8	1.02
(1,1089)	1:47:H:MET:N	1:47:H:MET:CA	1:47:H:MET:C	1:48:H:ASP:N	3	1.02
(1,1010)	1:37:H:GLY:C	1:38:H:ARG:N	1:38:H:ARG:CA	1:38:H:ARG:C	4	1.02
(1,948)	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	1:47:G:MET:N	9	1.02
(1,924)	1:18:G:ASP:N	1:18:G:ASP:CA	1:18:G:ASP:C	1:19:G:GLU:N	6	1.02
(1,878)	1:45:G:LEU:C	1:46:G:GLN:N	1:46:G:GLN:CA	1:46:G:GLN:C	7	1.02
(1,759)	1:70:F:MET:C	1:71:F:THR:N	1:71:F:THR:CA	1:71:F:THR:C	5	1.02
(1,668)	1:46:E:GLN:N	1:46:E:GLN:CA	1:46:E:GLN:C	1:47:E:MET:N	5	1.02
(1,310)	1:37:C:GLY:C	1:38:C:ARG:N	1:38:C:ARG:CA	1:38:C:ARG:C	4	1.02
(1,295)	1:18:C:ASP:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	10	1.02
(1,199)	1:70:B:MET:C	1:71:B:THR:N	1:71:B:THR:CA	1:71:B:THR:C	5	1.02
(1,8)	1:10:A:ASP:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	10	1.02
(1,2019)	1:70:O:MET:C	1:71:O:THR:N	1:71:O:THR:CA	1:71:O:THR:C	9	1.01
(1,1909)	1:23:N:PHE:N	1:23:N:PHE:CA	1:23:N:PHE:C	1:24:N:LYS:N	7	1.01
(1,1754)	1:7:M:ALA:N	1:7:M:ALA:CA	1:7:M:ALA:C	1:8:M:ILE:N	10	1.01
(1,1739)	1:70:M:MET:C	1:71:M:THR:N	1:71:M:THR:CA	1:71:M:THR:C	7	1.01
(1,1635)	1:29:L:THR:N	1:29:L:THR:CA	1:29:L:THR:C	1:30:L:VAL:N	8	1.01
(1,1614)	1:7:L:ALA:N	1:7:L:ALA:CA	1:7:L:ALA:C	1:8:L:ILE:N	10	1.01
(1,1570)	1:37:L:GLY:C	1:38:L:ARG:N	1:38:L:ARG:CA	1:38:L:ARG:C	2	1.01
(1,1508)	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	1:47:K:MET:N	2	1.01
(1,1438)	1:45:K:LEU:C	1:46:K:GLN:N	1:46:K:GLN:CA	1:46:K:GLN:C	7	1.01
(1,1319)	1:70:J:MET:C	1:71:J:THR:N	1:71:J:THR:CA	1:71:J:THR:C	1	1.01
(1,1268)	1:10:J:ASP:C	1:11:J:ALA:N	1:11:J:ALA:CA	1:11:J:ALA:C	10	1.01
(1,1158)	1:45:I:LEU:C	1:46:I:GLN:N	1:46:I:GLN:CA	1:46:I:GLN:C	7	1.01
(1,1102)	1:64:H:TYR:N	1:64:H:TYR:CA	1:64:H:TYR:C	1:65:H:GLY:N	6	1.01
(1,1075)	1:29:H:THR:N	1:29:H:THR:CA	1:29:H:THR:C	1:30:H:VAL:N	8	1.01
(1,1069)	1:23:H:PHE:N	1:23:H:PHE:CA	1:23:H:PHE:C	1:24:H:LYS:N	7	1.01
(1,1031)	1:58:H:SER:C	1:59:H:TYR:N	1:59:H:TYR:CA	1:59:H:TYR:C	7	1.01
(1,995)	1:18:H:ASP:C	1:19:H:GLU:N	1:19:H:GLU:CA	1:19:H:GLU:C	10	1.01
(1,935)	1:29:G:THR:N	1:29:G:THR:CA	1:29:G:THR:C	1:30:G:VAL:N	8	1.01
(1,708)	1:10:F:ASP:C	1:11:F:ALA:N	1:11:F:ALA:CA	1:11:F:ALA:C	10	1.01
(1,701)	1:3:F:ARG:C	1:4:F:ALA:N	1:4:F:ALA:CA	1:4:F:ALA:C	6	1.01
(1,443)	1:26:D:LYS:C	1:27:D:LEU:N	1:27:D:LEU:CA	1:27:D:LEU:C	9	1.01
(1,436)	1:19:D:GLU:C	1:20:D:LEU:N	1:20:D:LEU:CA	1:20:D:LEU:C	4	1.01
(1,435)	1:18:D:ASP:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	10	1.01
(1,318)	1:45:C:LEU:C	1:46:C:GLN:N	1:46:C:GLN:CA	1:46:C:GLN:C	5	1.01
(1,287)	1:9:C:LEU:C	1:10:C:ASP:N	1:10:C:ASP:CA	1:10:C:ASP:C	1	1.01
(1,249)	1:47:B:MET:N	1:47:B:MET:CA	1:47:B:MET:C	1:48:B:ASP:N	3	1.01
(1,249)	1:47:B:MET:N	1:47:B:MET:CA	1:47:B:MET:C	1:48:B:ASP:N	8	1.01
(1,59)	1:70:A:MET:C	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	3	1.01
(1,38)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	5	1.01
(1,1789)	1:47:M:MET:N	1:47:M:MET:CA	1:47:M:MET:C	1:48:M:ASP:N	8	1.0
(1,1629)	1:23:L:PHE:N	1:23:L:PHE:CA	1:23:L:PHE:C	1:24:L:LYS:N	7	1.0
(1,1547)	1:9:L:LEU:C	1:10:L:ASP:N	1:10:L:ASP:CA	1:10:L:ASP:C	1	1.0
(1,1522)	1:64:K:TYR:N	1:64:K:TYR:CA	1:64:K:TYR:C	1:65:K:GLY:N	6	1.0
(1,1495)	1:29:K:THR:N	1:29:K:THR:CA	1:29:K:THR:C	1:30:K:VAL:N	8	1.0
(1,1298)	1:45:J:LEU:C	1:46:J:GLN:N	1:46:J:GLN:CA	1:46:J:GLN:C	5	1.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,987)	1:9:H:LEU:C	1:10:H:ASP:N	1:10:H:ASP:CA	1:10:H:ASP:C	1	1.0
(1,808)	1:46:F:GLN:N	1:46:F:GLN:CA	1:46:F:GLN:C	1:47:F:MET:N	9	1.0
(1,759)	1:70:F:MET:C	1:71:F:THR:N	1:71:F:THR:CA	1:71:F:THR:C	7	1.0
(1,542)	1:64:D:TYR:N	1:64:D:TYR:CA	1:64:D:TYR:C	1:65:D:GLY:N	6	1.0
(1,339)	1:70:C:MET:C	1:71:C:THR:N	1:71:C:THR:CA	1:71:C:THR:C	3	1.0
(1,331)	1:58:C:SER:C	1:59:C:TYR:N	1:59:C:TYR:CA	1:59:C:TYR:C	7	1.0
(1,262)	1:64:B:TYR:N	1:64:B:TYR:CA	1:64:B:TYR:C	1:65:B:GLY:N	6	1.0
(1,191)	1:58:B:SER:C	1:59:B:TYR:N	1:59:B:TYR:CA	1:59:B:TYR:C	7	1.0
(1,74)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	10	1.0
(1,16)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	4	1.0
(1,1)	1:3:A:ARG:C	1:4:A:ALA:N	1:4:A:ALA:CA	1:4:A:ALA:C	6	1.0