



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:01 PM UTC

PDB ID : 2M3B / pdb_00002m3b
BMRB ID : 18952
Title : Serine 16 phosphorylated phospholamban pentamer, Hybrid solution and solid-state NMR structural ensemble
Authors : Vostrikov, V.V.; Verardi, R.; Veglia, G.
Deposited on : 2013-01-15

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

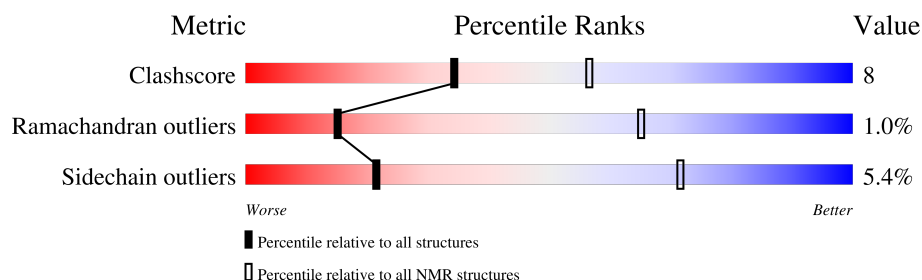
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 2%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	52	
1	B	52	
1	C	52	
1	D	52	
1	E	52	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:14 (10)	0.08	10
2	A:31-A:46, B:31-B:46, C:31-C:47, D:31-D:47, E:31-E:47 (83)	0.35	11
3	B:5-B:14 (10)	0.09	10
4	C:5-C:14 (10)	0.09	10
5	D:5-D:14 (10)	0.08	10
6	E:5-E:14 (10)	0.08	10

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4470 atoms, of which 2335 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cardiac phospholamban.

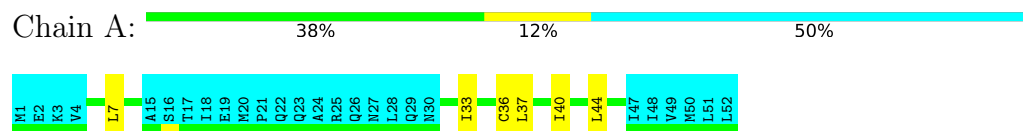
Mol	Chain	Residues	Atoms								Trace
1	A	52	Total	C	H	N	O	P	S		0
			894	274	467	73	73	1	6		
1	B	52	Total	C	H	N	O	P	S		0
			894	274	467	73	73	1	6		
1	C	52	Total	C	H	N	O	P	S		0
			894	274	467	73	73	1	6		
1	D	52	Total	C	H	N	O	P	S		0
			894	274	467	73	73	1	6		
1	E	52	Total	C	H	N	O	P	S		0
			894	274	467	73	73	1	6		

4 Residue-property plots

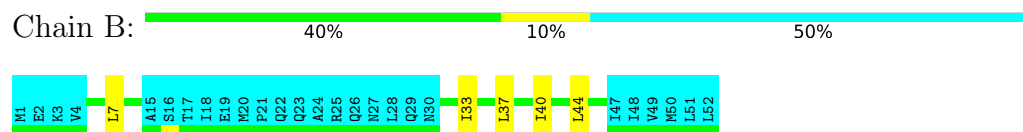
4.1 Average score per residue in the NMR ensemble

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

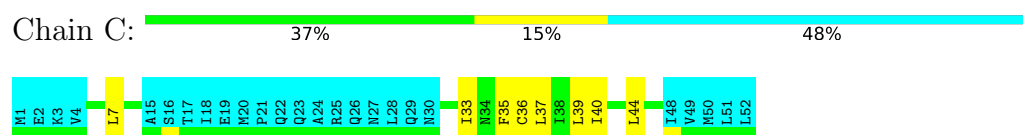
- Molecule 1: Cardiac phospholamban



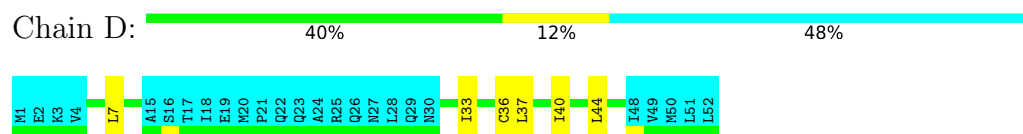
- Molecule 1: Cardiac phospholamban



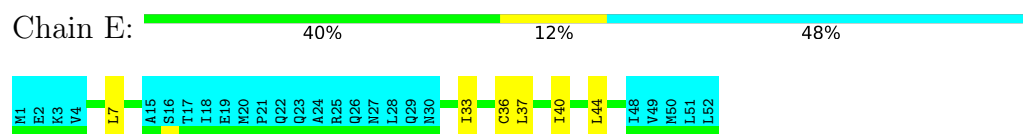
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Cardiac phospholamban

Chain A:  42% 50%



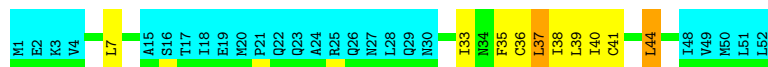
- Molecule 1: Cardiac phospholamban

Chain B:  40% 6% 50%



- Molecule 1: Cardiac phospholamban

Chain C:  33% 15% 48%

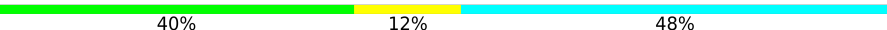


- Molecule 1: Cardiac phospholamban

Chain D:  44% 6% 48%



- Molecule 1: Cardiac phospholamban

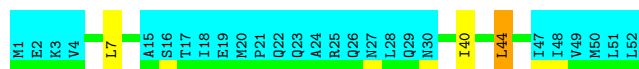
Chain E:  40% 12% 48%



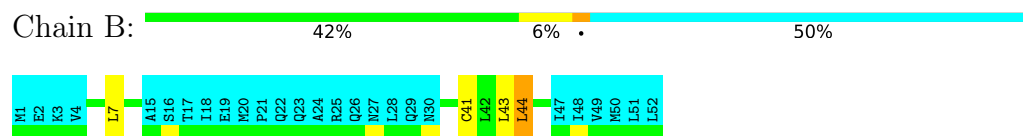
4.2.2 Score per residue for model 2

- Molecule 1: Cardiac phospholamban

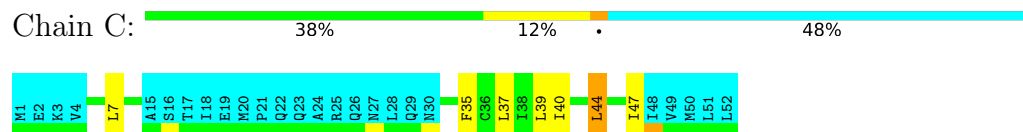
Chain A:  44% 50%



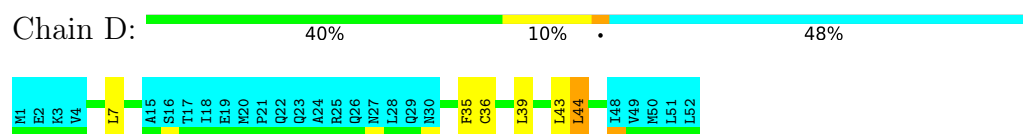
- Molecule 1: Cardiac phospholamban



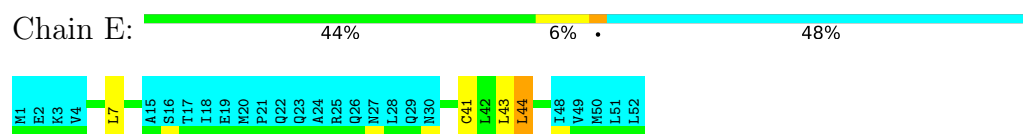
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

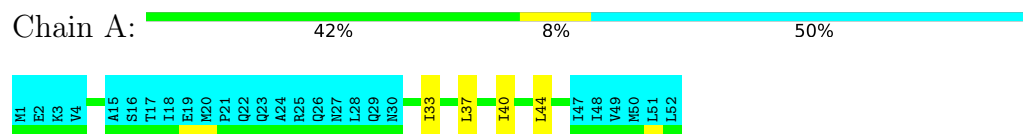


- Molecule 1: Cardiac phospholamban

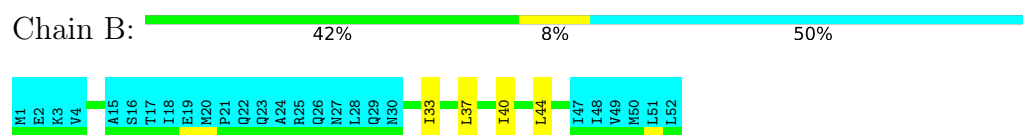


4.2.3 Score per residue for model 3

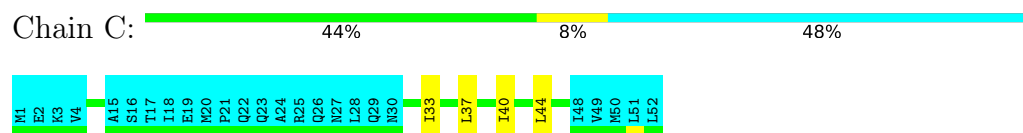
- Molecule 1: Cardiac phospholamban



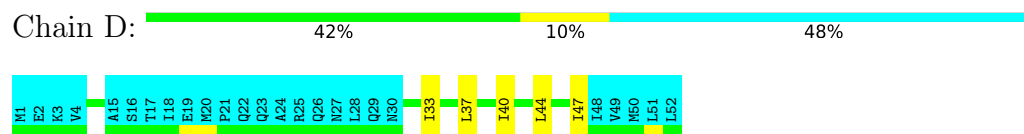
- Molecule 1: Cardiac phospholamban



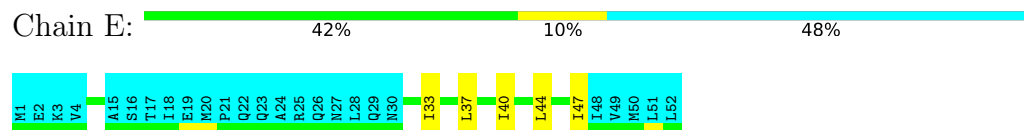
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

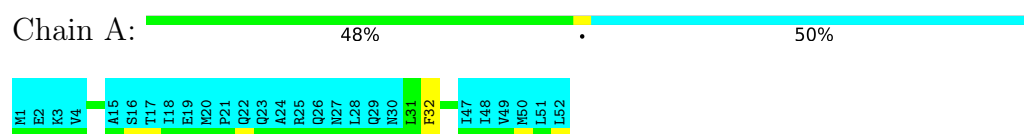


- Molecule 1: Cardiac phospholamban

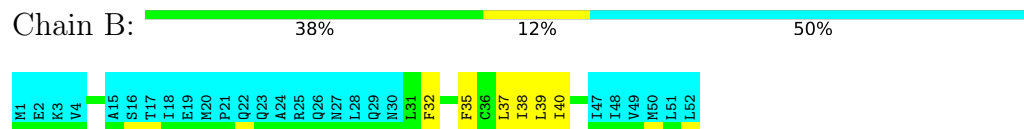


4.2.4 Score per residue for model 4

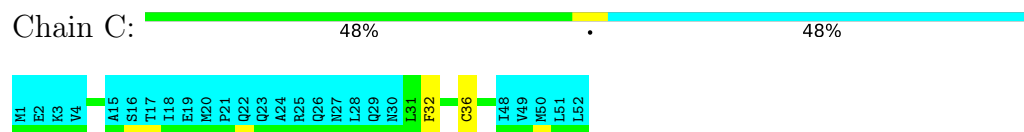
- Molecule 1: Cardiac phospholamban



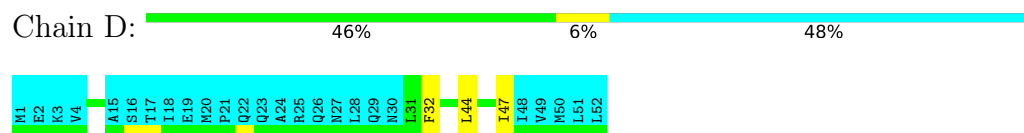
- Molecule 1: Cardiac phospholamban



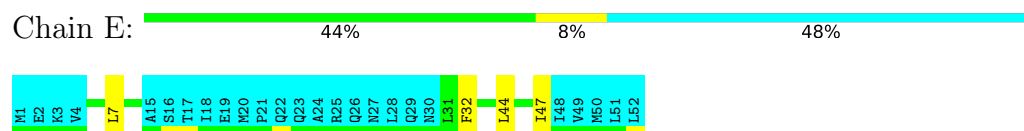
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

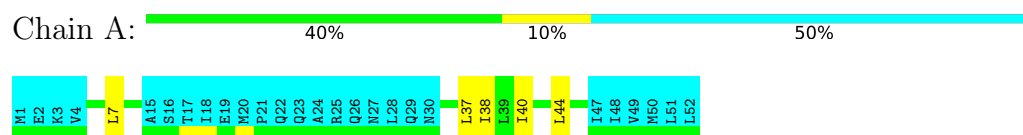


- Molecule 1: Cardiac phospholamban

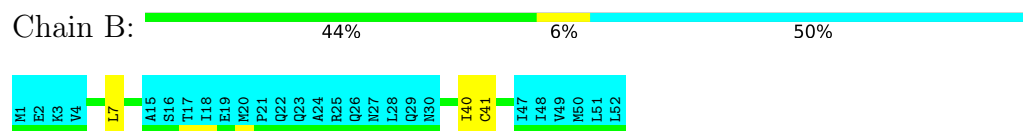


4.2.5 Score per residue for model 5

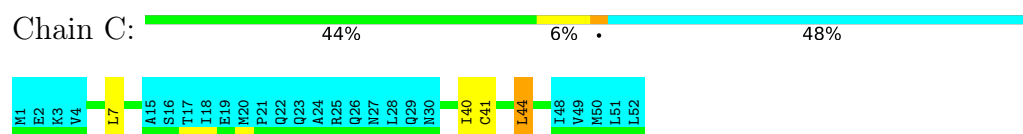
- Molecule 1: Cardiac phospholamban



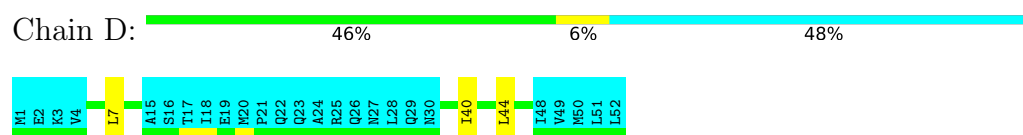
- Molecule 1: Cardiac phospholamban



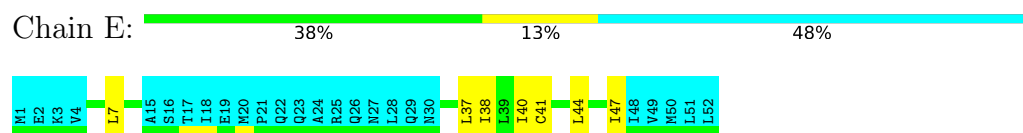
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

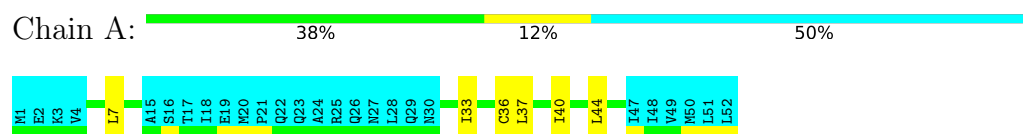


- Molecule 1: Cardiac phospholamban

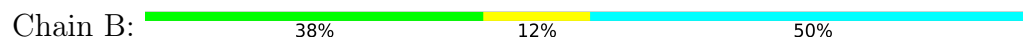


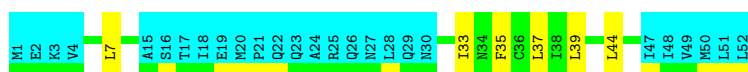
4.2.6 Score per residue for model 6

- Molecule 1: Cardiac phospholamban

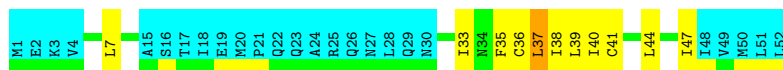
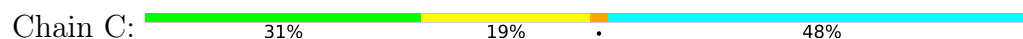


- Molecule 1: Cardiac phospholamban

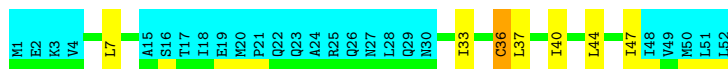
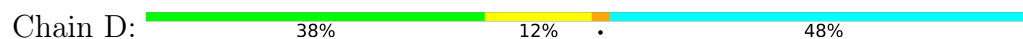




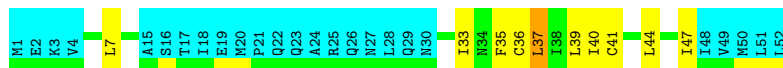
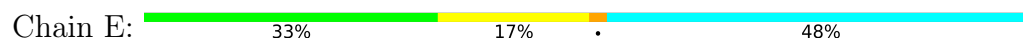
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

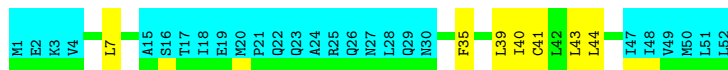
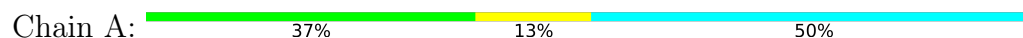


- Molecule 1: Cardiac phospholamban

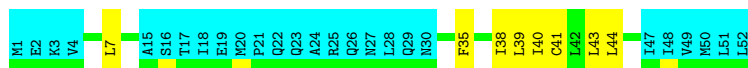
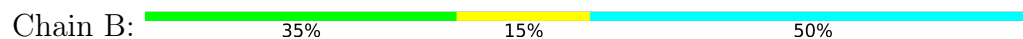


4.2.7 Score per residue for model 7

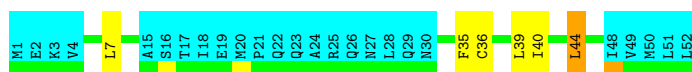
- Molecule 1: Cardiac phospholamban



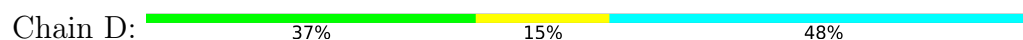
- Molecule 1: Cardiac phospholamban

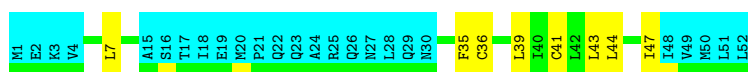


- Molecule 1: Cardiac phospholamban

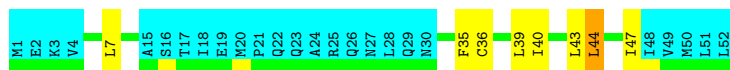
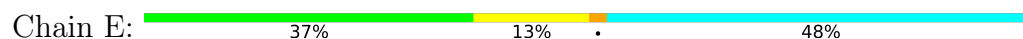


- Molecule 1: Cardiac phospholamban



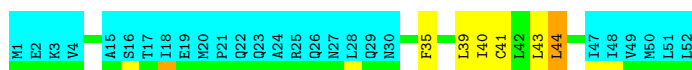
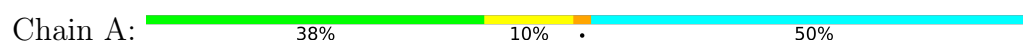


- Molecule 1: Cardiac phospholamban

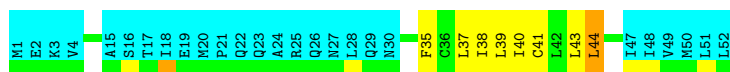
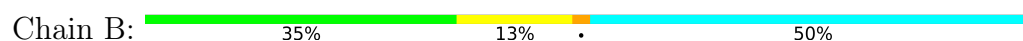


4.2.8 Score per residue for model 8

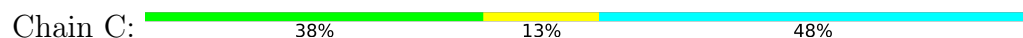
- Molecule 1: Cardiac phospholamban



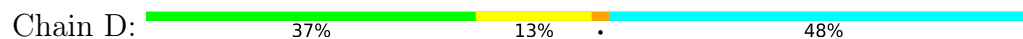
- Molecule 1: Cardiac phospholamban



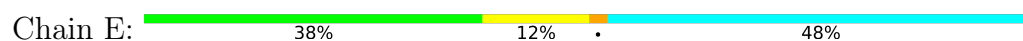
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

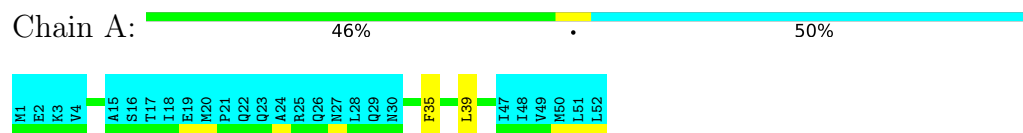


- Molecule 1: Cardiac phospholamban

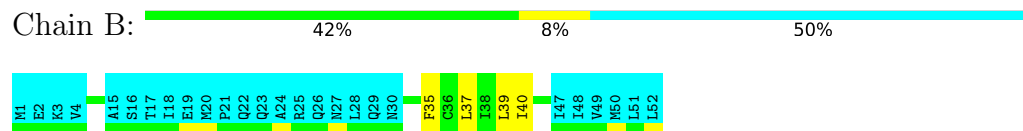


4.2.9 Score per residue for model 9

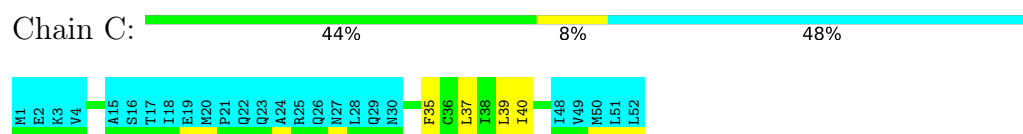
- Molecule 1: Cardiac phospholamban



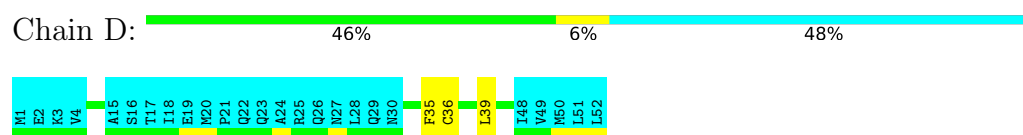
- Molecule 1: Cardiac phospholamban



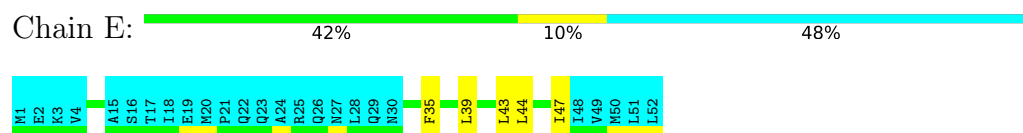
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

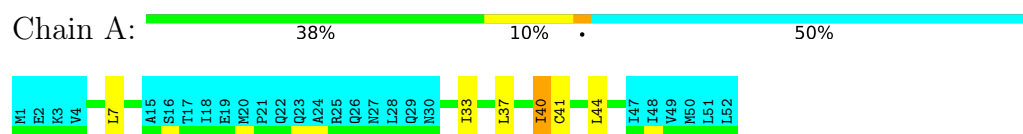


- Molecule 1: Cardiac phospholamban



4.2.10 Score per residue for model 10

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.11 Score per residue for model 11 (medoid)

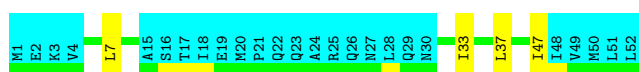
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

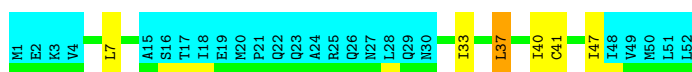


- Molecule 1: Cardiac phospholamban

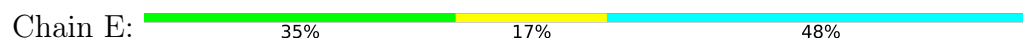


- Molecule 1: Cardiac phospholamban



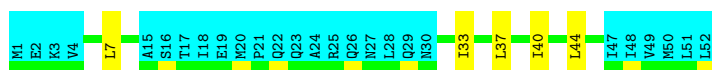


- Molecule 1: Cardiac phospholamban

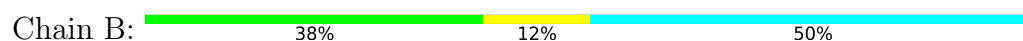


4.2.12 Score per residue for model 12

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



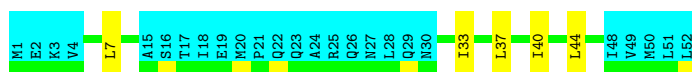
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

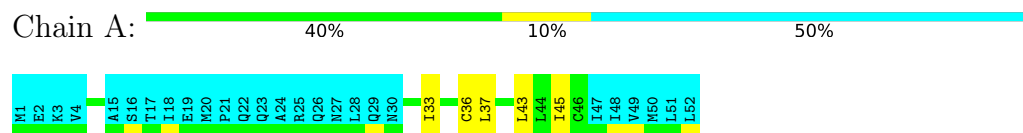


- Molecule 1: Cardiac phospholamban

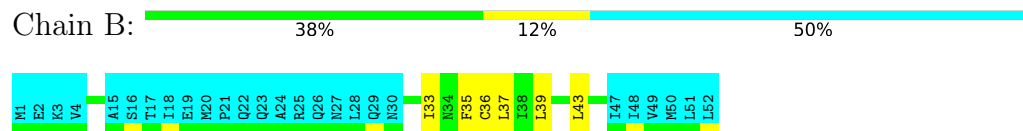


4.2.13 Score per residue for model 13

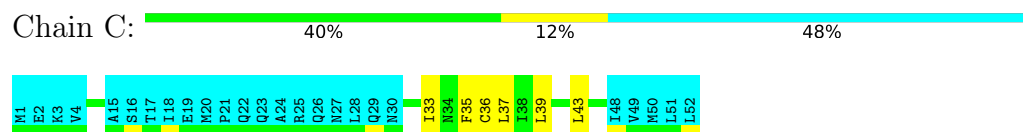
- Molecule 1: Cardiac phospholamban



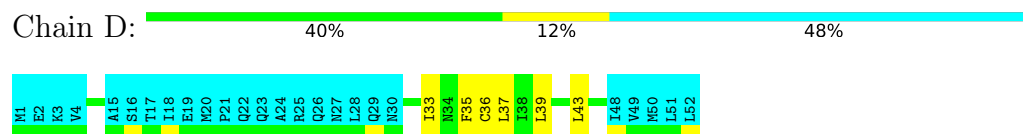
- Molecule 1: Cardiac phospholamban



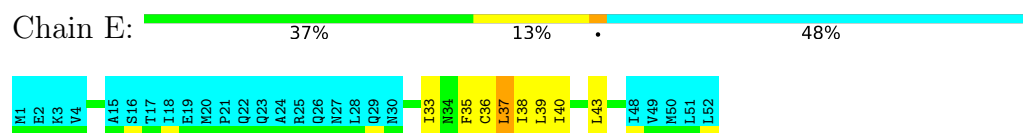
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

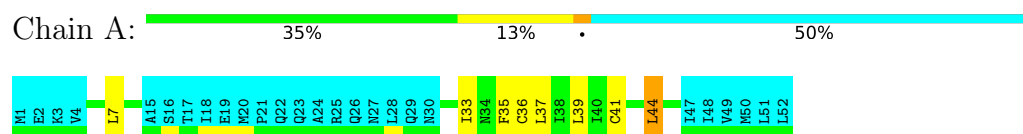


- Molecule 1: Cardiac phospholamban

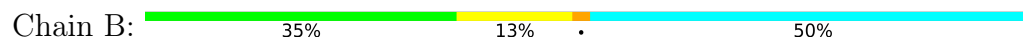


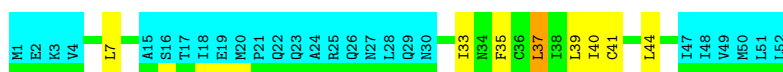
4.2.14 Score per residue for model 14

- Molecule 1: Cardiac phospholamban

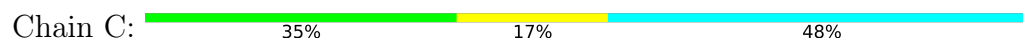


- Molecule 1: Cardiac phospholamban

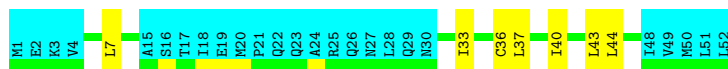
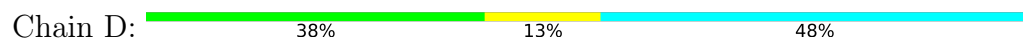




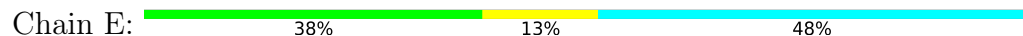
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

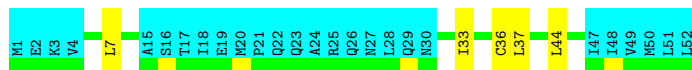


- Molecule 1: Cardiac phospholamban

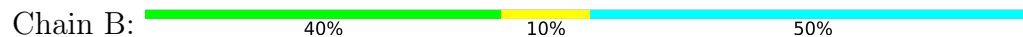


4.2.15 Score per residue for model 15

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



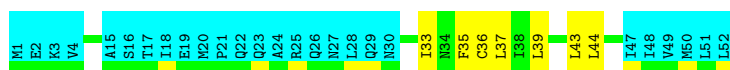
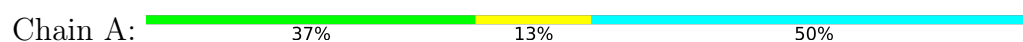


- Molecule 1: Cardiac phospholamban

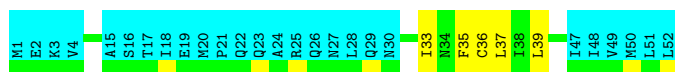


4.2.16 Score per residue for model 16

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



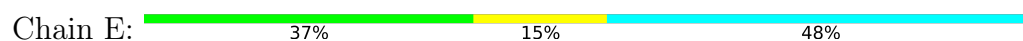
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

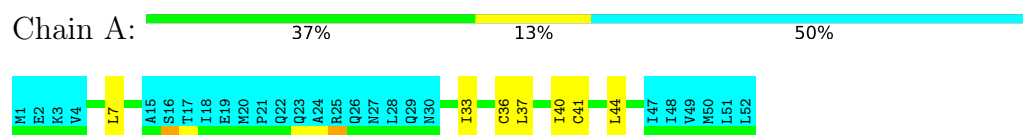


- Molecule 1: Cardiac phospholamban

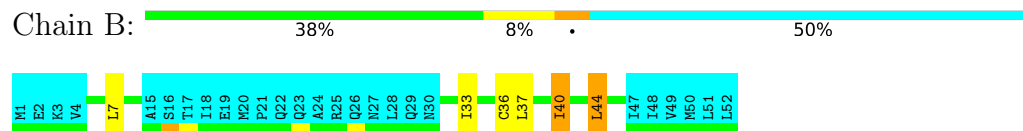


4.2.17 Score per residue for model 17

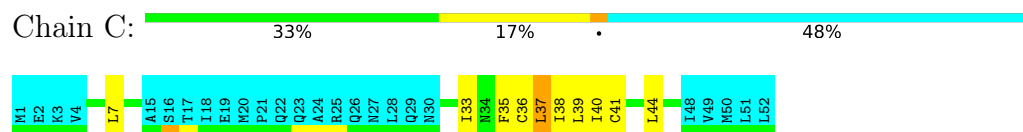
- Molecule 1: Cardiac phospholamban



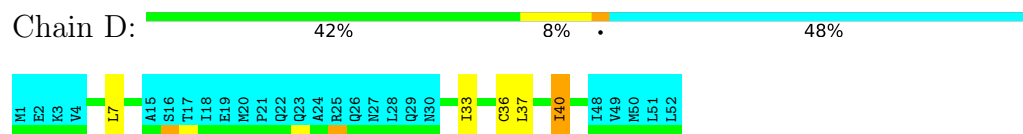
- Molecule 1: Cardiac phospholamban



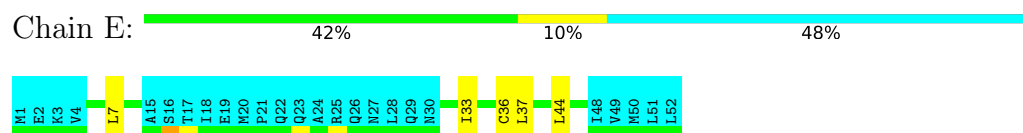
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

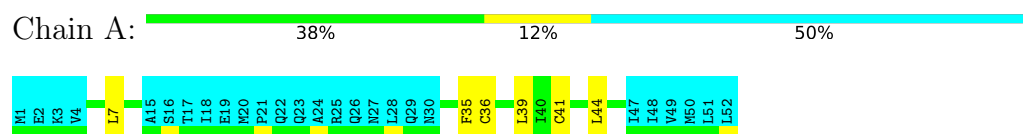


- Molecule 1: Cardiac phospholamban



4.2.18 Score per residue for model 18

- Molecule 1: Cardiac phospholamban

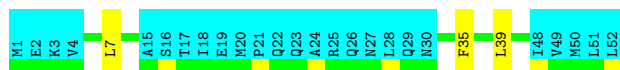


- Molecule 1: Cardiac phospholamban





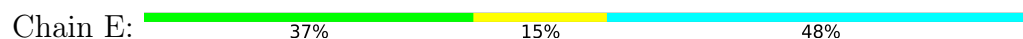
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

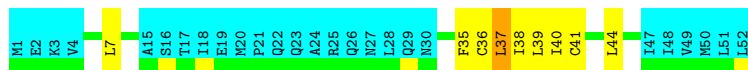
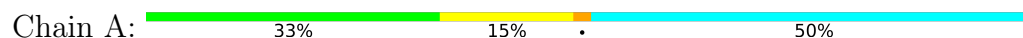


- Molecule 1: Cardiac phospholamban

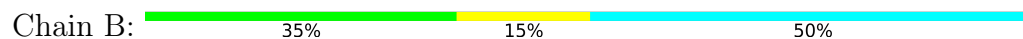


4.2.19 Score per residue for model 19

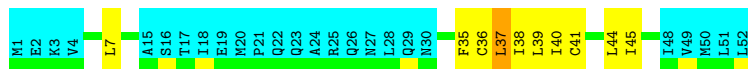
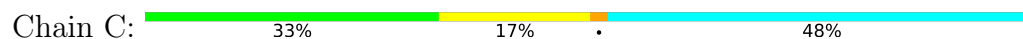
- Molecule 1: Cardiac phospholamban



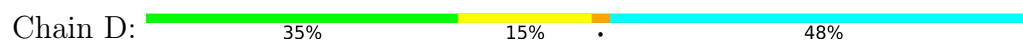
- Molecule 1: Cardiac phospholamban

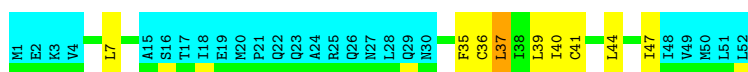


- Molecule 1: Cardiac phospholamban

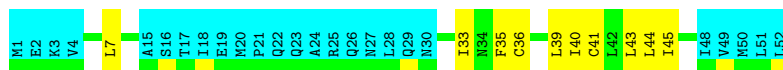
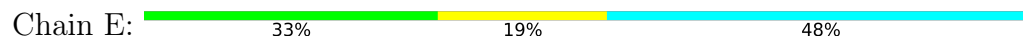


- Molecule 1: Cardiac phospholamban



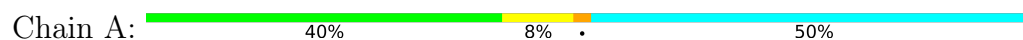


- Molecule 1: Cardiac phospholamban



4.2.20 Score per residue for model 20

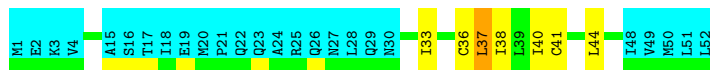
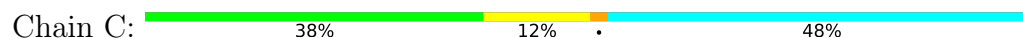
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



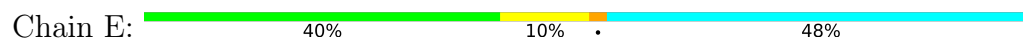
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	2.33
X-PLOR 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	98
Number of shifts mapped to atoms	98
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	2%

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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	216	244	244	6±3
1	B	216	244	244	6±2
1	C	224	255	255	6±3
1	D	224	255	255	6±3
1	E	224	255	255	7±3
All	All	22080	25060	25060	383

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:41:CYS:HG	1:D:36:CYS:HG	0.79	0.87	6	1
1:A:41:CYS:SG	1:B:40:ILE:HD11	0.72	2.24	18	7
1:B:41:CYS:SG	1:C:40:ILE:HD11	0.70	2.26	19	5
1:C:41:CYS:SG	1:D:40:ILE:HD11	0.70	2.27	19	7
1:D:41:CYS:SG	1:E:40:ILE:HD11	0.69	2.27	19	4
1:A:40:ILE:HD11	1:E:41:CYS:SG	0.68	2.28	11	7
1:A:37:LEU:CD1	1:B:33:ILE:HG23	0.65	2.21	10	11
1:B:37:LEU:CD1	1:C:33:ILE:HG23	0.64	2.21	10	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:37:LEU:CD1	1:E:33:ILE:HG23	0.64	2.22	10	13
1:A:33:ILE:HG23	1:E:37:LEU:CD1	0.63	2.23	10	11
1:C:37:LEU:CD1	1:D:33:ILE:HG23	0.63	2.22	10	11
1:A:40:ILE:HD12	1:E:44:LEU:CD1	0.59	2.27	11	4
1:C:44:LEU:HD23	1:D:43:LEU:HD23	0.58	1.73	2	1
1:A:37:LEU:HD11	1:B:33:ILE:HG23	0.58	1.74	10	6
1:C:44:LEU:CD1	1:D:40:ILE:HD12	0.58	2.27	20	4
1:B:37:LEU:HD11	1:C:33:ILE:HG23	0.58	1.74	10	8
1:A:44:LEU:HD23	1:B:43:LEU:HD23	0.57	1.75	2	1
1:D:44:LEU:HD23	1:E:43:LEU:HD23	0.57	1.75	2	1
1:D:37:LEU:HD11	1:E:33:ILE:HG23	0.57	1.77	10	9
1:C:37:LEU:HD11	1:D:33:ILE:HG23	0.56	1.76	10	7
1:A:33:ILE:HG23	1:E:37:LEU:HD11	0.56	1.77	10	7
1:D:44:LEU:CD1	1:E:40:ILE:HD12	0.56	2.31	19	3
1:A:44:LEU:CD1	1:B:40:ILE:HD12	0.56	2.30	18	3
1:B:44:LEU:CD1	1:C:40:ILE:HD12	0.55	2.31	19	1
1:A:44:LEU:CD1	1:B:40:ILE:HD13	0.54	2.33	1	2
1:A:44:LEU:HD11	1:B:40:ILE:HG23	0.54	1.77	3	4
1:D:44:LEU:HD11	1:E:40:ILE:HG23	0.53	1.79	3	4
1:B:41:CYS:HA	1:C:40:ILE:HD11	0.53	1.81	8	2
1:C:40:ILE:HG22	1:C:44:LEU:CD1	0.52	2.34	5	1
1:B:44:LEU:HD13	1:C:40:ILE:HD12	0.52	1.81	8	2
1:B:44:LEU:HD11	1:C:40:ILE:HG23	0.52	1.79	3	2
1:C:44:LEU:CD1	1:D:40:ILE:HD13	0.52	2.34	1	1
1:A:40:ILE:HG23	1:E:44:LEU:CD1	0.52	2.35	5	2
1:E:44:LEU:HA	1:E:47:ILE:HD12	0.52	1.82	6	8
1:D:44:LEU:HA	1:D:47:ILE:HD12	0.51	1.82	6	6
1:B:40:ILE:HG22	1:B:44:LEU:CD1	0.49	2.37	18	1
1:A:40:ILE:HD12	1:E:44:LEU:HD12	0.49	1.85	11	3
1:D:33:ILE:HG22	1:D:37:LEU:CD1	0.49	2.37	3	8
1:A:40:ILE:HG23	1:E:44:LEU:HD11	0.49	1.83	3	2
1:B:33:ILE:HG22	1:B:37:LEU:CD1	0.49	2.38	10	8
1:D:44:LEU:HB3	1:E:43:LEU:HD23	0.49	1.83	19	2
1:A:33:ILE:HG22	1:A:37:LEU:CD1	0.48	2.38	10	8
1:C:44:LEU:HD11	1:D:40:ILE:HG23	0.48	1.84	3	3
1:E:33:ILE:HG22	1:E:37:LEU:CD1	0.47	2.39	10	8
1:A:41:CYS:HA	1:B:40:ILE:HD11	0.47	1.86	8	1
1:D:35:PHE:CE2	1:D:39:LEU:HD11	0.47	2.45	16	5
1:C:33:ILE:HG22	1:C:37:LEU:CD1	0.47	2.40	10	7
1:E:37:LEU:O	1:E:40:ILE:N	0.47	2.48	5	7
1:A:40:ILE:HG23	1:E:44:LEU:HD13	0.47	1.87	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ILE:CD1	1:E:44:LEU:HD13	0.47	2.39	7	1
1:E:35:PHE:CE2	1:E:39:LEU:HD11	0.47	2.45	16	6
1:B:44:LEU:CD1	1:C:40:ILE:HG23	0.47	2.39	19	3
1:B:44:LEU:HD13	1:C:40:ILE:HG23	0.47	1.85	1	3
1:E:35:PHE:CZ	1:E:39:LEU:HD11	0.47	2.45	13	8
1:D:44:LEU:CD1	1:E:40:ILE:HG23	0.46	2.40	5	4
1:D:44:LEU:HD12	1:E:40:ILE:HD12	0.46	1.88	19	1
1:A:37:LEU:O	1:A:40:ILE:N	0.46	2.47	5	2
1:C:44:LEU:HA	1:C:47:ILE:HD12	0.46	1.86	6	1
1:B:35:PHE:CZ	1:B:39:LEU:HD11	0.46	2.46	14	5
1:B:35:PHE:CE2	1:B:39:LEU:HD11	0.46	2.45	9	8
1:C:44:LEU:HD12	1:D:40:ILE:HD12	0.46	1.88	19	2
1:A:40:ILE:HD12	1:E:44:LEU:HD13	0.46	1.86	8	2
1:B:37:LEU:O	1:B:40:ILE:N	0.46	2.48	19	5
1:B:44:LEU:HD12	1:C:40:ILE:HD12	0.46	1.87	19	1
1:D:33:ILE:HG22	1:D:37:LEU:HD11	0.45	1.88	10	2
1:C:35:PHE:CE2	1:C:39:LEU:HD11	0.45	2.46	16	5
1:C:44:LEU:HB3	1:D:43:LEU:HD23	0.45	1.88	7	2
1:A:7:LEU:C	1:A:7:LEU:HD13	0.45	2.36	1	3
1:D:44:LEU:HD13	1:E:40:ILE:HG23	0.45	1.89	6	4
1:D:35:PHE:CZ	1:D:39:LEU:HD11	0.45	2.47	9	6
1:A:44:LEU:CD1	1:B:40:ILE:HG23	0.45	2.42	19	3
1:C:44:LEU:HD13	1:D:40:ILE:HD12	0.45	1.89	5	1
1:B:7:LEU:HD13	1:B:7:LEU:C	0.45	2.37	17	3
1:C:35:PHE:CZ	1:C:39:LEU:HD11	0.45	2.47	14	11
1:A:44:LEU:HD13	1:B:40:ILE:HD12	0.45	1.89	8	1
1:C:7:LEU:C	1:C:7:LEU:HD13	0.44	2.37	1	3
1:E:7:LEU:C	1:E:7:LEU:HD13	0.44	2.37	17	3
1:C:41:CYS:HA	1:D:40:ILE:HD11	0.44	1.89	8	1
1:D:7:LEU:C	1:D:7:LEU:HD13	0.44	2.38	17	3
1:A:35:PHE:CE2	1:A:39:LEU:HD11	0.44	2.48	16	5
1:E:33:ILE:HG22	1:E:37:LEU:HD11	0.44	1.90	10	1
1:C:44:LEU:CD1	1:D:40:ILE:HG23	0.44	2.42	19	3
1:A:40:ILE:HD11	1:E:41:CYS:HA	0.43	1.90	8	2
1:C:33:ILE:HG22	1:C:37:LEU:HD11	0.43	1.90	10	1
1:C:44:LEU:HD13	1:D:40:ILE:HG23	0.43	1.88	14	2
1:D:44:LEU:HD13	1:E:40:ILE:HD12	0.43	1.90	8	1
1:B:33:ILE:HG22	1:B:37:LEU:HD11	0.43	1.91	10	2
1:D:37:LEU:O	1:D:40:ILE:N	0.43	2.51	11	2
1:C:37:LEU:O	1:C:40:ILE:N	0.43	2.51	19	6
1:A:44:LEU:HB3	1:B:43:LEU:HD23	0.43	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:PHE:CZ	1:A:39:LEU:HD11	0.43	2.49	9	5
1:A:40:ILE:HD13	1:E:44:LEU:CD1	0.42	2.45	1	1
1:D:41:CYS:HA	1:E:40:ILE:HD11	0.42	1.91	8	1
1:A:44:LEU:HD12	1:B:40:ILE:HD13	0.42	1.92	1	1
1:A:33:ILE:HG22	1:A:37:LEU:HD11	0.41	1.91	10	1
1:E:40:ILE:HG22	1:E:44:LEU:CD1	0.41	2.46	5	1
1:E:7:LEU:O	1:E:7:LEU:HD13	0.40	2.17	4	1
1:A:44:LEU:HD13	1:B:40:ILE:HG23	0.40	1.94	14	1

6.3 Torsion angles

6.3.1 Protein backbone

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	26/52 (50%)	26±1 (99±2%)	0±0 (0±1%)	0±0 (1±2%)	23	72
1	B	26/52 (50%)	25±1 (98±3%)	0±1 (2±2%)	0±0 (1±2%)	15	65
1	C	27/52 (52%)	26±1 (97±4%)	0±1 (1±3%)	0±1 (2±3%)	8	51
1	D	27/52 (52%)	27±1 (99±2%)	0±0 (1±1%)	0±0 (0±1%)	31	76
1	E	27/52 (52%)	26±1 (96±4%)	1±1 (2±3%)	0±1 (1±2%)	14	63
All	All	2660/5200 (51%)	2600 (98%)	34 (1%)	26 (1%)	15	65

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	37	LEU	5
1	C	38	ILE	5
1	B	38	ILE	4
1	E	38	ILE	3
1	E	37	LEU	3
1	A	38	ILE	2
1	D	37	LEU	2
1	B	37	LEU	1
1	A	37	LEU	1

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	25/48 (52%)	23±1 (94±4%)	2±1 (6±4%)	18	67
1	B	25/48 (52%)	24±1 (95±3%)	1±1 (5±3%)	25	76
1	C	26/48 (54%)	25±1 (94±3%)	1±1 (6±3%)	21	70
1	D	26/48 (54%)	25±1 (95±3%)	1±1 (5±3%)	22	72
1	E	26/48 (54%)	25±1 (95±3%)	1±1 (5±3%)	21	71
All	All	2560/4800 (53%)	2421 (95%)	139 (5%)	21	71

All 21 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	C	36	CYS	13
1	A	36	CYS	11
1	E	36	CYS	11
1	D	36	CYS	11
1	A	7	LEU	10
1	B	7	LEU	10
1	C	7	LEU	10
1	D	7	LEU	10
1	E	7	LEU	10
1	A	44	LEU	6
1	B	44	LEU	6
1	C	44	LEU	6
1	A	40	ILE	4
1	E	44	LEU	4
1	B	36	CYS	4
1	B	40	ILE	3
1	D	44	LEU	3
1	E	43	LEU	3
1	D	40	ILE	2
1	A	43	LEU	1
1	D	43	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	SEP	B	16	1	8,9,10	1.38±0.26	1±0 (7±6%)
1	SEP	D	16	1	8,9,10	1.38±0.27	1±0 (7±6%)
1	SEP	C	16	1	8,9,10	1.38±0.27	1±0 (7±6%)
1	SEP	E	16	1	8,9,10	1.38±0.26	1±0 (7±6%)
1	SEP	A	16	1	8,9,10	1.38±0.27	1±0 (7±6%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	SEP	B	16	1	7,12,14	1.12±0.19	0±0 (6±7%)
1	SEP	D	16	1	7,12,14	1.10±0.18	0±0 (7±7%)
1	SEP	C	16	1	7,12,14	1.11±0.19	0±0 (7±7%)
1	SEP	E	16	1	7,12,14	1.11±0.19	0±0 (7±7%)
1	SEP	A	16	1	7,12,14	1.13±0.21	1±0 (7±7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	16	1	-	0±0,6,8,10	-
1	SEP	D	16	1	-	0±0,6,8,10	-
1	SEP	A	16	1	-	0±0,6,8,10	-
1	SEP	E	16	1	-	0±0,6,8,10	-
1	SEP	C	16	1	-	0±0,6,8,10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	16	SEP	P-O1P	3.55	1.61	1.50	13	12
1	D	16	SEP	P-O1P	3.55	1.61	1.50	7	12
1	E	16	SEP	P-O1P	3.52	1.61	1.50	11	12
1	C	16	SEP	P-O1P	3.50	1.61	1.50	13	12
1	B	16	SEP	P-O1P	3.49	1.61	1.50	2	12

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	SEP	OG-CB-CA	4.03	112.07	108.14	11	11
1	E	16	SEP	OG-CB-CA	3.36	111.41	108.14	6	10
1	B	16	SEP	OG-CB-CA	3.35	111.40	108.14	11	9
1	C	16	SEP	OG-CB-CA	3.35	111.40	108.14	6	10
1	D	16	SEP	OG-CB-CA	3.29	111.34	108.14	6	10

There are no chirality outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	16	SEP	CA-CB-OG-P	2
1	B	16	SEP	CA-CB-OG-P	2
1	C	16	SEP	CA-CB-OG-P	2
1	D	16	SEP	CA-CB-OG-P	2
1	E	16	SEP	CA-CB-OG-P	2

There are no ring outliers.

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 2% for the well-defined parts and 2% 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	98
Number of shifts mapped to atoms	98
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
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	48	0.96 ± 0.26	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 2%, i.e. 52 atoms were assigned a chemical shift out of a possible 2139. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	52/665 (8%)	26/266 (10%)	0/266 (0%)	26/133 (20%)
Sidechain	0/1329 (0%)	0/887 (0%)	0/387 (0%)	0/55 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/145 (0%)	0/70 (0%)	0/75 (0%)	0/0 (—%)
Overall	52/2139 (2%)	26/1223 (2%)	0/728 (0%)	26/188 (14%)

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 2%, i.e. 96 atoms were assigned a chemical shift out of a possible 3950. 0 out of 60 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	96/1265 (8%)	48/505 (10%)	0/510 (0%)	48/250 (19%)
Sidechain	0/2540 (0%)	0/1680 (0%)	0/755 (0%)	0/105 (0%)
Aromatic	0/145 (0%)	0/70 (0%)	0/75 (0%)	0/0 (—%)
Overall	96/3950 (2%)	48/2255 (2%)	0/1340 (0%)	48/355 (14%)

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.

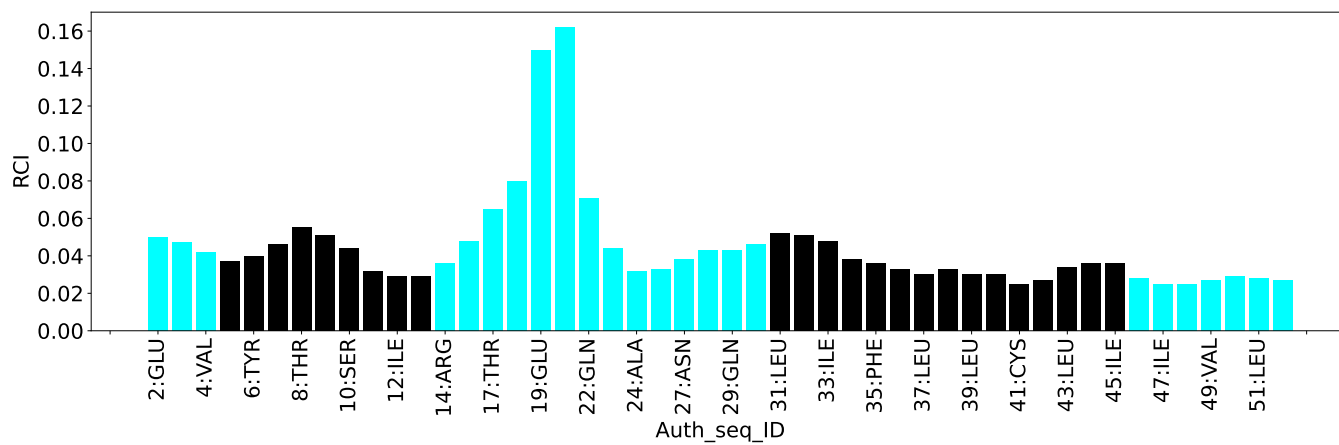
7.1.4 Statistically unusual chemical shifts [i](#)

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	2982
Intra-residue ($ i-j =0$)	875
Sequential ($ i-j =1$)	700
Medium range ($ i-j >1$ and $ i-j <5$)	495
Long range ($ i-j \geq 5$)	0
Inter-chain	912
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	430
Number of unmapped restraints	0
Number of restraints per residue	13.1
Number of long range restraints per residue ¹	0.0

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)	96.0	0.2
0.2-0.5 (Medium)	38.2	0.5
>0.5 (Large)	45.5	3.12

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	20.0	9.98
10.0-20.0 (Medium)	11.2	19.86
>20.0 (Large)	19.7	168.14

9 Distance violation analysis ⓘ

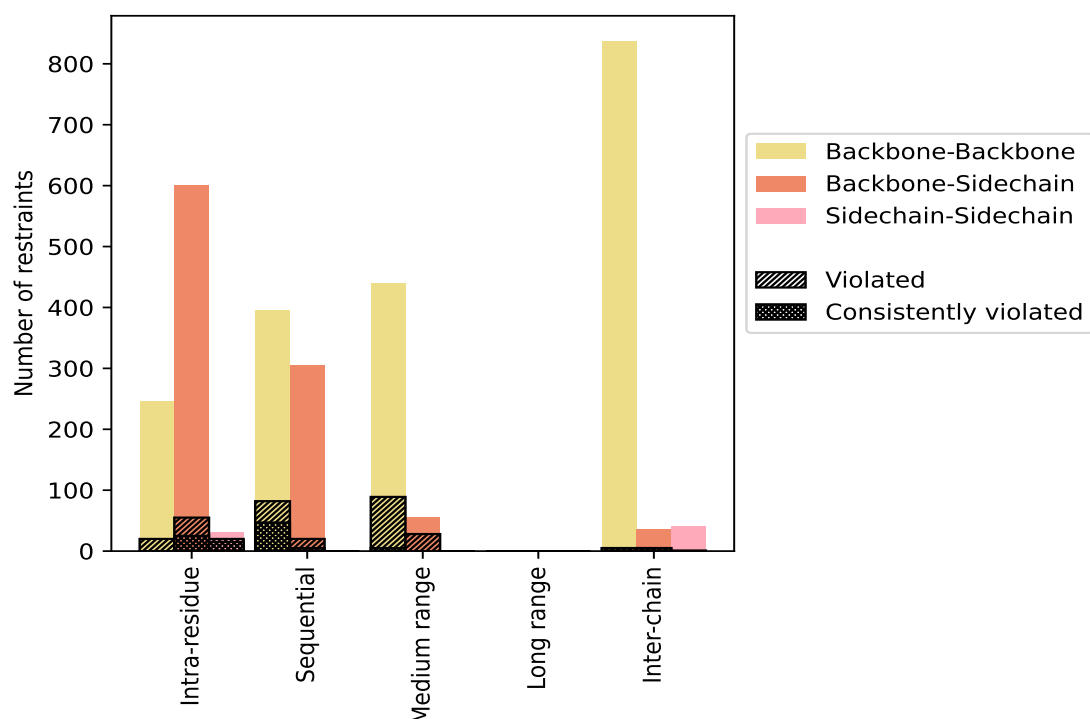
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	875	29.3	95	10.9	3.2	40	4.6	1.3
Backbone-Backbone	245	8.2	20	8.2	0.7	0	0.0	0.0
Backbone-Sidechain	600	20.1	55	9.2	1.8	25	4.2	0.8
Sidechain-Sidechain	30	1.0	20	66.7	0.7	15	50.0	0.5
Sequential ($i-j =1$)	700	23.5	102	14.6	3.4	52	7.4	1.7
Backbone-Backbone	395	13.2	82	20.8	2.7	47	11.9	1.6
Backbone-Sidechain	305	10.2	20	6.6	0.7	5	1.6	0.2
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	495	16.6	117	23.6	3.9	5	1.0	0.2
Backbone-Backbone	440	14.8	89	20.2	3.0	5	1.1	0.2
Backbone-Sidechain	55	1.8	28	50.9	0.9	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	912	30.6	11	1.2	0.4	10	1.1	0.3
Backbone-Backbone	837	28.1	5	0.6	0.2	5	0.6	0.2
Backbone-Sidechain	35	1.2	5	14.3	0.2	5	14.3	0.2
Sidechain-Sidechain	40	1.3	1	2.5	0.0	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	2982	100.0	325	10.9	10.9	107	3.6	3.6
Backbone-Backbone	1917	64.3	196	10.2	6.6	57	3.0	1.9
Backbone-Sidechain	995	33.4	108	10.9	3.6	35	3.5	1.2
Sidechain-Sidechain	70	2.3	21	30.0	0.7	15	21.4	0.5

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 disulfid 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	52	75	25	0	10	162	0.34	1.47	0.31	0.17
2	65	65	58	0	10	198	0.33	1.8	0.33	0.18
3	63	81	48	0	10	202	0.48	2.6	0.56	0.2
4	55	70	38	0	10	173	0.39	1.41	0.34	0.19
5	57	75	52	0	10	194	0.36	1.64	0.37	0.18
6	47	70	49	0	10	176	0.37	2.85	0.5	0.16
7	48	72	47	0	10	177	0.3	1.15	0.26	0.17
8	60	70	66	0	11	207	0.52	2.4	0.56	0.19
9	45	75	51	0	10	181	0.42	2.35	0.48	0.19
10	52	68	51	0	10	181	0.41	2.47	0.49	0.17

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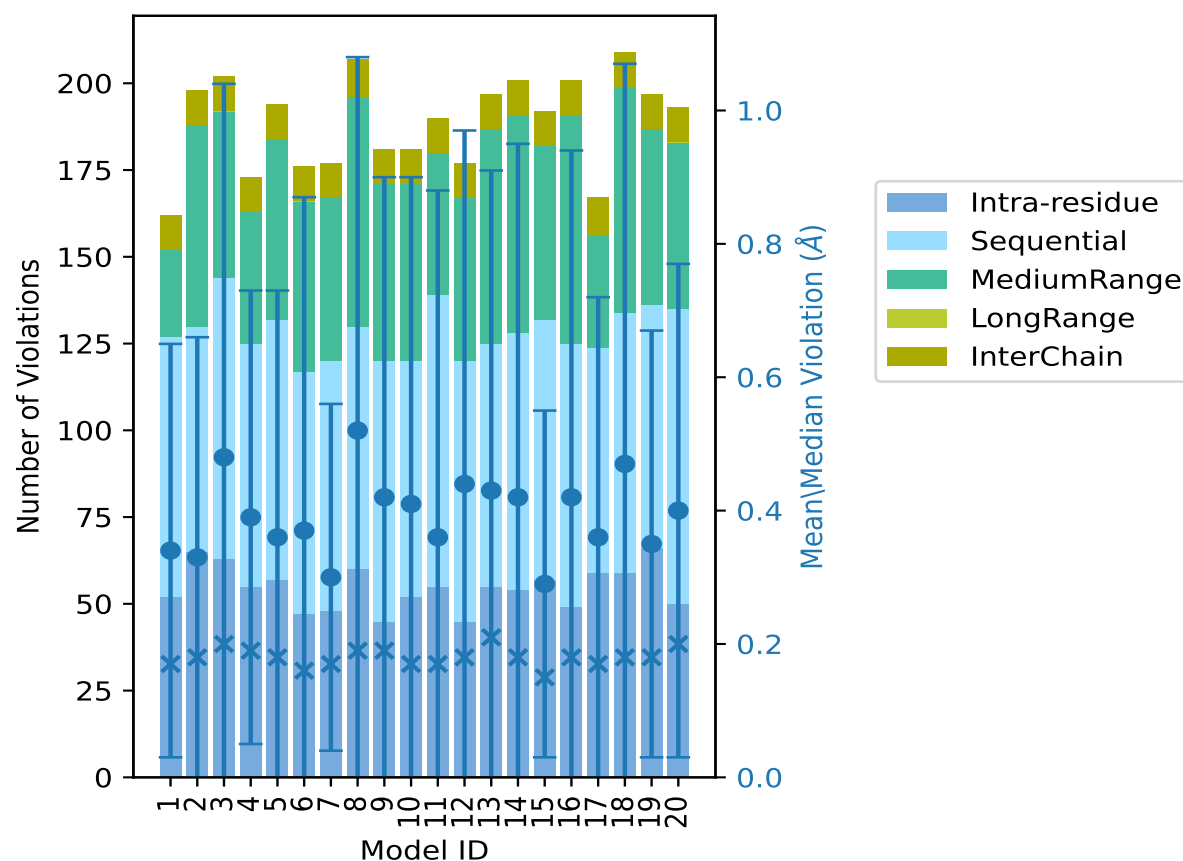
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	55	84	41	0	10	190	0.36	3.12	0.52	0.17
12	45	75	47	0	10	177	0.44	2.58	0.53	0.18
13	55	70	62	0	10	197	0.43	2.04	0.48	0.21
14	54	74	63	0	10	201	0.42	3.1	0.53	0.18
15	57	75	50	0	10	192	0.29	1.08	0.26	0.15
16	49	76	66	0	10	201	0.42	2.97	0.52	0.18
17	59	65	32	0	11	167	0.36	1.67	0.36	0.17
18	59	75	65	0	10	209	0.47	2.91	0.6	0.18
19	66	70	51	0	10	197	0.35	1.48	0.32	0.18
20	50	85	48	0	10	193	0.4	1.53	0.37	0.2

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

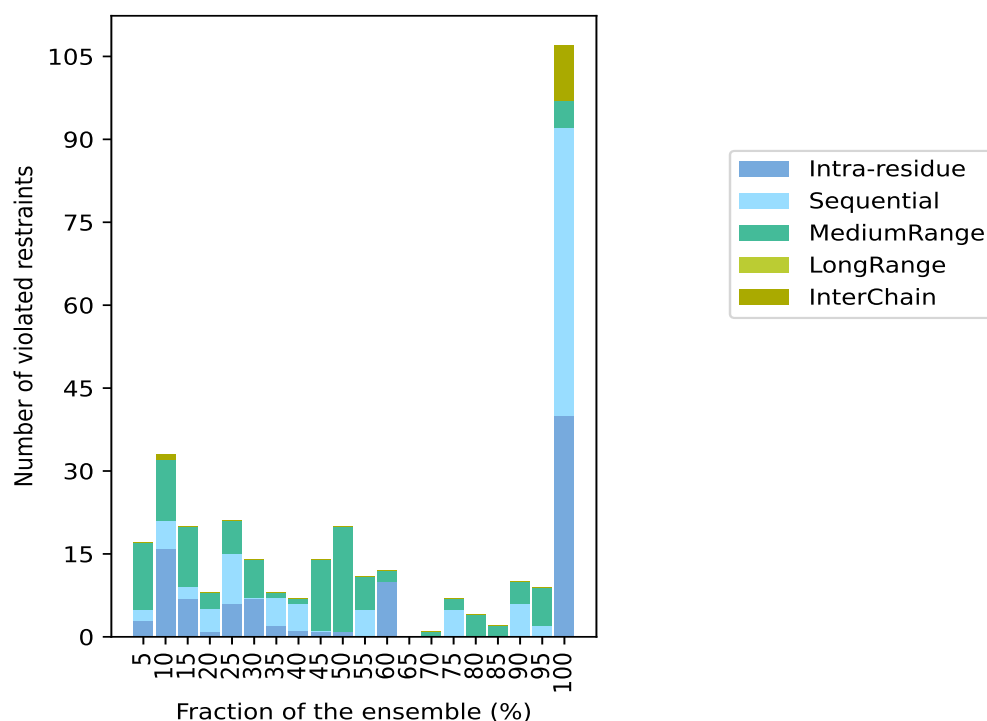
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2657(IR:780, SQ:598, MR:378, LR:0, IC:901) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	2	12	0	0	17	1	5.0
16	5	11	0	1	33	2	10.0
7	2	11	0	0	20	3	15.0
1	4	3	0	0	8	4	20.0
6	9	6	0	0	21	5	25.0
7	0	7	0	0	14	6	30.0
2	5	1	0	0	8	7	35.0
1	5	1	0	0	7	8	40.0
1	0	13	0	0	14	9	45.0
1	0	19	0	0	20	10	50.0
0	5	6	0	0	11	11	55.0
10	0	2	0	0	12	12	60.0
0	0	0	0	0	0	13	65.0
0	0	1	0	0	1	14	70.0
0	5	2	0	0	7	15	75.0
0	0	4	0	0	4	16	80.0
0	0	2	0	0	2	17	85.0
0	6	4	0	0	10	18	90.0
0	2	7	0	0	9	19	95.0
40	52	5	0	10	107	20	100.0

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

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

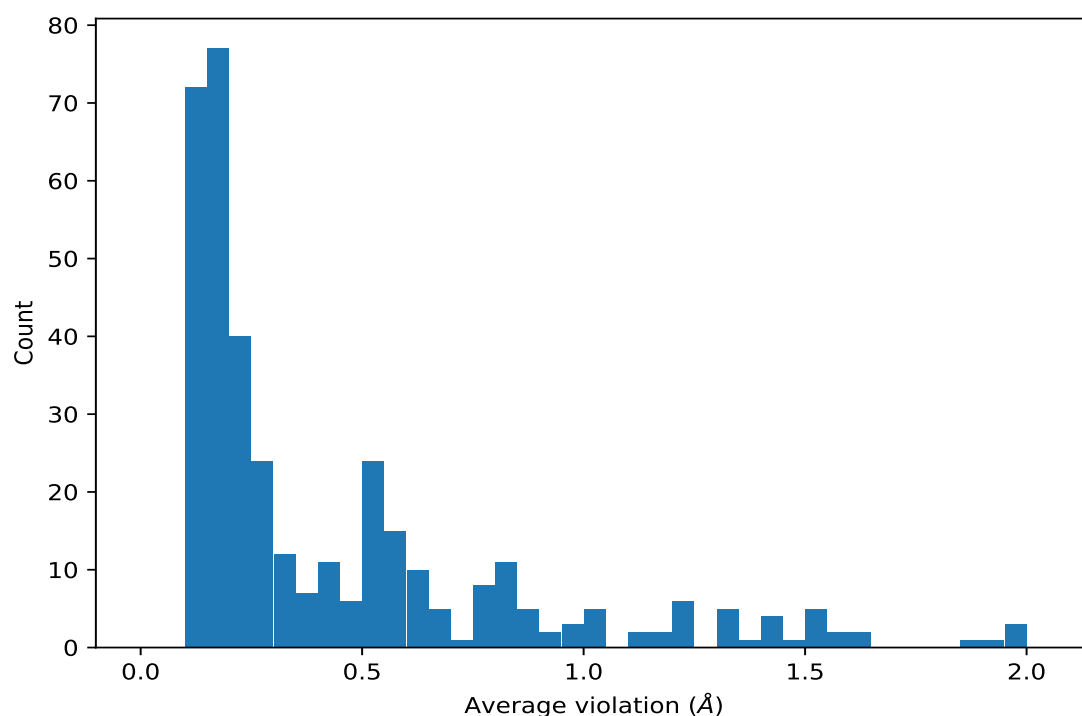
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	20	1.03	0.02	1.03
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	20	1.03	0.02	1.03
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	20	1.03	0.03	1.03
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	20	1.03	0.03	1.03
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	20	1.03	0.03	1.03
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	20	0.96	0.56	0.77
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	20	0.96	0.57	0.77
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	20	0.95	0.57	0.78
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	20	0.94	0.57	0.76
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	20	0.94	0.57	0.7
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	20	0.82	0.17	0.81
(2,2071)	1:40:A:ILE:CA	1:44:E:LEU:CA	20	0.82	0.17	0.81
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	20	0.81	0.18	0.8
(2,2072)	1:40:B:ILE:CA	1:44:A:LEU:CA	20	0.81	0.18	0.8
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	20	0.8	0.17	0.8
(2,2074)	1:40:D:ILE:CA	1:44:C:LEU:CA	20	0.8	0.17	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	20	0.8	0.19	0.77
(2,2073)	1:40:C:ILE:CA	1:44:B:LEU:CA	20	0.8	0.19	0.77
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	20	0.78	0.19	0.7
(2,2075)	1:40:E:ILE:CA	1:44:D:LEU:CA	20	0.78	0.19	0.7
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	20	0.64	0.17	0.62
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	20	0.64	0.17	0.62
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	20	0.59	0.21	0.52
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	20	0.59	0.21	0.52
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	20	0.58	0.17	0.52
(2,2110)	1:33:E:ILE:CG2	1:37:D:LEU:CA	20	0.58	0.17	0.52
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	20	0.58	0.19	0.52
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	20	0.58	0.19	0.52
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	20	0.58	0.15	0.56
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	20	0.58	0.15	0.56
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	20	0.53	0.06	0.52
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	20	0.53	0.06	0.52
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	20	0.53	0.06	0.53
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	20	0.53	0.06	0.53
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	20	0.53	0.06	0.52
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	20	0.53	0.06	0.52
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	20	0.53	0.06	0.52
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	20	0.53	0.06	0.52
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	20	0.53	0.06	0.52
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	20	0.53	0.06	0.52
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	20	0.49	0.05	0.5
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	20	0.49	0.05	0.5
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	20	0.49	0.05	0.5
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	20	0.49	0.05	0.49
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	20	0.49	0.05	0.49
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	20	0.24	0.2	0.15
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	20	0.24	0.2	0.15
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	20	0.24	0.2	0.15
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	20	0.24	0.2	0.15
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	20	0.24	0.2	0.15
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	20	0.23	0.04	0.23
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	20	0.22	0.03	0.23
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	20	0.22	0.03	0.23
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	20	0.22	0.03	0.23
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	20	0.22	0.03	0.23
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	20	0.19	0.02	0.18
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	20	0.19	0.02	0.19
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	20	0.19	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	20	0.19	0.02	0.18
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	20	0.19	0.02	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	20	0.18	0.01	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	20	0.18	0.01	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	20	0.18	0.01	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	20	0.18	0.01	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	20	0.18	0.01	0.18
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	20	0.18	0.01	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	20	0.17	0.01	0.18
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	20	0.17	0.03	0.16
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	20	0.17	0.03	0.17
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	20	0.17	0.02	0.17
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	20	0.17	0.01	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	20	0.17	0.01	0.17
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	20	0.17	0.01	0.16
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	20	0.16	0.03	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	20	0.16	0.01	0.16
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	20	0.16	0.03	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	20	0.16	0.01	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	20	0.16	0.01	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	20	0.16	0.01	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	20	0.16	0.01	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	20	0.16	0.01	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	20	0.15	0.01	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	20	0.15	0.01	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	20	0.15	0.01	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	20	0.15	0.01	0.15
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	20	0.15	0.01	0.15
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	20	0.15	0.01	0.15
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	20	0.15	0.01	0.15
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	20	0.15	0.01	0.15
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	20	0.15	0.01	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	20	0.15	0.01	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	20	0.15	0.01	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	20	0.15	0.01	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	20	0.15	0.01	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	20	0.15	0.0	0.15
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	20	0.15	0.01	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	20	0.15	0.01	0.15
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	20	0.15	0.01	0.14
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	20	0.15	0.01	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	20	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	20	0.14	0.02	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	20	0.14	0.01	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	20	0.14	0.0	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	20	0.14	0.01	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	20	0.14	0.0	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	20	0.14	0.0	0.14
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	20	0.14	0.02	0.14
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	20	0.13	0.03	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	20	0.12	0.01	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	20	0.12	0.01	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	20	0.12	0.01	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	20	0.12	0.01	0.12
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	20	0.1	0.0	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	20	0.1	0.0	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	20	0.1	0.0	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	20	0.1	0.0	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	20	0.1	0.0	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	20	0.1	0.0	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	20	0.1	0.0	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	20	0.1	0.0	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	20	0.1	0.0	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	20	0.1	0.0	0.1
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	19	0.87	0.34	0.75
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	19	0.87	0.33	0.78
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	19	0.87	0.33	0.75
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	19	0.86	0.33	0.76
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	19	0.86	0.33	0.74
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	19	0.17	0.05	0.17
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	19	0.16	0.05	0.14
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	19	0.13	0.02	0.13
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	19	0.13	0.02	0.13
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	18	0.24	0.08	0.24
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	18	0.2	0.07	0.19
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	18	0.17	0.04	0.16
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	18	0.16	0.04	0.15
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	18	0.13	0.01	0.13
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	18	0.13	0.02	0.13
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	18	0.13	0.01	0.13
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	18	0.13	0.01	0.13
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	18	0.13	0.01	0.13
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	18	0.13	0.01	0.13
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	17	0.25	0.08	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	17	0.2	0.08	0.19
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	16	0.25	0.07	0.24
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	16	0.24	0.06	0.22
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	16	0.21	0.08	0.2
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	16	0.17	0.04	0.18
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	15	0.35	0.08	0.33
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	15	0.34	0.08	0.32
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	15	0.34	0.08	0.34
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	15	0.33	0.08	0.33
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	15	0.33	0.08	0.32
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	15	0.26	0.07	0.24
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	15	0.2	0.08	0.18
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	14	0.21	0.08	0.2
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	12	1.12	0.97	0.99
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	12	1.12	0.97	0.99
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	12	0.29	0.09	0.27
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	12	0.29	0.1	0.27
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	12	0.29	0.09	0.27
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	12	0.29	0.09	0.26
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	12	0.29	0.09	0.27
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	12	0.16	0.02	0.16
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	12	0.16	0.02	0.16
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	12	0.15	0.01	0.16
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	12	0.15	0.01	0.16
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	12	0.15	0.02	0.16
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	12	0.12	0.02	0.12
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	11	1.51	0.65	1.69
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	11	1.5	0.67	1.73
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	11	1.49	0.66	1.71
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	11	1.22	0.97	1.01
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	11	1.22	0.97	1.01
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	11	1.22	0.97	1.01
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	11	1.22	0.97	1.01
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	11	0.69	0.1	0.72
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	11	0.69	0.1	0.71
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	11	0.69	0.1	0.72
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	11	0.68	0.1	0.72
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	11	0.68	0.1	0.72
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	11	0.3	0.17	0.29
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	10	1.6	0.81	1.5
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	10	1.6	0.78	1.51
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	10	1.58	0.78	1.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	10	1.56	0.67	1.8
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	10	1.54	0.8	1.38
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	10	1.53	0.8	1.38
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	10	1.52	0.63	1.8
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	10	1.34	0.94	1.04
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	10	1.34	0.94	1.04
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	10	1.34	0.95	1.04
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	10	1.34	0.95	1.04
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	10	0.6	0.11	0.58
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	10	0.34	0.16	0.3
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	10	0.33	0.16	0.3
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	10	0.33	0.17	0.29
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	10	0.31	0.16	0.28
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	10	0.21	0.08	0.23
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	10	0.21	0.08	0.2
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	10	0.13	0.02	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	10	0.13	0.02	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	10	0.13	0.02	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	10	0.13	0.02	0.12
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	10	0.12	0.02	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	10	0.12	0.01	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	10	0.12	0.01	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	10	0.12	0.01	0.12
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	9	1.97	0.8	1.94
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	9	1.97	0.8	1.92
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	9	1.96	0.8	1.92
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	9	1.9	0.75	1.93
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	9	1.88	0.75	1.93
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	9	0.26	0.08	0.26
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	9	0.22	0.07	0.22
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	9	0.21	0.06	0.2
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	9	0.17	0.04	0.16
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	9	0.17	0.04	0.16
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	9	0.17	0.04	0.16
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	9	0.15	0.05	0.13
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	9	0.15	0.05	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	9	0.13	0.01	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	9	0.13	0.01	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	9	0.13	0.01	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	9	0.13	0.01	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	9	0.13	0.01	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	9	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	9	0.12	0.02	0.11
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	9	0.12	0.01	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	9	0.12	0.01	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	9	0.12	0.01	0.12
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	8	0.43	0.16	0.4
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	8	0.37	0.09	0.36
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	8	0.37	0.09	0.36
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	8	0.37	0.08	0.37
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	8	0.36	0.1	0.38
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	8	0.36	0.09	0.37
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	8	0.13	0.02	0.12
(2,113)	1:18:A:ILE:H	1:17:A:THR:H	7	0.8	0.25	0.9
(2,941)	1:18:C:ILE:H	1:17:C:THR:H	7	0.8	0.28	0.9
(2,1769)	1:18:E:ILE:H	1:17:E:THR:H	7	0.8	0.28	0.9
(2,1355)	1:18:D:ILE:H	1:17:D:THR:H	7	0.79	0.28	0.9
(2,527)	1:18:B:ILE:H	1:17:B:THR:H	7	0.79	0.28	0.9
(2,1572)	1:44:D:LEU:H	1:44:D:LEU:HG	7	0.51	0.16	0.57
(2,330)	1:44:A:LEU:H	1:44:A:LEU:HG	7	0.5	0.22	0.54
(2,684)	1:39:B:LEU:H	1:36:B:CYS:HA	7	0.25	0.09	0.25
(2,744)	1:44:B:LEU:H	1:44:B:LEU:HG	6	0.6	0.07	0.62
(2,1813)	1:27:E:ASN:H	1:25:E:ARG:H	6	0.54	0.38	0.4
(2,571)	1:27:B:ASN:H	1:25:B:ARG:H	6	0.52	0.38	0.4
(2,985)	1:27:C:ASN:H	1:25:C:ARG:H	6	0.47	0.37	0.41
(2,157)	1:27:A:ASN:H	1:25:A:ARG:H	6	0.44	0.31	0.4
(2,664)	1:37:B:LEU:H	1:34:B:ASN:HA	6	0.19	0.04	0.18
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD11	6	0.18	0.05	0.16
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD12	6	0.18	0.05	0.16
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD13	6	0.18	0.05	0.16
(2,250)	1:37:A:LEU:H	1:34:A:ASN:HA	6	0.17	0.07	0.15
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB2	6	0.17	0.07	0.13
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB3	6	0.17	0.07	0.13
(2,938)	1:17:C:THR:H	1:17:C:THR:HA	6	0.13	0.01	0.13
(2,1352)	1:17:D:THR:H	1:17:D:THR:HA	6	0.13	0.01	0.13
(2,1766)	1:17:E:THR:H	1:17:E:THR:HA	6	0.13	0.01	0.14
(2,110)	1:17:A:THR:H	1:17:A:THR:HA	6	0.13	0.02	0.14
(2,524)	1:17:B:THR:H	1:17:B:THR:HA	6	0.13	0.01	0.13
(2,183)	1:30:A:ASN:H	1:26:A:GLN:HA	5	0.63	0.43	0.46
(2,1839)	1:30:E:ASN:H	1:26:E:GLN:HA	5	0.61	0.44	0.43
(2,1425)	1:30:D:ASN:H	1:26:D:GLN:HA	5	0.61	0.44	0.39
(2,1011)	1:30:C:ASN:H	1:26:C:GLN:HA	5	0.61	0.44	0.41
(2,1399)	1:27:D:ASN:H	1:25:D:ARG:H	5	0.61	0.36	0.43
(2,597)	1:30:B:ASN:H	1:26:B:GLN:HA	5	0.6	0.44	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB2	5	0.54	0.07	0.53
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB3	5	0.54	0.07	0.53
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB2	5	0.54	0.08	0.53
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB3	5	0.54	0.08	0.53
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB2	5	0.54	0.07	0.53
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB3	5	0.54	0.07	0.53
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB2	5	0.54	0.07	0.55
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB3	5	0.54	0.07	0.55
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB2	5	0.53	0.06	0.53
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB3	5	0.53	0.06	0.53
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD11	5	0.25	0.08	0.23
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD12	5	0.25	0.08	0.23
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD13	5	0.25	0.08	0.23
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD11	5	0.25	0.09	0.23
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD12	5	0.25	0.09	0.23
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD13	5	0.25	0.09	0.23
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD11	5	0.25	0.09	0.24
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD12	5	0.25	0.09	0.24
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD13	5	0.25	0.09	0.24
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD11	5	0.24	0.08	0.23
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD12	5	0.24	0.08	0.23
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD13	5	0.24	0.08	0.23
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD11	5	0.24	0.08	0.23
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD12	5	0.24	0.08	0.23
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD13	5	0.24	0.08	0.23
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD11	5	0.22	0.11	0.15
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD12	5	0.22	0.11	0.15
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD13	5	0.22	0.11	0.15
(2,517)	1:16:B:SEP:H	1:15:B:ALA:HA	5	0.13	0.01	0.13
(2,1345)	1:16:D:SEP:H	1:15:D:ALA:HA	5	0.13	0.01	0.13
(2,931)	1:16:C:SEP:H	1:15:C:ALA:HA	5	0.13	0.01	0.13
(2,1759)	1:16:E:SEP:H	1:15:E:ALA:HA	5	0.13	0.01	0.13
(2,542)	1:20:B:MET:H	1:19:B:GLU:HA	4	0.37	0.22	0.32
(2,956)	1:20:C:MET:H	1:19:C:GLU:HA	4	0.34	0.24	0.26
(2,128)	1:20:A:MET:H	1:19:A:GLU:HA	4	0.33	0.24	0.24
(2,1370)	1:20:D:MET:H	1:19:D:GLU:HA	4	0.33	0.25	0.24
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD11	4	0.15	0.03	0.15
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD12	4	0.15	0.03	0.15
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD13	4	0.15	0.03	0.15
(2,1946)	1:41:E:CYS:H	1:38:E:ILE:HA	4	0.15	0.03	0.15
(2,1941)	1:40:E:ILE:H	1:37:E:LEU:HA	4	0.14	0.02	0.15
(2,1113)	1:40:C:ILE:H	1:37:C:LEU:HA	4	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1242)	1:52:C:LEU:H	1:52:C:LEU:HG	3	1.44	0.17	1.4
(2,2070)	1:52:E:LEU:H	1:52:E:LEU:HG	3	1.44	0.17	1.39
(2,414)	1:52:A:LEU:H	1:52:A:LEU:HG	3	1.43	0.17	1.39
(2,1656)	1:52:D:LEU:H	1:52:D:LEU:HG	3	1.43	0.17	1.39
(2,828)	1:52:B:LEU:H	1:52:B:LEU:HG	3	1.37	0.19	1.27
(2,989)	1:28:C:LEU:H	1:25:C:ARG:HA	3	1.32	0.45	1.51
(2,161)	1:28:A:LEU:H	1:25:A:ARG:HA	3	1.2	0.61	1.48
(2,1817)	1:28:E:LEU:H	1:25:E:ARG:HA	3	1.2	0.6	1.46
(2,575)	1:28:B:LEU:H	1:25:B:ARG:HA	3	1.17	0.62	1.44
(2,1403)	1:28:D:LEU:H	1:25:D:ARG:HA	3	1.17	0.6	1.43
(2,1529)	1:39:D:LEU:H	1:35:D:PHE:HD1	3	0.44	0.38	0.21
(2,1529)	1:39:D:LEU:H	1:35:D:PHE:HD2	3	0.44	0.38	0.21
(2,287)	1:39:A:LEU:H	1:35:A:PHE:HD1	3	0.41	0.4	0.14
(2,287)	1:39:A:LEU:H	1:35:A:PHE:HD2	3	0.41	0.4	0.14
(2,1115)	1:39:C:LEU:H	1:35:C:PHE:HD1	3	0.41	0.38	0.17
(2,1115)	1:39:C:LEU:H	1:35:C:PHE:HD2	3	0.41	0.38	0.17
(2,1784)	1:20:E:MET:H	1:19:E:GLU:HA	3	0.41	0.24	0.33
(2,1943)	1:39:E:LEU:H	1:35:E:PHE:HD1	3	0.4	0.37	0.17
(2,1943)	1:39:E:LEU:H	1:35:E:PHE:HD2	3	0.4	0.37	0.17
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD11	3	0.25	0.02	0.26
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD12	3	0.25	0.02	0.26
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD13	3	0.25	0.02	0.26
(2,270)	1:39:A:LEU:H	1:36:A:CYS:HA	3	0.21	0.08	0.22
(2,738)	1:44:B:LEU:H	1:41:B:CYS:HB2	3	0.13	0.02	0.13
(2,738)	1:44:B:LEU:H	1:41:B:CYS:HB3	3	0.13	0.02	0.13
(2,103)	1:16:A:SEP:H	1:15:A:ALA:HA	3	0.13	0.01	0.13
(2,1156)	1:44:C:LEU:H	1:44:C:LEU:HA	3	0.1	0.0	0.1
(2,1228)	1:51:C:LEU:H	1:51:C:LEU:HB3	2	0.76	0.0	0.76
(2,814)	1:51:B:LEU:H	1:51:B:LEU:HB3	2	0.76	0.01	0.76
(2,2056)	1:51:E:LEU:H	1:51:E:LEU:HB3	2	0.76	0.01	0.76
(2,400)	1:51:A:LEU:H	1:51:A:LEU:HB3	2	0.75	0.0	0.75
(2,1642)	1:51:D:LEU:H	1:51:D:LEU:HB3	2	0.74	0.01	0.74
(2,120)	1:19:A:GLU:H	1:18:A:ILE:HA	2	0.58	0.1	0.58
(2,948)	1:19:C:GLU:H	1:18:C:ILE:HA	2	0.58	0.1	0.58
(2,701)	1:39:B:LEU:H	1:35:B:PHE:HD1	2	0.58	0.42	0.58
(2,701)	1:39:B:LEU:H	1:35:B:PHE:HD2	2	0.58	0.42	0.58
(2,534)	1:19:B:GLU:H	1:18:B:ILE:HA	2	0.57	0.11	0.57
(2,1362)	1:19:D:GLU:H	1:18:D:ILE:HA	2	0.57	0.11	0.57
(2,1776)	1:19:E:GLU:H	1:18:E:ILE:HA	2	0.57	0.11	0.57
(2,1512)	1:39:D:LEU:H	1:36:D:CYS:HA	2	0.26	0.0	0.26
(2,1447)	1:32:D:PHE:H	1:29:D:GLN:HA	2	0.25	0.04	0.25
(2,1033)	1:32:C:PHE:H	1:29:C:GLN:HA	2	0.24	0.04	0.24

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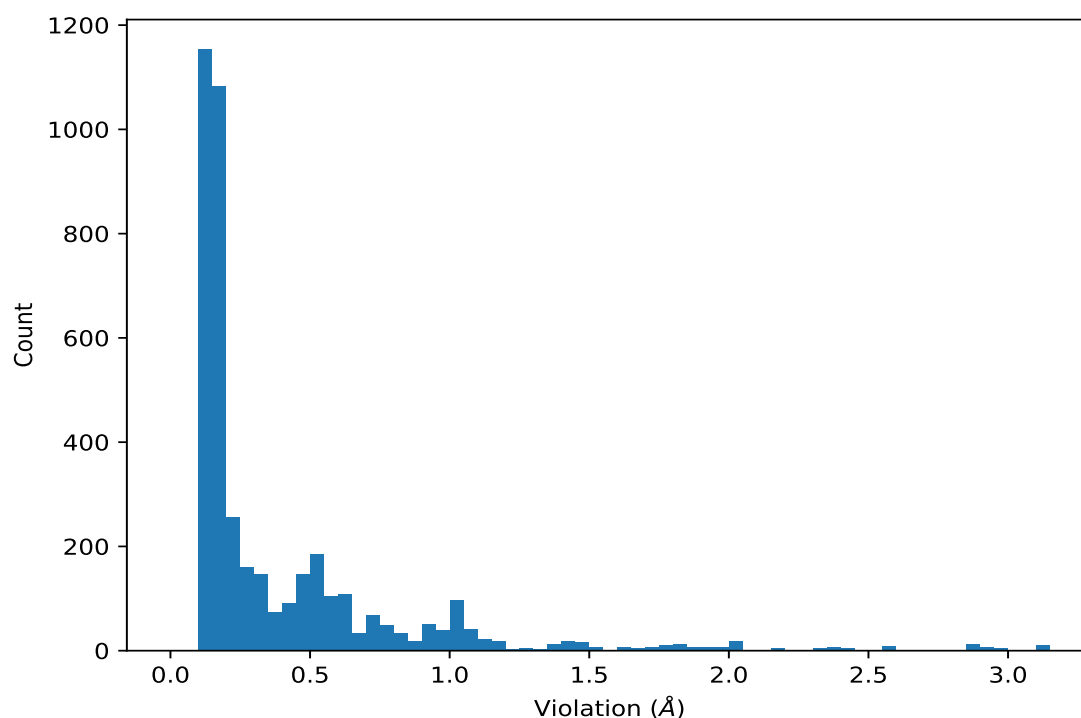
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,619)	1:32:B:PHE:H	1:29:B:GLN:HA	2	0.24	0.03	0.24
(2,1861)	1:32:E:PHE:H	1:29:E:GLN:HA	2	0.24	0.03	0.24
(2,205)	1:32:A:PHE:H	1:29:A:GLN:HA	2	0.23	0.04	0.23
(2,225)	1:27:A:ASN:HD21	1:27:A:ASN:HB3	2	0.22	0.02	0.22
(2,1467)	1:27:D:ASN:HD21	1:27:D:ASN:HB3	2	0.22	0.02	0.22
(2,639)	1:27:B:ASN:HD21	1:27:B:ASN:HB3	2	0.22	0.01	0.22
(2,1881)	1:27:E:ASN:HD21	1:27:E:ASN:HB3	2	0.22	0.01	0.22
(2,1053)	1:27:C:ASN:HD21	1:27:C:ASN:HB3	2	0.22	0.02	0.22
(2,411)	1:52:A:LEU:H	1:52:A:LEU:HA	2	0.16	0.0	0.16
(2,699)	1:40:B:ILE:H	1:37:B:LEU:HA	2	0.16	0.03	0.16
(2,2067)	1:52:E:LEU:H	1:52:E:LEU:HA	2	0.16	0.0	0.16
(2,825)	1:52:B:LEU:H	1:52:B:LEU:HA	2	0.16	0.01	0.16
(2,1239)	1:52:C:LEU:H	1:52:C:LEU:HA	2	0.16	0.01	0.16
(2,1653)	1:52:D:LEU:H	1:52:D:LEU:HA	2	0.16	0.01	0.16
(2,324)	1:44:A:LEU:H	1:41:A:CYS:HB2	2	0.13	0.02	0.13
(2,324)	1:44:A:LEU:H	1:41:A:CYS:HB3	2	0.13	0.02	0.13
(2,1527)	1:40:D:ILE:H	1:37:D:LEU:HA	2	0.13	0.02	0.13
(2,297)	1:42:A:LEU:H	1:39:A:LEU:HB2	2	0.12	0.0	0.12
(2,297)	1:42:A:LEU:H	1:39:A:LEU:HB3	2	0.12	0.0	0.12
(2,813)	1:51:B:LEU:H	1:51:B:LEU:HA	2	0.11	0.01	0.11
(2,2127)	1:47:C:ILE:CG2	1:44:B:LEU:CD2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	11	3.12
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	11	3.12
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	11	3.12
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	11	3.12
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	11	3.11
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	11	3.11
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	11	3.11
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	11	3.11
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	14	3.1
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	11	3.1
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	11	3.1
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	14	2.99
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	16	2.97
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	16	2.95
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	16	2.95
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	14	2.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	14	2.91
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	18	2.91
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	18	2.9
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	18	2.9
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	18	2.9
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	18	2.89
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	14	2.88
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	6	2.85
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	6	2.85
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	6	2.85
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	6	2.85
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	6	2.85
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	6	2.85
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	6	2.85
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	6	2.85
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	6	2.85
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	6	2.85
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	3	2.6
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	3	2.59
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	12	2.58
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	3	2.57
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	3	2.57
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	3	2.56
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	12	2.56
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	12	2.55
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	12	2.55
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	12	2.55
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	10	2.47
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	10	2.44
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	10	2.44
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	10	2.43
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	8	2.4
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	8	2.4
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	8	2.39
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	8	2.39
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	8	2.38
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	16	2.37
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	16	2.37
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	9	2.35
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	9	2.33
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	9	2.32
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	9	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	9	2.31
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	18	2.19
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	18	2.18
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	18	2.18
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	18	2.17
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	18	2.17
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	10	2.12
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	3	2.07
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	3	2.04
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	3	2.04
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	8	2.04
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	12	2.04
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	12	2.04
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	8	2.04
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	3	2.04
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	13	2.04
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	13	2.04
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	3	2.03
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	8	2.03
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	8	2.02
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	13	2.02
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	8	2.02
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	13	2.01
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	12	2.01
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	12	2.01
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	12	2.0
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	12	2.0
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	13	1.99
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	12	1.99
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	12	1.99
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	12	1.98
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	12	1.98
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	16	1.96
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	13	1.94
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	13	1.93
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	13	1.93
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	13	1.92
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	16	1.92
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	13	1.92
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	3	1.88
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	3	1.87
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	3	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	3	1.87
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	16	1.86
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	3	1.86
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	18	1.84
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	18	1.84
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	18	1.83
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	18	1.83
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	18	1.83
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	16	1.82
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	16	1.82
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	13	1.81
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	2	1.8
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	13	1.8
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	13	1.8
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	13	1.8
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	2	1.79
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	2	1.79
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	2	1.78
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	13	1.78
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	2	1.77
(2,161)	1:28:A:LEU:H	1:25:A:ARG:HA	9	1.77
(2,1817)	1:28:E:LEU:H	1:25:E:ARG:HA	9	1.76
(2,575)	1:28:B:LEU:H	1:25:B:ARG:HA	9	1.76
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	10	1.75
(2,989)	1:28:C:LEU:H	1:25:C:ARG:HA	9	1.75
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	10	1.75
(2,1403)	1:28:D:LEU:H	1:25:D:ARG:HA	9	1.74
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	8	1.74
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	10	1.73
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	8	1.73
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	8	1.72
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	10	1.72
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	8	1.71
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	8	1.69
(2,2070)	1:52:E:LEU:H	1:52:E:LEU:HG	17	1.67
(2,1656)	1:52:D:LEU:H	1:52:D:LEU:HG	17	1.66
(2,1242)	1:52:C:LEU:H	1:52:C:LEU:HG	17	1.66
(2,414)	1:52:A:LEU:H	1:52:A:LEU:HG	17	1.66
(2,828)	1:52:B:LEU:H	1:52:B:LEU:HG	17	1.64
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	5	1.64
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	5	1.63
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	5	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	5	1.63
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	5	1.63
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	10	1.57
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	20	1.53
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	20	1.52
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	20	1.52
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	20	1.51
(2,989)	1:28:C:LEU:H	1:25:C:ARG:HA	14	1.51
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	20	1.5
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	18	1.49
(2,1839)	1:30:E:ASN:H	1:26:E:GLN:HA	8	1.48
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	19	1.48
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	18	1.48
(2,1425)	1:30:D:ASN:H	1:26:D:GLN:HA	8	1.48
(2,1011)	1:30:C:ASN:H	1:26:C:GLN:HA	8	1.48
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	18	1.48
(2,161)	1:28:A:LEU:H	1:25:A:ARG:HA	14	1.48
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	1	1.47
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	18	1.47
(2,597)	1:30:B:ASN:H	1:26:B:GLN:HA	8	1.47
(2,183)	1:30:A:ASN:H	1:26:A:GLN:HA	8	1.47
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	19	1.47
(2,1817)	1:28:E:LEU:H	1:25:E:ARG:HA	14	1.46
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	18	1.46
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	20	1.45
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	19	1.45
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	1	1.44
(2,575)	1:28:B:LEU:H	1:25:B:ARG:HA	14	1.44
(2,1403)	1:28:D:LEU:H	1:25:D:ARG:HA	14	1.43
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	20	1.43
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	20	1.42
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	20	1.42
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	19	1.42
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	12	1.41
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	1	1.41
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	4	1.41
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	1	1.41
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	4	1.41
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	20	1.41
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	4	1.4
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	12	1.4
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	1	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1242)	1:52:C:LEU:H	1:52:C:LEU:HG	8	1.4
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	19	1.4
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	12	1.4
(2,2070)	1:52:E:LEU:H	1:52:E:LEU:HG	8	1.39
(2,1656)	1:52:D:LEU:H	1:52:D:LEU:HG	8	1.39
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	4	1.39
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	16	1.39
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	4	1.39
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	16	1.39
(2,414)	1:52:A:LEU:H	1:52:A:LEU:HG	8	1.39
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	5	1.38
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	12	1.38
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	16	1.37
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	12	1.37
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	5	1.37
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	14	1.36
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	5	1.33
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	5	1.31
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	5	1.3
(2,828)	1:52:B:LEU:H	1:52:B:LEU:HG	8	1.27
(2,2070)	1:52:E:LEU:H	1:52:E:LEU:HG	20	1.25
(2,1656)	1:52:D:LEU:H	1:52:D:LEU:HG	20	1.25
(2,1242)	1:52:C:LEU:H	1:52:C:LEU:HG	20	1.25
(2,414)	1:52:A:LEU:H	1:52:A:LEU:HG	20	1.25
(2,985)	1:27:C:ASN:H	1:25:C:ARG:H	10	1.24
(2,828)	1:52:B:LEU:H	1:52:B:LEU:HG	20	1.2
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	6	1.2
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	14	1.19
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	11	1.18
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	11	1.17
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	14	1.17
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	6	1.17
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	6	1.16
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	7	1.15
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	11	1.15
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	17	1.15
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	3	1.15
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	4	1.15
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	4	1.15
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	17	1.15
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	6	1.15
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	11	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	17	1.15
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	4	1.15
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	4	1.15
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	14	1.14
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	6	1.14
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	17	1.14
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	3	1.14
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	11	1.14
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	4	1.14
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	4	1.14
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	4	1.13
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	4	1.13
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	3	1.13
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	3	1.13
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	14	1.13
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	8	1.12
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	8	1.12
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	3	1.12
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	17	1.11
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	8	1.1
(2,2072)	1:40:B:ILE:CA	1:44:A:LEU:CA	5	1.1
(2,2072)	1:40:B:ILE:CA	1:44:A:LEU:CA	8	1.1
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	6	1.1
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	6	1.1
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	4	1.1
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	4	1.1
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	9	1.09
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	14	1.09
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	6	1.09
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	14	1.09
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	6	1.09
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	6	1.09
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	5	1.08
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	7	1.08
(2,1813)	1:27:E:ASN:H	1:25:E:ARG:H	10	1.08
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	15	1.08
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	15	1.08
(2,157)	1:27:A:ASN:H	1:25:A:ARG:H	10	1.08
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	9	1.07
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	8	1.07
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	18	1.07
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	15	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	15	1.07
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	10	1.07
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	18	1.07
(2,1399)	1:27:D:ASN:H	1:25:D:ARG:H	10	1.07
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	14	1.07
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	18	1.07
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	18	1.07
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	15	1.07
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	15	1.07
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	9	1.06
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	10	1.06
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	18	1.06
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	10	1.06
(2,571)	1:27:B:ASN:H	1:25:B:ARG:H	10	1.06
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	8	1.06
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	10	1.05
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	11	1.05
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	15	1.05
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	15	1.05
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	1	1.05
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	8	1.05
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	20	1.05
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	15	1.05
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	15	1.05
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	1	1.05
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	10	1.05
(2,2071)	1:40:A:ILE:CA	1:44:E:LEU:CA	5	1.04
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	1	1.04
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	4	1.04
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	8	1.04
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	11	1.04
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	20	1.04
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	1	1.04
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	4	1.04
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	8	1.04
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	20	1.04
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	3	1.04
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	4	1.04
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	11	1.04
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	20	1.04
(2,941)	1:18:C:ILE:H	1:17:C:THR:H	19	1.04
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	1	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	3	1.04
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	11	1.04
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	17	1.04
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	4	1.04
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	11	1.04
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	13	1.04
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	5	1.03
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	9	1.03
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	13	1.03
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	17	1.03
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	5	1.03
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	9	1.03
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	13	1.03
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	17	1.03
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	5	1.03
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	9	1.03
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	13	1.03
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	17	1.03
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	4	1.03
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	5	1.03
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	8	1.03
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	9	1.03
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	13	1.03
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	14	1.03
(2,571)	1:27:B:ASN:H	1:25:B:ARG:H	16	1.03
(2,527)	1:18:B:ILE:H	1:17:B:THR:H	19	1.03
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	14	1.03
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	3	1.03
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	5	1.03
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	9	1.03
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	12	1.03
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	17	1.03
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	20	1.03
(2,2073)	1:40:C:ILE:CA	1:44:B:LEU:CA	7	1.02
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	18	1.02
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	2	1.02
(2,1769)	1:18:E:ILE:H	1:17:E:THR:H	19	1.02
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	2	1.02
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	5	1.02
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	5	1.02
(2,1355)	1:18:D:ILE:H	1:17:D:THR:H	19	1.02
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	2	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	2	1.02
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	2	1.02
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	18	1.01
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	3	1.01
(2,1813)	1:27:E:ASN:H	1:25:E:ARG:H	16	1.01
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	5	1.01
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	5	1.01
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	3	1.01
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	14	1.01
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	15	1.01
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	7	1.01
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	14	1.01
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	5	1.01
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	5	1.01
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	7	1.01
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	5	1.01
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	5	1.01
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	7	1.01
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	14	1.01
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	5	1.01
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	5	1.01
(2,113)	1:18:A:ILE:H	1:17:A:THR:H	19	1.01
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	9	1.0
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	7	1.0
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	12	1.0
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	14	1.0
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	15	1.0
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	7	1.0
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	12	1.0
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	19	1.0
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	16	1.0
(2,701)	1:39:B:LEU:H	1:35:B:PHE:HD1	10	1.0
(2,701)	1:39:B:LEU:H	1:35:B:PHE:HD2	10	1.0
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	12	1.0
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	15	1.0
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	19	1.0
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	16	1.0
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	19	1.0
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	8	0.99
(2,2075)	1:40:E:ILE:CA	1:44:D:LEU:CA	2	0.99
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	18	0.99
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	16	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1858)	1:31:E:LEU:H	1:31:E:LEU:HG	19	0.99
(2,1444)	1:31:D:LEU:H	1:31:D:LEU:HG	16	0.99
(2,1399)	1:27:D:ASN:H	1:25:D:ARG:H	16	0.99
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	14	0.99
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	12	0.99
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	15	0.99
(2,1030)	1:31:C:LEU:H	1:31:C:LEU:HG	19	0.99
(2,616)	1:31:B:LEU:H	1:31:B:LEU:HG	16	0.99
(2,202)	1:31:A:LEU:H	1:31:A:LEU:HG	15	0.99
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	1	0.98
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	9	0.98
(2,1529)	1:39:D:LEU:H	1:35:D:PHE:HD1	10	0.98
(2,1529)	1:39:D:LEU:H	1:35:D:PHE:HD2	10	0.98
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	19	0.98
(2,287)	1:39:A:LEU:H	1:35:A:PHE:HD1	10	0.98
(2,287)	1:39:A:LEU:H	1:35:A:PHE:HD2	10	0.98
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	8	0.98
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	8	0.98
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	18	0.97
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	18	0.97
(2,2072)	1:40:B:ILE:CA	1:44:A:LEU:CA	7	0.97
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	8	0.97
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	8	0.97
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	8	0.97
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	8	0.97
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	8	0.97
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	8	0.97
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	8	0.97
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	8	0.97
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	9	0.96
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	4	0.96
(2,2075)	1:40:E:ILE:CA	1:44:D:LEU:CA	5	0.96
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	18	0.96
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	19	0.96
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	19	0.95
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	4	0.94
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	4	0.94
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	4	0.94
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	1	0.94
(2,2071)	1:40:A:ILE:CA	1:44:E:LEU:CA	2	0.94
(2,1769)	1:18:E:ILE:H	1:17:E:THR:H	3	0.94
(2,1355)	1:18:D:ILE:H	1:17:D:THR:H	3	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1115)	1:39:C:LEU:H	1:35:C:PHE:HD1	10	0.94
(2,1115)	1:39:C:LEU:H	1:35:C:PHE:HD2	10	0.94
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	19	0.94
(2,941)	1:18:C:ILE:H	1:17:C:THR:H	3	0.94
(2,113)	1:18:A:ILE:H	1:17:A:THR:H	3	0.94
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	4	0.93
(2,2074)	1:40:D:ILE:CA	1:44:C:LEU:CA	2	0.93
(2,2072)	1:40:B:ILE:CA	1:44:A:LEU:CA	2	0.93
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	4	0.93
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	19	0.93
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	9	0.93
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	8	0.92
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	4	0.92
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	8	0.92
(2,1943)	1:39:E:LEU:H	1:35:E:PHE:HD1	10	0.92
(2,1943)	1:39:E:LEU:H	1:35:E:PHE:HD2	10	0.92
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	2	0.92
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	9	0.92
(2,527)	1:18:B:ILE:H	1:17:B:THR:H	3	0.92
(2,2110)	1:33:E:ILE:CG2	1:37:D:LEU:CA	4	0.91
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	4	0.91
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	18	0.91
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	9	0.91
(2,2073)	1:40:C:ILE:CA	1:44:B:LEU:CA	2	0.91
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	20	0.91
(2,1769)	1:18:E:ILE:H	1:17:E:THR:H	7	0.91
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	3	0.91
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	20	0.91
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	9	0.91
(2,330)	1:44:A:LEU:H	1:44:A:LEU:HG	2	0.91
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	9	0.9
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	18	0.9
(2,1769)	1:18:E:ILE:H	1:17:E:THR:H	15	0.9
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	9	0.9
(2,1355)	1:18:D:ILE:H	1:17:D:THR:H	7	0.9
(2,1355)	1:18:D:ILE:H	1:17:D:THR:H	15	0.9
(2,941)	1:18:C:ILE:H	1:17:C:THR:H	7	0.9
(2,941)	1:18:C:ILE:H	1:17:C:THR:H	15	0.9
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	3	0.9
(2,527)	1:18:B:ILE:H	1:17:B:THR:H	7	0.9
(2,527)	1:18:B:ILE:H	1:17:B:THR:H	15	0.9
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	3	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,113)	1:18:A:ILE:H	1:17:A:THR:H	7	0.9
(2,113)	1:18:A:ILE:H	1:17:A:THR:H	15	0.9
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	8	0.89
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	1	0.89
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	19	0.89
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	9	0.89
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	20	0.89
(2,2074)	1:40:D:ILE:CA	1:44:C:LEU:CA	5	0.88
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	19	0.88
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	3	0.88
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	9	0.87
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	3	0.87
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	19	0.85
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	17	0.85
(2,1769)	1:18:E:ILE:H	1:17:E:THR:H	20	0.85
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	20	0.85
(2,1355)	1:18:D:ILE:H	1:17:D:THR:H	20	0.85
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	8	0.85
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	8	0.85
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	8	0.85
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	8	0.84
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	17	0.84
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	16	0.84
(2,941)	1:18:C:ILE:H	1:17:C:THR:H	20	0.84
(2,527)	1:18:B:ILE:H	1:17:B:THR:H	1	0.84
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	20	0.84
(2,113)	1:18:A:ILE:H	1:17:A:THR:H	20	0.84
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	4	0.83
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	9	0.83
(2,2074)	1:40:D:ILE:CA	1:44:C:LEU:CA	7	0.83
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	3	0.83
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	17	0.83
(2,1769)	1:18:E:ILE:H	1:17:E:THR:H	1	0.83
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	8	0.83
(2,1355)	1:18:D:ILE:H	1:17:D:THR:H	1	0.83
(2,941)	1:18:C:ILE:H	1:17:C:THR:H	1	0.83
(2,527)	1:18:B:ILE:H	1:17:B:THR:H	20	0.83
(2,113)	1:18:A:ILE:H	1:17:A:THR:H	1	0.83
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	3	0.82
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	14	0.82
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	3	0.82
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	19	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	16	0.82
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	6	0.82
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	16	0.82
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	8	0.81
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	17	0.81
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	18	0.8
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	3	0.8
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	20	0.8
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	3	0.8
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	14	0.8
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	17	0.8
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	20	0.79
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	17	0.79
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	17	0.79
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	14	0.78
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	20	0.78
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	14	0.78
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	16	0.78
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	8	0.78
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	7	0.78
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	6	0.77
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	16	0.77
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	16	0.77
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	16	0.77
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	6	0.77
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	16	0.77
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	16	0.77
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	16	0.77
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	16	0.77
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	17	0.76
(2,2056)	1:51:E:LEU:H	1:51:E:LEU:HB3	19	0.76
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	9	0.76
(2,1228)	1:51:C:LEU:H	1:51:C:LEU:HB3	5	0.76
(2,1228)	1:51:C:LEU:H	1:51:C:LEU:HB3	19	0.76
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	7	0.76
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	9	0.76
(2,814)	1:51:B:LEU:H	1:51:B:LEU:HB3	19	0.76
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	9	0.76
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	18	0.76
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	5	0.75
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	20	0.75
(2,2056)	1:51:E:LEU:H	1:51:E:LEU:HB3	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	8	0.75
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	18	0.75
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	4	0.75
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	9	0.75
(2,1642)	1:51:D:LEU:H	1:51:D:LEU:HB3	19	0.75
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	18	0.75
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	6	0.75
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	17	0.75
(2,814)	1:51:B:LEU:H	1:51:B:LEU:HB3	5	0.75
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	6	0.75
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	16	0.75
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	4	0.75
(2,400)	1:51:A:LEU:H	1:51:A:LEU:HB3	5	0.75
(2,400)	1:51:A:LEU:H	1:51:A:LEU:HB3	19	0.75
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	8	0.75
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	4	0.75
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	9	0.75
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	11	0.74
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	7	0.74
(2,1642)	1:51:D:LEU:H	1:51:D:LEU:HB3	5	0.74
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	5	0.74
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	7	0.74
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	4	0.74
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	13	0.74
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	5	0.74
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	8	0.74
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	4	0.74
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	18	0.74
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	7	0.74
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	13	0.74
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	19	0.73
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	5	0.73
(2,1784)	1:20:E:MET:H	1:19:E:GLU:HA	18	0.73
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	12	0.73
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	13	0.73
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	19	0.73
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	8	0.73
(2,1370)	1:20:D:MET:H	1:19:D:GLU:HA	18	0.73
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	19	0.73
(2,956)	1:20:C:MET:H	1:19:C:GLU:HA	18	0.73
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	13	0.73
(2,542)	1:20:B:MET:H	1:19:B:GLU:HA	18	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	13	0.73
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	19	0.73
(2,128)	1:20:A:MET:H	1:19:A:GLU:HA	18	0.73
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	6	0.72
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	20	0.72
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	14	0.72
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	14	0.72
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	12	0.72
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	14	0.72
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	18	0.72
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	12	0.72
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	14	0.72
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	14	0.72
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	19	0.72
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	5	0.72
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	12	0.72
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	5	0.72
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	6	0.72
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	12	0.72
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	14	0.72
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	7	0.71
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	14	0.71
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	6	0.71
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	14	0.71
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	6	0.71
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	14	0.71
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	6	0.71
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	2	0.71
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	6	0.71
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	14	0.71
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	14	0.71
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	2	0.7
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	11	0.7
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	11	0.7
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	11	0.7
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	11	0.7
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	17	0.7
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	2	0.7
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	2	0.7
(2,1572)	1:44:D:LEU:H	1:44:D:LEU:HG	2	0.7
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	2	0.7
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,744)	1:44:B:LEU:H	1:44:B:LEU:HG	2	0.7
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	2	0.7
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	2	0.69
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	14	0.69
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	17	0.69
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	6	0.69
(2,989)	1:28:C:LEU:H	1:25:C:ARG:HA	10	0.69
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	6	0.68
(2,1776)	1:19:E:GLU:H	1:18:E:ILE:HA	13	0.68
(2,1362)	1:19:D:GLU:H	1:18:D:ILE:HA	13	0.68
(2,948)	1:19:C:GLU:H	1:18:C:ILE:HA	13	0.68
(2,534)	1:19:B:GLU:H	1:18:B:ILE:HA	13	0.68
(2,120)	1:19:A:GLU:H	1:18:A:ILE:HA	13	0.68
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	17	0.67
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	2	0.67
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	1	0.67
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	6	0.67
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	17	0.67
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	1	0.67
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	6	0.67
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	10	0.67
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	10	0.67
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	4	0.67
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	10	0.67
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	10	0.67
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	10	0.67
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	5	0.66
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	10	0.66
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	3	0.65
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	2	0.65
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	3	0.65
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	20	0.65
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	15	0.65
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB2	3	0.65
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB3	3	0.65
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	17	0.65
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	5	0.64
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	13	0.64
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	11	0.64
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	15	0.64
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB2	3	0.64
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB3	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	16	0.64
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	16	0.64
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	11	0.64
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	16	0.64
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	16	0.64
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	4	0.64
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	11	0.64
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	3	0.63
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	14	0.63
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	18	0.63
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	4	0.63
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	17	0.63
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	16	0.63
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	16	0.63
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	7	0.63
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	11	0.63
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	15	0.63
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	17	0.63
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB2	3	0.63
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB3	3	0.63
(2,744)	1:44:B:LEU:H	1:44:B:LEU:HG	13	0.63
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	17	0.63
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	15	0.63
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	4	0.63
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	17	0.63
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	3	0.62
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	1	0.62
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	3	0.62
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	20	0.62
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	17	0.62
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	13	0.62
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	16	0.62
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	16	0.62
(2,1572)	1:44:D:LEU:H	1:44:D:LEU:HG	13	0.62
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	15	0.62
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	12	0.62
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	12	0.62
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	4	0.62
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	17	0.62
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	12	0.62
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	12	0.62
(2,744)	1:44:B:LEU:H	1:44:B:LEU:HG	9	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,744)	1:44:B:LEU:H	1:44:B:LEU:HG	18	0.62
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	7	0.62
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	4	0.62
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	12	0.62
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	12	0.62
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	12	0.62
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	12	0.62
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	16	0.62
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	16	0.62
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	11	0.61
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	16	0.61
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	16	0.61
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	10	0.61
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	16	0.61
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB2	3	0.61
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB3	3	0.61
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	4	0.61
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	12	0.61
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	12	0.61
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	20	0.61
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	11	0.61
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	13	0.61
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	13	0.61
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	13	0.61
(2,990)	1:28:C:LEU:H	1:24:C:ALA:HA	13	0.61
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	15	0.61
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	13	0.61
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	13	0.61
(2,576)	1:28:B:LEU:H	1:24:B:ALA:HA	13	0.61
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB2	3	0.61
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB3	3	0.61
(2,330)	1:44:A:LEU:H	1:44:A:LEU:HG	9	0.61
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	4	0.61
(2,162)	1:28:A:LEU:H	1:24:A:ALA:HA	13	0.61
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	11	0.6
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	11	0.6
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	17	0.6
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	10	0.6
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	10	0.6
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	10	0.6
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	13	0.6
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	15	0.6
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	13	0.6
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	13	0.6
(2,1572)	1:44:D:LEU:H	1:44:D:LEU:HG	9	0.6
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	7	0.6
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	13	0.6
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	13	0.6
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	15	0.6
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	15	0.6
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	9	0.6
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	15	0.6
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	15	0.6
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	15	0.6
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	15	0.6
(2,330)	1:44:A:LEU:H	1:44:A:LEU:HG	4	0.6
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	15	0.6
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	10	0.6
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	13	0.6
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	13	0.6
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	13	0.59
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	15	0.59
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	16	0.59
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	10	0.59
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	3	0.59
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	3	0.59
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	15	0.59
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	15	0.59
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	4	0.59
(2,1404)	1:28:D:LEU:H	1:24:D:ALA:HA	13	0.59
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	4	0.59
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	7	0.59
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	10	0.59
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	15	0.59
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	15	0.59
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	20	0.59
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	10	0.59
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	7	0.59
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	15	0.59
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	15	0.59
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	20	0.58
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	1	0.58
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	15	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	19	0.58
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	15	0.58
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	13	0.58
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	15	0.58
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB2	12	0.58
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB3	12	0.58
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	10	0.58
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	10	0.58
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	19	0.58
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	19	0.58
(2,1818)	1:28:E:LEU:H	1:24:E:ALA:HA	13	0.58
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB2	12	0.58
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB3	12	0.58
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	10	0.58
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	3	0.58
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	3	0.58
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	20	0.58
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB2	12	0.58
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB3	12	0.58
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	16	0.58
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	18	0.58
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	3	0.58
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	3	0.58
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	19	0.58
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	19	0.58
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	10	0.58
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	3	0.58
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	3	0.58
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	19	0.58
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	19	0.58
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	20	0.58
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB2	12	0.58
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB3	12	0.58
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	10	0.58
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	10	0.58
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	20	0.58
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	11	0.57
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	13	0.57
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	15	0.57
(2,1572)	1:44:D:LEU:H	1:44:D:LEU:HG	16	0.57
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	10	0.57
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	10	0.57
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	10	0.57
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB2	12	0.57
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB3	12	0.57
(2,744)	1:44:B:LEU:H	1:44:B:LEU:HG	4	0.57
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	10	0.57
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	10	0.57
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	10	0.57
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	3	0.57
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	3	0.57
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	19	0.57
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	19	0.57
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	2	0.56
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	1	0.56
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	14	0.56
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	16	0.56
(2,2071)	1:33:A:ILE:CA	1:37:E:LEU:CA	12	0.56
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	1	0.56
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	10	0.56
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	19	0.56
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	19	0.56
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	1	0.56
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	10	0.56
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	10	0.56
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	14	0.56
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	14	0.56
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	14	0.56
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	19	0.55
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	20	0.55
(2,2075)	1:33:E:ILE:CA	1:37:D:LEU:CA	12	0.55
(2,2073)	1:33:C:ILE:CA	1:37:B:LEU:CA	12	0.55
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	12	0.55
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	1	0.55
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	14	0.55
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB2	13	0.55
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB3	13	0.55
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	4	0.55
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	14	0.55
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	14	0.55
(2,2072)	1:33:B:ILE:CA	1:37:A:LEU:CA	12	0.54
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	2	0.54
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	7	0.54
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	7	0.54
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	14	0.54
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	14	0.54
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	4	0.54
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	14	0.54
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	12	0.54
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	1	0.54
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	2	0.54
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	2	0.54
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	14	0.54
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	14	0.54
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	4	0.54
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	14	0.54
(2,330)	1:44:A:LEU:H	1:44:A:LEU:HG	8	0.54
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	4	0.54
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	1	0.54
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	1	0.54
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	20	0.53
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB2	11	0.53
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB3	11	0.53
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB2	13	0.53
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB3	13	0.53
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	4	0.53
(2,1839)	1:30:E:ASN:H	1:26:E:GLN:HA	2	0.53
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB2	11	0.53
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB3	11	0.53
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB2	13	0.53
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB3	13	0.53
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	1	0.53
(2,1425)	1:30:D:ASN:H	1:26:D:GLN:HA	2	0.53
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	7	0.53
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	7	0.53
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB2	11	0.53
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB3	11	0.53
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB2	13	0.53
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB3	13	0.53
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	10	0.53
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	12	0.53
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	4	0.53
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	14	0.53
(2,1011)	1:30:C:ASN:H	1:26:C:GLN:HA	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	7	0.53
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	7	0.53
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	11	0.53
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	11	0.53
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB2	11	0.53
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB3	11	0.53
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB2	13	0.53
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB3	13	0.53
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	4	0.53
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	12	0.53
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	1	0.53
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	2	0.53
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	12	0.53
(2,2110)	1:33:E:ILE:CG2	1:37:D:LEU:CA	11	0.52
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	14	0.52
(2,2074)	1:33:D:ILE:CA	1:37:C:LEU:CA	12	0.52
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	8	0.52
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	20	0.52
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	2	0.52
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	2	0.52
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	11	0.52
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	11	0.52
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	4	0.52
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	2	0.52
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	11	0.52
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	1	0.52
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	2	0.52
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	2	0.52
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	11	0.52
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	11	0.52
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	2	0.52
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	20	0.52
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	2	0.52
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	2	0.52
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	2	0.52
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	11	0.52
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	11	0.52
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB2	11	0.52
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB3	11	0.52
(2,183)	1:30:A:ASN:H	1:26:A:GLN:HA	2	0.52
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	2	0.52
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	2	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	7	0.52
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	7	0.52
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	8	0.52
(2,2110)	1:33:E:ILE:CG2	1:37:D:LEU:CA	12	0.51
(2,2110)	1:33:E:ILE:CG2	1:37:D:LEU:CA	15	0.51
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	15	0.51
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	19	0.51
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	15	0.51
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	12	0.51
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	19	0.51
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	7	0.51
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	11	0.51
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	17	0.51
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	8	0.51
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	8	0.51
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	9	0.51
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	9	0.51
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	18	0.51
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	18	0.51
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	8	0.51
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	12	0.51
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	7	0.51
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	17	0.51
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	20	0.51
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	8	0.51
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	8	0.51
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	14	0.51
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	14	0.51
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	8	0.51
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	5	0.51
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	1	0.51
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	7	0.51
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	11	0.51
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	12	0.51
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	8	0.51
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	8	0.51
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	8	0.51
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	11	0.51
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	7	0.51
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	7	0.51
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	8	0.51
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	11	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	17	0.51
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	20	0.51
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	9	0.51
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	9	0.51
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	11	0.51
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	11	0.51
(2,2110)	1:33:E:ILE:CG2	1:37:D:LEU:CA	13	0.5
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	19	0.5
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	16	0.5
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	13	0.5
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	15	0.5
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	1	0.5
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	16	0.5
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	19	0.5
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	12	0.5
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	1	0.5
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	1	0.5
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	17	0.5
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	17	0.5
(2,1572)	1:44:D:LEU:H	1:44:D:LEU:HG	8	0.5
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	1	0.5
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	16	0.5
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	3	0.5
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	16	0.5
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	9	0.5
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	9	0.5
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	18	0.5
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	18	0.5
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	4	0.5
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	19	0.5
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	1	0.5
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	1	0.5
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	9	0.5
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	9	0.5
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	18	0.5
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	18	0.5
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	1	0.5
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	17	0.5
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	20	0.5
(2,597)	1:30:B:ASN:H	1:26:B:GLN:HA	2	0.5
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	8	0.5
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	8	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	9	0.5
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	9	0.5
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	18	0.5
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	18	0.5
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	1	0.5
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	3	0.5
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	7	0.5
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	19	0.5
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	8	0.5
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	8	0.5
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	17	0.5
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	17	0.5
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	18	0.5
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	18	0.5
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	15	0.49
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	12	0.49
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	13	0.49
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	19	0.49
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	16	0.49
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	3	0.49
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	5	0.49
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	5	0.49
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	8	0.49
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	12	0.49
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	1	0.49
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	1	0.49
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	17	0.49
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	17	0.49
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	8	0.49
(2,1158)	1:44:C:LEU:H	1:44:C:LEU:HG	8	0.49
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	3	0.49
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	12	0.49
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	16	0.49
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	17	0.49
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	4	0.49
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	18	0.49
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	18	0.49
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	8	0.49
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	3	0.49
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	7	0.49
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	12	0.49
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	16	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	19	0.49
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	12	0.49
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	1	0.49
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	1	0.49
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	8	0.49
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	16	0.49
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	16	0.49
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	12	0.49
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	1	0.49
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	1	0.49
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	8	0.49
(2,2110)	1:33:E:ILE:CG2	1:37:D:LEU:CA	16	0.48
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	12	0.48
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	16	0.48
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	12	0.48
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	6	0.48
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	9	0.48
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	12	0.48
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	1	0.48
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	6	0.48
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	6	0.48
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	6	0.48
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	19	0.48
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	5	0.48
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	5	0.48
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	18	0.48
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	18	0.48
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	16	0.48
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	9	0.48
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	5	0.48
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	5	0.48
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	17	0.48
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	17	0.48
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	3	0.48
(2,948)	1:19:C:GLU:H	1:18:C:ILE:HA	16	0.48
(2,744)	1:44:B:LEU:H	1:44:B:LEU:HG	8	0.48
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	16	0.48
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	9	0.48
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	1	0.48
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	5	0.48
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	5	0.48
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	17	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	17	0.48
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	3	0.48
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	5	0.48
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	5	0.48
(2,120)	1:19:A:GLU:H	1:18:A:ILE:HA	16	0.48
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	13	0.47
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	13	0.47
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	16	0.47
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	19	0.47
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	15	0.47
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	18	0.47
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	18	0.47
(2,1776)	1:19:E:GLU:H	1:18:E:ILE:HA	16	0.47
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	13	0.47
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	9	0.47
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	13	0.47
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	1	0.47
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	6	0.47
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	6	0.47
(2,1362)	1:19:D:GLU:H	1:18:D:ILE:HA	16	0.47
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	6	0.47
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	15	0.47
(2,985)	1:27:C:ASN:H	1:25:C:ARG:H	3	0.47
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	19	0.47
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	6	0.47
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	18	0.47
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	18	0.47
(2,534)	1:19:B:GLU:H	1:18:B:ILE:HA	16	0.47
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	6	0.47
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	9	0.47
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	13	0.47
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	15	0.47
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	4	0.47
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	18	0.47
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	18	0.47
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	3	0.47
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	5	0.46
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	7	0.46
(2,1874)	1:34:E:ASN:H	1:31:E:LEU:HA	13	0.46
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	13	0.46
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	15	0.46
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	13	0.46
(2,1046)	1:34:C:ASN:H	1:31:C:LEU:HA	19	0.46
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	13	0.46
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	4	0.46
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	6	0.46
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	6	0.46
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	2	0.46
(2,632)	1:34:B:ASN:H	1:31:B:LEU:HA	13	0.46
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	13	0.46
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	15	0.46
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	1	0.46
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	4	0.46
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	6	0.46
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	6	0.46
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	19	0.46
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	12	0.46
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	1	0.46
(2,183)	1:30:A:ASN:H	1:26:A:GLN:HA	9	0.46
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	6	0.46
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	6	0.46
(2,2106)	1:33:A:ILE:CG2	1:37:E:LEU:CA	10	0.45
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	5	0.45
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	8	0.45
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	4	0.45
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	3	0.45
(2,1460)	1:34:D:ASN:H	1:31:D:LEU:HA	19	0.45
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	4	0.45
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	20	0.45
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	5	0.45
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	1	0.45
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	20	0.45
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	5	0.45
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	8	0.45
(2,218)	1:34:A:ASN:H	1:31:A:LEU:HA	13	0.45
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	8	0.45
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	7	0.44
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	7	0.44
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	16	0.44
(2,2106)	1:40:A:ILE:CG2	1:44:E:LEU:CA	6	0.44
(2,1813)	1:27:E:ASN:H	1:25:E:ARG:H	3	0.44
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	2	0.44
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	8	0.44
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	17	0.44
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	4	0.44
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	4	0.44
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	8	0.44
(2,985)	1:27:C:ASN:H	1:25:C:ARG:H	16	0.44
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	20	0.44
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	5	0.44
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	4	0.44
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	4	0.44
(2,157)	1:27:A:ASN:H	1:25:A:ARG:H	16	0.44
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	14	0.43
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	17	0.43
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	6	0.43
(2,2109)	1:33:D:ILE:CG2	1:37:C:LEU:CA	10	0.43
(2,2108)	1:33:C:ILE:CG2	1:37:B:LEU:CA	10	0.43
(2,2107)	1:33:B:ILE:CG2	1:37:A:LEU:CA	10	0.43
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	2	0.43
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	17	0.43
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	20	0.43
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	12	0.43
(2,1839)	1:30:E:ASN:H	1:26:E:GLN:HA	9	0.43
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	4	0.43
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	4	0.43
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	15	0.43
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	14	0.43
(2,1399)	1:27:D:ASN:H	1:25:D:ARG:H	3	0.43
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	15	0.43
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB2	19	0.43
(2,1240)	1:52:C:LEU:H	1:52:C:LEU:HB3	19	0.43
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	4	0.43
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	4	0.43
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB2	19	0.43
(2,826)	1:52:B:LEU:H	1:52:B:LEU:HB3	19	0.43
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	4	0.43
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	4	0.43
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG2	20	0.43
(2,594)	1:29:B:GLN:H	1:29:B:GLN:HG3	20	0.43
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	18	0.43
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	15	0.43
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	20	0.43
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	18	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	15	0.43
(2,2110)	1:33:E:ILE:CG2	1:37:D:LEU:CA	10	0.42
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	6	0.42
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB2	19	0.42
(2,2068)	1:52:E:LEU:H	1:52:E:LEU:HB3	19	0.42
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	18	0.42
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	2	0.42
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG2	20	0.42
(2,1422)	1:29:D:GLN:H	1:29:D:GLN:HG3	20	0.42
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	2	0.42
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	15	0.42
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	2	0.42
(2,571)	1:27:B:ASN:H	1:25:B:ARG:H	3	0.42
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB2	19	0.42
(2,412)	1:52:A:LEU:H	1:52:A:LEU:HB3	19	0.42
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	2	0.42
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG2	20	0.42
(2,180)	1:29:A:GLN:H	1:29:A:GLN:HG3	20	0.42
(2,157)	1:27:A:ASN:H	1:25:A:ARG:H	3	0.42
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	1	0.41
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	2	0.41
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG2	20	0.41
(2,1836)	1:29:E:GLN:H	1:29:E:GLN:HG3	20	0.41
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB2	19	0.41
(2,1654)	1:52:D:LEU:H	1:52:D:LEU:HB3	19	0.41
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	12	0.41
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	17	0.41
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	12	0.41
(2,1011)	1:30:C:ASN:H	1:26:C:GLN:HA	9	0.41
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG2	20	0.41
(2,1008)	1:29:C:GLN:H	1:29:C:GLN:HG3	20	0.41
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	18	0.41
(2,597)	1:30:B:ASN:H	1:26:B:GLN:HA	9	0.41
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	12	0.4
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	18	0.4
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	20	0.4
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	14	0.4
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	12	0.4
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	12	0.4
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	17	0.4
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	12	0.4
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	12	0.39
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	14	0.39
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	1	0.39
(2,1425)	1:30:D:ASN:H	1:26:D:GLN:HA	9	0.39
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	20	0.39
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	7	0.39
(2,684)	1:39:B:LEU:H	1:36:B:CYS:HA	9	0.39
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	17	0.39
(2,526)	1:18:B:ILE:H	1:17:B:THR:HA	11	0.39
(2,157)	1:27:A:ASN:H	1:25:A:ARG:H	8	0.39
(2,1859)	1:32:E:PHE:H	1:31:E:LEU:HB2	18	0.38
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	3	0.38
(2,1768)	1:18:E:ILE:H	1:17:E:THR:HA	11	0.38
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	7	0.38
(2,1399)	1:27:D:ASN:H	1:25:D:ARG:H	8	0.38
(2,1354)	1:18:D:ILE:H	1:17:D:THR:HA	11	0.38
(2,985)	1:27:C:ASN:H	1:25:C:ARG:H	8	0.38
(2,940)	1:18:C:ILE:H	1:17:C:THR:HA	11	0.38
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	20	0.38
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	2	0.38
(2,112)	1:18:A:ILE:H	1:17:A:THR:HA	11	0.38
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	6	0.37
(2,1817)	1:28:E:LEU:H	1:25:E:ARG:HA	10	0.37
(2,1813)	1:27:E:ASN:H	1:25:E:ARG:H	8	0.37
(2,1445)	1:32:D:PHE:H	1:31:D:LEU:HB2	18	0.37
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	12	0.37
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD11	20	0.37
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD12	20	0.37
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD13	20	0.37
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	7	0.37
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	1	0.37
(2,1031)	1:32:C:PHE:H	1:31:C:LEU:HB2	18	0.37
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	1	0.37
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	12	0.37
(2,617)	1:32:B:PHE:H	1:31:B:LEU:HB2	18	0.37
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	6	0.37
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	14	0.37
(2,571)	1:27:B:ASN:H	1:25:B:ARG:H	8	0.37
(2,203)	1:32:A:PHE:H	1:31:A:LEU:HB2	18	0.37
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	3	0.37
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	1	0.37
(2,2110)	1:40:E:ILE:CG2	1:44:D:LEU:CA	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	14	0.36
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD11	20	0.36
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD12	20	0.36
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD13	20	0.36
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	6	0.36
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	7	0.36
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	6	0.36
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	3	0.36
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	11	0.36
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	17	0.35
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	7	0.35
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	6	0.35
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	20	0.35
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	13	0.35
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	13	0.35
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	14	0.35
(2,1403)	1:28:D:LEU:H	1:25:D:ARG:HA	10	0.35
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	2	0.35
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	3	0.35
(2,956)	1:20:C:MET:H	1:19:C:GLU:HA	20	0.35
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD11	20	0.35
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD12	20	0.35
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD13	20	0.35
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	6	0.35
(2,684)	1:39:B:LEU:H	1:36:B:CYS:HA	7	0.35
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	11	0.35
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	13	0.35
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	13	0.35
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	6	0.35
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	9	0.35
(2,161)	1:28:A:LEU:H	1:25:A:ARG:HA	10	0.35
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	5	0.34
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	19	0.34
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	19	0.34
(2,1839)	1:30:E:ASN:H	1:26:E:GLN:HA	18	0.34
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	11	0.34
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG12	16	0.34
(2,1783)	1:20:E:MET:H	1:18:E:ILE:HG13	16	0.34
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD11	5	0.34
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD12	5	0.34
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD13	5	0.34
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1425)	1:30:D:ASN:H	1:26:D:GLN:HA	5	0.34
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	1	0.34
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	13	0.34
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	13	0.34
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD11	5	0.34
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD12	5	0.34
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD13	5	0.34
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD11	20	0.34
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD12	20	0.34
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD13	20	0.34
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD11	10	0.34
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD12	10	0.34
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD13	10	0.34
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	6	0.34
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	19	0.34
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	12	0.34
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	13	0.34
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	13	0.34
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD11	5	0.34
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD12	5	0.34
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD13	5	0.34
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	1	0.34
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD11	5	0.34
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD12	5	0.34
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD13	5	0.34
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD11	20	0.34
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD12	20	0.34
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD13	20	0.34
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	6	0.34
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	7	0.34
(2,183)	1:30:A:ASN:H	1:26:A:GLN:HA	5	0.34
(2,183)	1:30:A:ASN:H	1:26:A:GLN:HA	18	0.34
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	20	0.34
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	13	0.34
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	13	0.34
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD11	5	0.34
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD12	5	0.34
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD13	5	0.34
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD11	20	0.34
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD12	20	0.34
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD13	20	0.34
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	8	0.33
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	6	0.33
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	7	0.33
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	9	0.33
(2,1811)	1:27:E:ASN:H	1:24:E:ALA:HA	14	0.33
(2,1784)	1:20:E:MET:H	1:19:E:GLU:HA	20	0.33
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	3	0.33
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	11	0.33
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	11	0.33
(2,1370)	1:20:D:MET:H	1:19:D:GLU:HA	20	0.33
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG12	16	0.33
(2,1369)	1:20:D:MET:H	1:18:D:ILE:HG13	16	0.33
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	17	0.33
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	9	0.33
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	15	0.33
(2,1011)	1:30:C:ASN:H	1:26:C:GLN:HA	18	0.33
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	11	0.33
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	16	0.33
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	16	0.33
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	8	0.33
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	7	0.33
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	14	0.33
(2,597)	1:30:B:ASN:H	1:26:B:GLN:HA	18	0.33
(2,542)	1:20:B:MET:H	1:19:B:GLU:HA	3	0.33
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	16	0.33
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	16	0.33
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	11	0.33
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	14	0.33
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	15	0.33
(2,128)	1:20:A:MET:H	1:19:A:GLU:HA	20	0.33
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	16	0.33
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	16	0.33
(2,2108)	1:40:C:ILE:CG2	1:44:B:LEU:CA	1	0.32
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	4	0.32
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	8	0.32
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	15	0.32
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	14	0.32
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	4	0.32
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	8	0.32
(2,1425)	1:30:D:ASN:H	1:26:D:GLN:HA	18	0.32
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	14	0.32
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	7	0.32
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	14	0.32
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	14	0.32
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	8	0.32
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	12	0.32
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	9	0.32
(2,575)	1:28:B:LEU:H	1:25:B:ARG:HA	10	0.32
(2,542)	1:20:B:MET:H	1:19:B:GLU:HA	20	0.32
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	14	0.32
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	8	0.32
(2,250)	1:37:A:LEU:H	1:34:A:ASN:HA	19	0.32
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	8	0.32
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	7	0.32
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	16	0.32
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	14	0.32
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	15	0.31
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	14	0.31
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	9	0.31
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	11	0.31
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	12	0.31
(2,1851)	1:31:E:LEU:H	1:27:E:ASN:HA	14	0.31
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	3	0.31
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	6	0.31
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	8	0.31
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	7	0.31
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	9	0.31
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	9	0.31
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	15	0.31
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	3	0.31
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	8	0.31
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	7	0.31
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	9	0.31
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	3	0.31
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	9	0.31
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	15	0.31
(2,597)	1:30:B:ASN:H	1:26:B:GLN:HA	5	0.31
(2,569)	1:27:B:ASN:H	1:24:B:ALA:HA	14	0.31
(2,330)	1:44:A:LEU:H	1:44:A:LEU:HG	13	0.31
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	9	0.31
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	12	0.31
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	5	0.3
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1397)	1:27:D:ASN:H	1:24:D:ALA:HA	14	0.3
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	11	0.3
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	6	0.3
(2,1011)	1:30:C:ASN:H	1:26:C:GLN:HA	5	0.3
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	11	0.3
(2,609)	1:31:B:LEU:H	1:27:B:ASN:HA	14	0.3
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	6	0.3
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	15	0.3
(2,270)	1:39:A:LEU:H	1:36:A:CYS:HA	19	0.3
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	3	0.3
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	13	0.29
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	13	0.29
(2,1839)	1:30:E:ASN:H	1:26:E:GLN:HA	5	0.29
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	2	0.29
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	16	0.29
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	3	0.29
(2,1572)	1:44:D:LEU:H	1:44:D:LEU:HG	4	0.29
(2,1447)	1:32:D:PHE:H	1:29:D:GLN:HA	18	0.29
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	9	0.29
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	2	0.29
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	16	0.29
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	20	0.29
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	6	0.29
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	19	0.29
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	9	0.29
(2,983)	1:27:C:ASN:H	1:24:C:ALA:HA	14	0.29
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	2	0.29
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	2	0.29
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	16	0.29
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	19	0.29
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	13	0.29
(2,152)	1:26:A:GLN:H	1:24:A:ALA:H	2	0.29
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	2	0.29
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	16	0.29
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	20	0.29
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	4	0.28
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	18	0.28
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	17	0.28
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	11	0.28
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	7	0.28
(2,1808)	1:26:E:GLN:H	1:24:E:ALA:H	2	0.28
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD11	10	0.28
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD12	10	0.28
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD13	10	0.28
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	15	0.28
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB2	3	0.28
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB3	3	0.28
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	19	0.28
(2,1437)	1:31:D:LEU:H	1:27:D:ASN:HA	14	0.28
(2,1394)	1:26:D:GLN:H	1:24:D:ALA:H	2	0.28
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	4	0.28
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	16	0.28
(2,1033)	1:32:C:PHE:H	1:29:C:GLN:HA	18	0.28
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	16	0.28
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	16	0.28
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD11	20	0.28
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD12	20	0.28
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD13	20	0.28
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	3	0.28
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	19	0.28
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	9	0.28
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	13	0.28
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	3	0.28
(2,330)	1:44:A:LEU:H	1:44:A:LEU:HG	7	0.28
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	9	0.28
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	3	0.27
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	3	0.27
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	14	0.27
(2,1861)	1:32:E:PHE:H	1:29:E:GLN:HA	18	0.27
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	6	0.27
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	18	0.27
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	5	0.27
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	14	0.27
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	18	0.27
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	6	0.27
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	13	0.27
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	17	0.27
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	5	0.27
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	14	0.27
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	13	0.27
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	20	0.27
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	15	0.27
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,619)	1:32:B:PHE:H	1:29:B:GLN:HA	18	0.27
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	3	0.27
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	4	0.27
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	16	0.27
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	3	0.27
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	11	0.27
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	14	0.27
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	17	0.27
(2,205)	1:32:A:PHE:H	1:29:A:GLN:HA	18	0.27
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	6	0.27
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	3	0.26
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	3	0.26
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	6	0.26
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	11	0.26
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	17	0.26
(2,1572)	1:44:D:LEU:H	1:44:D:LEU:HG	18	0.26
(2,1512)	1:39:D:LEU:H	1:36:D:CYS:HA	11	0.26
(2,1512)	1:39:D:LEU:H	1:36:D:CYS:HA	19	0.26
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	3	0.26
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	6	0.26
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	11	0.26
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	17	0.26
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	20	0.26
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	13	0.26
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	3	0.26
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	15	0.26
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	19	0.26
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	2	0.26
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	3	0.26
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	11	0.26
(2,980)	1:26:C:GLN:H	1:24:C:ALA:H	2	0.26
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD11	10	0.26
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD12	10	0.26
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD13	10	0.26
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	11	0.26
(2,684)	1:39:B:LEU:H	1:36:B:CYS:HA	19	0.26
(2,664)	1:37:B:LEU:H	1:34:B:ASN:HA	5	0.26
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	3	0.26
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	11	0.26
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	17	0.26
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	20	0.26
(2,566)	1:26:B:GLN:H	1:24:B:ALA:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	18	0.26
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	11	0.26
(2,330)	1:44:A:LEU:H	1:44:A:LEU:HG	16	0.26
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	20	0.26
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	18	0.26
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	19	0.26
(2,155)	1:27:A:ASN:H	1:24:A:ALA:HA	14	0.26
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	13	0.26
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	10	0.25
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	10	0.25
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	10	0.25
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	7	0.25
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	9	0.25
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	16	0.25
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	18	0.25
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	6	0.25
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	20	0.25
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	18	0.25
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	16	0.25
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	19	0.25
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	4	0.25
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	13	0.25
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	18	0.25
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	13	0.25
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	1	0.25
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	4	0.25
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	18	0.25
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	1	0.25
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	20	0.25
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	6	0.25
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	17	0.25
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	20	0.25
(2,1023)	1:31:C:LEU:H	1:27:C:ASN:HA	14	0.25
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	4	0.25
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	18	0.25
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	4	0.25
(2,684)	1:39:B:LEU:H	1:36:B:CYS:HA	4	0.25
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	5	0.25
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	4	0.25
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	13	0.25
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	17	0.25
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	6	0.25
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	4	0.25
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	18	0.25
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	19	0.24
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	1	0.24
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	20	0.24
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	8	0.24
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	9	0.24
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	7	0.24
(2,1829)	1:29:E:GLN:H	1:28:E:LEU:HG	5	0.24
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	13	0.24
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	19	0.24
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	5	0.24
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	16	0.24
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	19	0.24
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB2	5	0.24
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB3	5	0.24
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	17	0.24
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	8	0.24
(2,1467)	1:27:D:ASN:HD21	1:27:D:ASN:HB3	19	0.24
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	2	0.24
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	7	0.24
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	16	0.24
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	13	0.24
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	19	0.24
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	1	0.24
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	9	0.24
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	5	0.24
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	5	0.24
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD11	15	0.24
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD12	15	0.24
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD13	15	0.24
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	13	0.24
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	13	0.24
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	6	0.24
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	9	0.24
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	1	0.24
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	2	0.24
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	6	0.24
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	9	0.24
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	16	0.24
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	8	0.24
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	9	0.24
(2,225)	1:27:A:ASN:HD21	1:27:A:ASN:HB3	19	0.24
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	7	0.24
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	13	0.24
(2,1986)	1:44:E:LEU:H	1:44:E:LEU:HG	16	0.23
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	18	0.23
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	1	0.23
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	2	0.23
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	5	0.23
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	10	0.23
(2,1881)	1:27:E:ASN:HD21	1:27:E:ASN:HB3	19	0.23
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD11	15	0.23
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD12	15	0.23
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD13	15	0.23
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	17	0.23
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	1	0.23
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	2	0.23
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	5	0.23
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	9	0.23
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	5	0.23
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD11	15	0.23
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD12	15	0.23
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD13	15	0.23
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	17	0.23
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	10	0.23
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	11	0.23
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	2	0.23
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	4	0.23
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	5	0.23
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	8	0.23
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	10	0.23
(2,1053)	1:27:C:ASN:HD21	1:27:C:ASN:HB3	19	0.23
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	17	0.23
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	19	0.23
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	18	0.23
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	19	0.23
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	5	0.23
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	8	0.23
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	10	0.23
(2,639)	1:27:B:ASN:HD21	1:27:B:ASN:HB3	19	0.23
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,587)	1:29:B:GLN:H	1:28:B:LEU:HG	19	0.23
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD11	15	0.23
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD12	15	0.23
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD13	15	0.23
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	17	0.23
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	19	0.23
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	13	0.23
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	2	0.23
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	4	0.23
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	5	0.23
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	10	0.23
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	5	0.23
(2,195)	1:31:A:LEU:H	1:27:A:ASN:HA	14	0.23
(2,173)	1:29:A:GLN:H	1:28:A:LEU:HG	5	0.23
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD11	15	0.23
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD12	15	0.23
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD13	15	0.23
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	17	0.23
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	11	0.22
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	13	0.22
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	5	0.22
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	12	0.22
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	4	0.22
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	18	0.22
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	11	0.22
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	14	0.22
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	2	0.22
(2,1852)	1:31:E:LEU:H	1:30:E:ASN:HD21	5	0.22
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD11	2	0.22
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD12	2	0.22
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD13	2	0.22
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	9	0.22
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	12	0.22
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	4	0.22
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	10	0.22
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	18	0.22
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	1	0.22
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	11	0.22
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	14	0.22
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	17	0.22
(2,1438)	1:31:D:LEU:H	1:30:D:ASN:HD21	5	0.22
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	13	0.22
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	18	0.22
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	9	0.22
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	12	0.22
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	18	0.22
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	11	0.22
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	18	0.22
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD11	2	0.22
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD12	2	0.22
(2,775)	1:47:B:ILE:H	1:47:B:ILE:HD13	2	0.22
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	9	0.22
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	13	0.22
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	1	0.22
(2,684)	1:39:B:LEU:H	1:36:B:CYS:HA	14	0.22
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	4	0.22
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	3	0.22
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	11	0.22
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	14	0.22
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	18	0.22
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	13	0.22
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	6	0.22
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	1	0.22
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	9	0.22
(2,270)	1:39:A:LEU:H	1:36:A:CYS:HA	5	0.22
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	18	0.22
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	6	0.22
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	14	0.22
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	17	0.22
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	7	0.21
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	5	0.21
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	18	0.21
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	10	0.21
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	13	0.21
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	2	0.21
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	3	0.21
(2,1881)	1:27:E:ASN:HD21	1:27:E:ASN:HB3	14	0.21
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	6	0.21
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	17	0.21
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	20	0.21
(2,1861)	1:32:E:PHE:H	1:29:E:GLN:HA	2	0.21
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	6	0.21
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1529)	1:39:D:LEU:H	1:35:D:PHE:HD1	20	0.21
(2,1529)	1:39:D:LEU:H	1:35:D:PHE:HD2	20	0.21
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	13	0.21
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	3	0.21
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	20	0.21
(2,1467)	1:27:D:ASN:HD21	1:27:D:ASN:HB3	14	0.21
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	6	0.21
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	20	0.21
(2,1447)	1:32:D:PHE:H	1:29:D:GLN:HA	2	0.21
(2,1415)	1:29:D:GLN:H	1:28:D:LEU:HG	19	0.21
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	13	0.21
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	2	0.21
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	6	0.21
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	14	0.21
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	17	0.21
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	20	0.21
(2,1033)	1:32:C:PHE:H	1:29:C:GLN:HA	2	0.21
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	2	0.21
(2,1024)	1:31:C:LEU:H	1:30:C:ASN:HD21	7	0.21
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	4	0.21
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	16	0.21
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	17	0.21
(2,664)	1:37:B:LEU:H	1:34:B:ASN:HA	12	0.21
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	18	0.21
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	2	0.21
(2,639)	1:27:B:ASN:HD21	1:27:B:ASN:HB3	14	0.21
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	1	0.21
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	6	0.21
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	17	0.21
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	20	0.21
(2,619)	1:32:B:PHE:H	1:29:B:GLN:HA	2	0.21
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	2	0.21
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	9	0.21
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	18	0.21
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	2	0.21
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	3	0.21
(2,225)	1:27:A:ASN:HD21	1:27:A:ASN:HB3	14	0.21
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	3	0.21
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	11	0.21
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	20	0.21
(2,2109)	1:40:D:ILE:CG2	1:44:C:LEU:CA	7	0.2
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	2	0.2
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	2	0.2
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	2	0.2
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	19	0.2
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	19	0.2
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	5	0.2
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	18	0.2
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	1	0.2
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	3	0.2
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	13	0.2
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	9	0.2
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	16	0.2
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	8	0.2
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	2	0.2
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	3	0.2
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	13	0.2
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	1	0.2
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	4	0.2
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	13	0.2
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	6	0.2
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	16	0.2
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	2	0.2
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	8	0.2
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	2	0.2
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	3	0.2
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	20	0.2
(2,1053)	1:27:C:ASN:HD21	1:27:C:ASN:HB3	14	0.2
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	3	0.2
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	13	0.2
(2,1001)	1:29:C:GLN:H	1:28:C:LEU:HG	19	0.2
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	19	0.2
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	13	0.2
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	13	0.2
(2,684)	1:39:B:LEU:H	1:36:B:CYS:HA	8	0.2
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	13	0.2
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	20	0.2
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	3	0.2
(2,610)	1:31:B:LEU:H	1:30:B:ASN:HD21	7	0.2
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	20	0.2
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	7	0.2
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	14	0.2
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	2	0.2
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	20	0.2
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	1	0.2
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	13	0.2
(2,196)	1:31:A:LEU:H	1:30:A:ASN:HD21	2	0.2
(2,113)	1:18:A:ILE:H	1:17:A:THR:H	11	0.2
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	4	0.2
(2,2107)	1:40:B:ILE:CG2	1:44:A:LEU:CA	7	0.19
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	3	0.19
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	4	0.19
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	11	0.19
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	12	0.19
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	6	0.19
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	2	0.19
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	3	0.19
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	4	0.19
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	8	0.19
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	15	0.19
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	20	0.19
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	9	0.19
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	13	0.19
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	16	0.19
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	19	0.19
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	1	0.19
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	3	0.19
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	4	0.19
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	8	0.19
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	14	0.19
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	16	0.19
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	7	0.19
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	7	0.19
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	10	0.19
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	3	0.19
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	5	0.19
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	15	0.19
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	9	0.19
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	16	0.19
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	19	0.19
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	3	0.19
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	8	0.19
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	16	0.19
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	9	0.19
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	20	0.19
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	13	0.19
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	19	0.19
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	9	0.19
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	9	0.19
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	14	0.19
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	15	0.19
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	1	0.19
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	9	0.19
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	16	0.19
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	3	0.19
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	20	0.19
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	7	0.19
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	10	0.19
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	20	0.19
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	16	0.19
(2,699)	1:40:B:ILE:H	1:37:B:LEU:HA	7	0.19
(2,664)	1:37:B:LEU:H	1:34:B:ASN:HA	18	0.19
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	2	0.19
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	8	0.19
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	15	0.19
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	9	0.19
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	13	0.19
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	15	0.19
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	16	0.19
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	19	0.19
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	1	0.19
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	3	0.19
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	4	0.19
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	8	0.19
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	20	0.19
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	16	0.19
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	3	0.19
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	12	0.19
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	5	0.19
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	10	0.19
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	19	0.19
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	2	0.19
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	15	0.19
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	16	0.19
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:32:A:PHE:H	1:29:A:GLN:HA	2	0.19
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	19	0.19
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	19	0.19
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	1	0.19
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	3	0.19
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	8	0.19
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	20	0.18
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	20	0.18
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	20	0.18
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	10	0.18
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	5	0.18
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	5	0.18
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	2	0.18
(2,1946)	1:41:E:CYS:H	1:38:E:ILE:HA	13	0.18
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	2	0.18
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	7	0.18
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	9	0.18
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	11	0.18
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	16	0.18
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	20	0.18
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	8	0.18
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	7	0.18
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	16	0.18
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	12	0.18
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	15	0.18
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	7	0.18
(2,1813)	1:27:E:ASN:H	1:25:E:ARG:H	13	0.18
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	16	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	3	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	7	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	9	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	11	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	17	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	18	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	19	0.18
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	20	0.18
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	4	0.18
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	11	0.18
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	12	0.18
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD11	20	0.18
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD12	20	0.18
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD13	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	13	0.18
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	2	0.18
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	4	0.18
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	8	0.18
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	9	0.18
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	11	0.18
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	8	0.18
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	7	0.18
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	16	0.18
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	4	0.18
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	5	0.18
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	12	0.18
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	15	0.18
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	7	0.18
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD11	12	0.18
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD12	12	0.18
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD13	12	0.18
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	9	0.18
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	17	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	3	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	4	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	5	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	6	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	7	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	8	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	9	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	11	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	14	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	15	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	16	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	17	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	18	0.18
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	19	0.18
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	4	0.18
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	7	0.18
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	11	0.18
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	2	0.18
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	10	0.18
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	14	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	1	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	3	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	5	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	6	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	7	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	8	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	19	0.18
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	20	0.18
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	7	0.18
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	16	0.18
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	4	0.18
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	12	0.18
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	15	0.18
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	7	0.18
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	17	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	3	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	4	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	5	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	6	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	7	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	9	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	14	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	15	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	16	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	17	0.18
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	18	0.18
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	1	0.18
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	4	0.18
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	8	0.18
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	17	0.18
(2,750)	1:45:B:ILE:H	1:42:B:LEU:HA	5	0.18
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	2	0.18
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	3	0.18
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	4	0.18
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	5	0.18
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	7	0.18
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	14	0.18
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	7	0.18
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	16	0.18
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	5	0.18
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	12	0.18
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	17	0.18
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	19	0.18
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	11	0.18
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	18	0.18
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	9	0.18
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	16	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	3	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	4	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	6	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	7	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	9	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	10	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	11	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	14	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	17	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	18	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	19	0.18
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	20	0.18
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	4	0.18
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	11	0.18
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	16	0.18
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD11	20	0.18
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD12	20	0.18
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD13	20	0.18
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	5	0.18
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	3	0.18
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	5	0.18
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	19	0.18
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	12	0.18
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	15	0.18
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	16	0.18
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	7	0.18
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	9	0.18
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	16	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	3	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	4	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	6	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	7	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	8	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	9	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	10	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	11	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	14	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	16	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	17	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	18	0.18
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	20	0.18
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	5	0.17
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	8	0.17
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	14	0.17
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	18	0.17
(2,2025)	1:48:E:ILE:H	1:45:E:ILE:HA	12	0.17
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	19	0.17
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	19	0.17
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	19	0.17
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	15	0.17
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	15	0.17
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	9	0.17
(2,1943)	1:39:E:LEU:H	1:35:E:PHE:HD1	20	0.17
(2,1943)	1:39:E:LEU:H	1:35:E:PHE:HD2	20	0.17
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	8	0.17
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	6	0.17
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	12	0.17
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	13	0.17
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	5	0.17
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	9	0.17
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	14	0.17
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	12	0.17
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	4	0.17
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	5	0.17
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	8	0.17
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	18	0.17
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	15	0.17
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	16	0.17
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	19	0.17
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	5	0.17
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	11	0.17
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	18	0.17
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	20	0.17
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	9	0.17
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	10	0.17
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	1	0.17
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	2	0.17
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	4	0.17
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	6	0.17
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	8	0.17
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	10	0.17
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	13	0.17
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	15	0.17
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	3	0.17
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	5	0.17
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	8	0.17
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	10	0.17
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	11	0.17
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	2	0.17
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	7	0.17
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	12	0.17
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	16	0.17
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	19	0.17
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	7	0.17
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	12	0.17
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	2	0.17
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	8	0.17
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	10	0.17
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	3	0.17
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	12	0.17
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	15	0.17
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	17	0.17
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	20	0.17
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	11	0.17
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	17	0.17
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	18	0.17
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	10	0.17
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	1	0.17
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	2	0.17
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	10	0.17
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	13	0.17
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	20	0.17
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	3	0.17
(2,1197)	1:48:C:ILE:H	1:45:C:ILE:HA	12	0.17
(2,1115)	1:39:C:LEU:H	1:35:C:PHE:HD1	20	0.17
(2,1115)	1:39:C:LEU:H	1:35:C:PHE:HD2	20	0.17
(2,1113)	1:40:C:ILE:H	1:37:C:LEU:HA	17	0.17
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	16	0.17
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	17	0.17
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	3	0.17
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	5	0.17
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	8	0.17
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	12	0.17
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	5	0.17
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	8	0.17
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	10	0.17
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	18	0.17
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	4	0.17
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	12	0.17
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	15	0.17
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	5	0.17
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	11	0.17
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	18	0.17
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	20	0.17
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	1	0.17
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	8	0.17
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	1	0.17
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	2	0.17
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	8	0.17
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	10	0.17
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	11	0.17
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	13	0.17
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	19	0.17
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	3	0.17
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	5	0.17
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	11	0.17
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	12	0.17
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	14	0.17
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	18	0.17
(2,783)	1:48:B:ILE:H	1:45:B:ILE:HA	12	0.17
(2,664)	1:37:B:LEU:H	1:34:B:ASN:HA	2	0.17
(2,664)	1:37:B:LEU:H	1:34:B:ASN:HA	19	0.17
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	16	0.17
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	19	0.17
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	5	0.17
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	3	0.17
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	12	0.17
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	2	0.17
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	4	0.17
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	8	0.17
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	18	0.17
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	1	0.17
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	7	0.17
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	12	0.17
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	15	0.17
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	16	0.17
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	3	0.17
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	5	0.17
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	11	0.17
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	17	0.17
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	18	0.17
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	10	0.17
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	1	0.17
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	2	0.17
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	5	0.17
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	8	0.17
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	13	0.17
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	15	0.17
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	14	0.17
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	1	0.17
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	5	0.17
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	8	0.17
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	14	0.17
(2,369)	1:48:A:ILE:H	1:45:A:ILE:HA	12	0.17
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	10	0.17
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	20	0.17
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	13	0.17
(2,250)	1:37:A:LEU:H	1:34:A:ASN:HA	2	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	4	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	7	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	8	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	9	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	11	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	12	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	14	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	15	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	16	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	18	0.17
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	20	0.17
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	2	0.17
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	7	0.17
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	18	0.17
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	7	0.17
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	12	0.17
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	4	0.17
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	5	0.17
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	8	0.17
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	10	0.17
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	4	0.17
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	12	0.17
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	14	0.17
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	15	0.17
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	16	0.17
(2,157)	1:27:A:ASN:H	1:25:A:ARG:H	13	0.17
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	11	0.17
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	17	0.17
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	18	0.17
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	17	0.17
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	1	0.17
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	2	0.17
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	5	0.17
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	13	0.17
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	19	0.17
(2,2067)	1:52:E:LEU:H	1:52:E:LEU:HA	7	0.16
(2,2067)	1:52:E:LEU:H	1:52:E:LEU:HA	19	0.16
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	1	0.16
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	3	0.16
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	9	0.16
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	17	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	1	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	2	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	3	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	6	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	8	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	10	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	11	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	13	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	14	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	15	0.16
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	20	0.16
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	6	0.16
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	6	0.16
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	16	0.16
(2,1946)	1:41:E:CYS:H	1:38:E:ILE:HA	20	0.16
(2,1941)	1:40:E:ILE:H	1:37:E:LEU:HA	14	0.16
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	16	0.16
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	1	0.16
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	14	0.16
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	15	0.16
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	17	0.16
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	2	0.16
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	7	0.16
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	10	0.16
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	14	0.16
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	3	0.16
(2,1885)	1:34:E:ASN:H	1:34:E:ASN:HB3	19	0.16
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	13	0.16
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	16	0.16
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	2	0.16
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	10	0.16
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	19	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	1	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	3	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	4	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	5	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	8	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	9	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	11	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	12	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	14	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	17	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	18	0.16
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	20	0.16
(2,1784)	1:20:E:MET:H	1:19:E:GLU:HA	3	0.16
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	2	0.16
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	3	0.16
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	6	0.16
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	17	0.16
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD11	12	0.16
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD12	12	0.16
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD13	12	0.16
(2,1771)	1:18:E:ILE:H	1:18:E:ILE:HB	5	0.16
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	17	0.16
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	3	0.16
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	13	0.16
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	20	0.16
(2,1663)	1:3:E:LYS:H	1:3:E:LYS:HB3	12	0.16
(2,1653)	1:52:D:LEU:H	1:52:D:LEU:HA	19	0.16
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	8	0.16
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	3	0.16
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	17	0.16
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	1	0.16
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	2	0.16
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	3	0.16
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	8	0.16
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	13	0.16
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	15	0.16
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	20	0.16
(2,1611)	1:48:D:ILE:H	1:45:D:ILE:HA	12	0.16
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	2	0.16
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	10	0.16
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	14	0.16
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	18	0.16
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	6	0.16
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	14	0.16
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	15	0.16
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	18	0.16
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	20	0.16
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	2	0.16
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	3	0.16
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	5	0.16
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	9	0.16
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	14	0.16
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	18	0.16
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	3	0.16
(2,1471)	1:34:D:ASN:H	1:34:D:ASN:HB3	19	0.16
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	13	0.16
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	18	0.16
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	19	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	1	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	4	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	5	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	6	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	8	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	11	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	14	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	16	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	18	0.16
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	19	0.16
(2,1399)	1:27:D:ASN:H	1:25:D:ARG:H	13	0.16
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	2	0.16
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	3	0.16
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	5	0.16
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	6	0.16
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD11	7	0.16
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD12	7	0.16
(2,1363)	1:19:D:GLU:H	1:18:D:ILE:HD13	7	0.16
(2,1357)	1:18:D:ILE:H	1:18:D:ILE:HB	5	0.16
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	20	0.16
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	6	0.16
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	16	0.16
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	20	0.16
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	3	0.16
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	8	0.16
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	13	0.16
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	20	0.16
(2,1239)	1:52:C:LEU:H	1:52:C:LEU:HA	19	0.16
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	3	0.16
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	5	0.16
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	9	0.16
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	14	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	1	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	2	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	3	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	4	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	10	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	13	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	14	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	15	0.16
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	20	0.16
(2,1164)	1:45:C:ILE:H	1:42:C:LEU:HA	8	0.16
(2,1118)	1:41:C:CYS:H	1:38:C:ILE:HA	20	0.16
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	18	0.16
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	11	0.16
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	12	0.16
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	4	0.16
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	7	0.16
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	18	0.16
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	3	0.16
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	13	0.16
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	2	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	3	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	8	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	9	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	11	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	14	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	16	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	17	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	18	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	19	0.16
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	20	0.16
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	19	0.16
(2,956)	1:20:C:MET:H	1:19:C:GLU:HA	3	0.16
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	2	0.16
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	3	0.16
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	6	0.16
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	17	0.16
(2,943)	1:18:C:ILE:H	1:18:C:ILE:HB	5	0.16
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	16	0.16
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	1	0.16
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	3	0.16
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	13	0.16
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	20	0.16
(2,825)	1:52:B:LEU:H	1:52:B:LEU:HA	19	0.16
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	5	0.16
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	3	0.16
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	9	0.16
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	2	0.16
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	3	0.16
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	4	0.16
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	8	0.16
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	10	0.16
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	13	0.16
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	14	0.16
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	20	0.16
(2,738)	1:44:B:LEU:H	1:41:B:CYS:HB2	11	0.16
(2,738)	1:44:B:LEU:H	1:41:B:CYS:HB3	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	4	0.16
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	10	0.16
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	14	0.16
(2,701)	1:39:B:LEU:H	1:35:B:PHE:HD1	20	0.16
(2,701)	1:39:B:LEU:H	1:35:B:PHE:HD2	20	0.16
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	1	0.16
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	12	0.16
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	15	0.16
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	18	0.16
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	20	0.16
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	2	0.16
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	3	0.16
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	7	0.16
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	8	0.16
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	9	0.16
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	18	0.16
(2,643)	1:34:B:ASN:H	1:34:B:ASN:HB3	19	0.16
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	16	0.16
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	7	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	3	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	4	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	5	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	8	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	9	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	11	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	14	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	18	0.16
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	20	0.16
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	6	0.16
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD11	12	0.16
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD12	12	0.16
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD13	12	0.16
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	20	0.16
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	17	0.16
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	20	0.16
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	6	0.16
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	3	0.16
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	13	0.16
(2,421)	1:3:B:LYS:H	1:3:B:LYS:HB3	12	0.16
(2,411)	1:52:A:LEU:H	1:52:A:LEU:HA	7	0.16
(2,411)	1:52:A:LEU:H	1:52:A:LEU:HA	19	0.16
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	16	0.16
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	17	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	2	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	3	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	4	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	6	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	8	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	10	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	13	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	15	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	17	0.16
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	20	0.16
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD11	10	0.16
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD12	10	0.16
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD13	10	0.16
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	18	0.16
(2,250)	1:37:A:LEU:H	1:34:A:ASN:HA	18	0.16
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	1	0.16
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	5	0.16
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	9	0.16
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	10	0.16
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	9	0.16
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	13	0.16
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	2	0.16
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	7	0.16
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	18	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	1	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	3	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	5	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	11	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	17	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	18	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	19	0.16
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	20	0.16
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	2	0.16
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	3	0.16
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	5	0.16
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	6	0.16
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	10	0.16
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD11	12	0.16
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD12	12	0.16
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD13	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:18:A:ILE:H	1:18:A:ILE:HB	5	0.16
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	20	0.16
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	6	0.16
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	20	0.16
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	3	0.16
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	13	0.16
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	20	0.16
(2,7)	1:3:A:LYS:H	1:3:A:LYS:HB3	12	0.16
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	1	0.15
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	5	0.15
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	8	0.15
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	14	0.15
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	15	0.15
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	18	0.15
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	6	0.15
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	15	0.15
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	16	0.15
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	4	0.15
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	7	0.15
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	9	0.15
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	12	0.15
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	16	0.15
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	17	0.15
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	18	0.15
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	19	0.15
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	15	0.15
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	15	0.15
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	15	0.15
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	17	0.15
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	17	0.15
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	17	0.15
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	20	0.15
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	13	0.15
(2,1941)	1:40:E:ILE:H	1:37:E:LEU:HA	6	0.15
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	15	0.15
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	10	0.15
(2,1898)	1:36:E:CYS:H	1:35:E:PHE:HA	19	0.15
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	1	0.15
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	3	0.15
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	15	0.15
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	17	0.15
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	19	0.15
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	9	0.15
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	11	0.15
(2,1876)	1:34:E:ASN:H	1:33:E:ILE:HA	7	0.15
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	2	0.15
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	6	0.15
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	13	0.15
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	19	0.15
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	8	0.15
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	10	0.15
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD11	7	0.15
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD12	7	0.15
(2,1777)	1:19:E:GLU:H	1:18:E:ILE:HD13	7	0.15
(2,1766)	1:17:E:THR:H	1:17:E:THR:HA	1	0.15
(2,1759)	1:16:E:SEP:H	1:15:E:ALA:HA	11	0.15
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	4	0.15
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	5	0.15
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	4	0.15
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	20	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	3	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	4	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	6	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	8	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	9	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	10	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	13	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	17	0.15
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	18	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	1	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	4	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	6	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	8	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	9	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	10	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	16	0.15
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	17	0.15
(2,1653)	1:52:D:LEU:H	1:52:D:LEU:HA	7	0.15
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	5	0.15
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	17	0.15
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	6	0.15
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	9	0.15
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	16	0.15
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	18	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	4	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	6	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	7	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	9	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	11	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	12	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	14	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	16	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	17	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	18	0.15
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	19	0.15
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD11	6	0.15
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD12	6	0.15
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD13	6	0.15
(2,1527)	1:40:D:ILE:H	1:37:D:LEU:HA	7	0.15
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	15	0.15
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	1	0.15
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	10	0.15
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	13	0.15
(2,1484)	1:36:D:CYS:H	1:35:D:PHE:HA	17	0.15
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	4	0.15
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	6	0.15
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	10	0.15
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	13	0.15
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	15	0.15
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	19	0.15
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	20	0.15
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	14	0.15
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	9	0.15
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	11	0.15
(2,1462)	1:34:D:ASN:H	1:33:D:ILE:HA	7	0.15
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	2	0.15
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	13	0.15
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	19	0.15
(2,1370)	1:20:D:MET:H	1:19:D:GLU:HA	3	0.15
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	8	0.15
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	10	0.15
(2,1352)	1:17:D:THR:H	1:17:D:THR:HA	1	0.15
(2,1352)	1:17:D:THR:H	1:17:D:THR:HA	3	0.15
(2,1345)	1:16:D:SEP:H	1:15:D:ALA:HA	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	5	0.15
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	4	0.15
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	20	0.15
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	7	0.15
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	7	0.15
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	7	0.15
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	19	0.15
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	19	0.15
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	19	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	3	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	4	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	5	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	8	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	9	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	13	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	17	0.15
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	18	0.15
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	1	0.15
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	6	0.15
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	9	0.15
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	10	0.15
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	16	0.15
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	17	0.15
(2,1249)	1:3:D:LYS:H	1:3:D:LYS:HB3	12	0.15
(2,1239)	1:52:C:LEU:H	1:52:C:LEU:HA	7	0.15
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	5	0.15
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	8	0.15
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	17	0.15
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	6	0.15
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	8	0.15
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	16	0.15
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	17	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	6	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	7	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	8	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	9	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	11	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	12	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	16	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	17	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	18	0.15
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD11	17	0.15
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD12	17	0.15
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD13	17	0.15
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	4	0.15
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	18	0.15
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	10	0.15
(2,1070)	1:36:C:CYS:H	1:35:C:PHE:HA	13	0.15
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	2	0.15
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	9	0.15
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	10	0.15
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	11	0.15
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	13	0.15
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	14	0.15
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	19	0.15
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	13	0.15
(2,1057)	1:34:C:ASN:H	1:34:C:ASN:HB3	19	0.15
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	8	0.15
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	9	0.15
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	7	0.15
(2,1048)	1:34:C:ASN:H	1:33:C:ILE:HA	19	0.15
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	1	0.15
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	2	0.15
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	5	0.15
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	6	0.15
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	13	0.15
(2,985)	1:27:C:ASN:H	1:25:C:ARG:H	13	0.15
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	8	0.15
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	10	0.15
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD11	7	0.15
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD12	7	0.15
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD13	7	0.15
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD11	12	0.15
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD12	12	0.15
(2,949)	1:19:C:GLU:H	1:18:C:ILE:HD13	12	0.15
(2,938)	1:17:C:THR:H	1:17:C:THR:HA	1	0.15
(2,938)	1:17:C:THR:H	1:17:C:THR:HA	3	0.15
(2,931)	1:16:C:SEP:H	1:15:C:ALA:HA	11	0.15
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	5	0.15
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	9	0.15
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	1	0.15
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	4	0.15
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	14	0.15
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	16	0.15
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	20	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	1	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	3	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	4	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	5	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	6	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	7	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	8	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	9	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	13	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	16	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	17	0.15
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	20	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	4	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	5	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	6	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	8	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	9	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	10	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	11	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	16	0.15
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	17	0.15
(2,835)	1:3:C:LYS:H	1:3:C:LYS:HB3	12	0.15
(2,825)	1:52:B:LEU:H	1:52:B:LEU:HA	7	0.15
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	17	0.15
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	18	0.15
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	6	0.15
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	10	0.15
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	15	0.15
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	16	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	1	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	6	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	7	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	9	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	11	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	12	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	15	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	16	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	17	0.15
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,664)	1:37:B:LEU:H	1:34:B:ASN:HA	7	0.15
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	6	0.15
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	9	0.15
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	10	0.15
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	11	0.15
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	13	0.15
(2,656)	1:36:B:CYS:H	1:35:B:PHE:HA	17	0.15
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	1	0.15
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	6	0.15
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	10	0.15
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	11	0.15
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	14	0.15
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	19	0.15
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	9	0.15
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	11	0.15
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	13	0.15
(2,634)	1:34:B:ASN:H	1:33:B:ILE:HA	19	0.15
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	2	0.15
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	6	0.15
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	13	0.15
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	19	0.15
(2,608)	1:31:B:LEU:H	1:28:B:LEU:HA	2	0.15
(2,571)	1:27:B:ASN:H	1:25:B:ARG:H	13	0.15
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	1	0.15
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	2	0.15
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	8	0.15
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	10	0.15
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD11	7	0.15
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD12	7	0.15
(2,535)	1:19:B:GLU:H	1:18:B:ILE:HD13	7	0.15
(2,529)	1:18:B:ILE:H	1:18:B:ILE:HB	5	0.15
(2,524)	1:17:B:THR:H	1:17:B:THR:HA	1	0.15
(2,517)	1:16:B:SEP:H	1:15:B:ALA:HA	11	0.15
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	5	0.15
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	4	0.15
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	12	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	1	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	3	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	4	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	5	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	7	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	9	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	10	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	13	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	16	0.15
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	20	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	1	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	4	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	6	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	8	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	9	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	10	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	16	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	17	0.15
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	20	0.15
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	1	0.15
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	5	0.15
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	10	0.15
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	15	0.15
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	17	0.15
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	6	0.15
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	9	0.15
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	10	0.15
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	15	0.15
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	1	0.15
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	7	0.15
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	9	0.15
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	11	0.15
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	12	0.15
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	16	0.15
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	18	0.15
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	19	0.15
(2,324)	1:44:A:LEU:H	1:41:A:CYS:HB2	15	0.15
(2,324)	1:44:A:LEU:H	1:41:A:CYS:HB3	15	0.15
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	20	0.15
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	13	0.15
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	17	0.15
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	1	0.15
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	3	0.15
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	13	0.15
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	14	0.15
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	15	0.15
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	19	0.15
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	13	0.15
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	14	0.15
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	17	0.15
(2,229)	1:34:A:ASN:H	1:34:A:ASN:HB3	19	0.15
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	11	0.15
(2,220)	1:34:A:ASN:H	1:33:A:ILE:HA	19	0.15
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	2	0.15
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	6	0.15
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	8	0.15
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	9	0.15
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	13	0.15
(2,128)	1:20:A:MET:H	1:19:A:GLU:HA	3	0.15
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	1	0.15
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	4	0.15
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	8	0.15
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD11	7	0.15
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD12	7	0.15
(2,121)	1:19:A:GLU:H	1:18:A:ILE:HD13	7	0.15
(2,110)	1:17:A:THR:H	1:17:A:THR:HA	1	0.15
(2,110)	1:17:A:THR:H	1:17:A:THR:HA	3	0.15
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	4	0.15
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	3	0.15
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	4	0.15
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	20	0.15
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	1	0.15
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	7	0.15
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	8	0.15
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	9	0.15
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	12	0.15
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	13	0.15
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	16	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	1	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	6	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	8	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	9	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	10	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	11	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	16	0.15
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	17	0.15
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	2	0.14
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	17	0.14
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	19	0.14
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	10	0.14
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	20	0.14
(2,2030)	1:49:E:VAL:H	1:48:E:ILE:HA	5	0.14
(2,1946)	1:41:E:CYS:H	1:38:E:ILE:HA	16	0.14
(2,1941)	1:40:E:ILE:H	1:37:E:LEU:HA	17	0.14
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	1	0.14
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	4	0.14
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	6	0.14
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	11	0.14
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	12	0.14
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	13	0.14
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	8	0.14
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	12	0.14
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	17	0.14
(2,1850)	1:31:E:LEU:H	1:28:E:LEU:HA	2	0.14
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	1	0.14
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	4	0.14
(2,1766)	1:17:E:THR:H	1:17:E:THR:HA	3	0.14
(2,1766)	1:17:E:THR:H	1:17:E:THR:HA	18	0.14
(2,1759)	1:16:E:SEP:H	1:15:E:ALA:HA	15	0.14
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	9	0.14
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	10	0.14
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	11	0.14
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	14	0.14
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	16	0.14
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	15	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	1	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	2	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	3	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	5	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	6	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	7	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	8	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	9	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	10	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	11	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	12	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	13	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	14	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	17	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	18	0.14
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	19	0.14
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	14	0.14
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	14	0.14
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	14	0.14
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	15	0.14
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	15	0.14
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	15	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	1	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	2	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	5	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	7	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	11	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	12	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	14	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	15	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	16	0.14
(2,1687)	1:7:E:LEU:H	1:6:E:TYR:HA	19	0.14
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	2	0.14
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	7	0.14
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	11	0.14
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	14	0.14
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	15	0.14
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	18	0.14
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	19	0.14
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	14	0.14
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	19	0.14
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	1	0.14
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	10	0.14
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	15	0.14
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	20	0.14
(2,1616)	1:49:D:VAL:H	1:48:D:ILE:HA	5	0.14
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD11	17	0.14
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD12	17	0.14
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD13	17	0.14
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	4	0.14
(2,1529)	1:39:D:LEU:H	1:35:D:PHE:HD1	11	0.14
(2,1529)	1:39:D:LEU:H	1:35:D:PHE:HD2	11	0.14
(2,1492)	1:37:D:LEU:H	1:34:D:ASN:HA	9	0.14
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	1	0.14
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	12	0.14
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	16	0.14
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	6	0.14
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	17	0.14
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	8	0.14
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	1	0.14
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	4	0.14
(2,1345)	1:16:D:SEP:H	1:15:D:ALA:HA	15	0.14
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	4	0.14
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	9	0.14
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	11	0.14
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	14	0.14
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	16	0.14
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	6	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	1	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	2	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	3	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	5	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	6	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	7	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	8	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	9	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	10	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	12	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	13	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	14	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	16	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	17	0.14
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	18	0.14
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	14	0.14
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	14	0.14
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	14	0.14
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	15	0.14
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	15	0.14
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	15	0.14
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	1	0.14
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	2	0.14
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	7	0.14
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	10	0.14
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	11	0.14
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	12	0.14
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	15	0.14
(2,1273)	1:7:D:LEU:H	1:6:D:TYR:HA	19	0.14
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	2	0.14
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	4	0.14
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	7	0.14
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	11	0.14
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	14	0.14
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	15	0.14
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	18	0.14
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	19	0.14
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	6	0.14
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	9	0.14
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	19	0.14
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	1	0.14
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	15	0.14
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	18	0.14
(2,1202)	1:49:C:VAL:H	1:48:C:ILE:HA	5	0.14
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD11	1	0.14
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD12	1	0.14
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD13	1	0.14
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	15	0.14
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	1	0.14
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	12	0.14
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	15	0.14
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	17	0.14
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	14	0.14
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	11	0.14
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	12	0.14
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	1	0.14
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	4	0.14
(2,931)	1:16:C:SEP:H	1:15:C:ALA:HA	15	0.14
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	4	0.14
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	9	0.14
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	11	0.14
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	14	0.14
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	10	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	2	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	3	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	5	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	6	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	7	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	10	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	11	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	12	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	13	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	18	0.14
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	19	0.14
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	18	0.14
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	18	0.14
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	18	0.14
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	2	0.14
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	10	0.14
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	11	0.14
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	12	0.14
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	14	0.14
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	15	0.14
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	18	0.14
(2,859)	1:7:C:LEU:H	1:6:C:TYR:HA	19	0.14
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	2	0.14
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	7	0.14
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	14	0.14
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	15	0.14
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	18	0.14
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	15	0.14
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	19	0.14
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	20	0.14
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	5	0.14
(2,788)	1:49:B:VAL:H	1:48:B:ILE:HA	18	0.14
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	18	0.14
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	4	0.14
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	12	0.14
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	13	0.14
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	15	0.14
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	16	0.14
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	17	0.14
(2,649)	1:35:B:PHE:H	1:34:B:ASN:HA	20	0.14
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	14	0.14
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	8	0.14
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	12	0.14
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	4	0.14
(2,524)	1:17:B:THR:H	1:17:B:THR:HA	3	0.14
(2,517)	1:16:B:SEP:H	1:15:B:ALA:HA	15	0.14
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	9	0.14
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	14	0.14
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	16	0.14
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	6	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	1	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	2	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	3	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	5	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	7	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	8	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	9	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	10	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	11	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	13	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	14	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	16	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	18	0.14
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	19	0.14
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	14	0.14
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	14	0.14
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	14	0.14
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	15	0.14
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	15	0.14
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	15	0.14
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	2	0.14
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	11	0.14
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	12	0.14
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	14	0.14
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	15	0.14
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	17	0.14
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	18	0.14
(2,445)	1:7:B:LEU:H	1:6:B:TYR:HA	19	0.14
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	2	0.14
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	5	0.14
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	7	0.14
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	11	0.14
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	15	0.14
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	18	0.14
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	19	0.14
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	6	0.14
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	19	0.14
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	3	0.14
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	18	0.14
(2,389)	1:50:A:MET:H	1:50:A:MET:HB3	20	0.14
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	5	0.14
(2,374)	1:49:A:VAL:H	1:48:A:ILE:HA	14	0.14
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD11	15	0.14
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD12	15	0.14
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD13	15	0.14
(2,336)	1:45:A:ILE:H	1:42:A:LEU:HA	8	0.14
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	11	0.14
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	16	0.14
(2,287)	1:39:A:LEU:H	1:35:A:PHE:HD1	20	0.14
(2,287)	1:39:A:LEU:H	1:35:A:PHE:HD2	20	0.14
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	6	0.14
(2,242)	1:36:A:CYS:H	1:35:A:PHE:HA	10	0.14
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	4	0.14
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	6	0.14
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	11	0.14
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	12	0.14
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	17	0.14
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	3	0.14
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	8	0.14
(2,194)	1:31:A:LEU:H	1:28:A:LEU:HA	2	0.14
(2,110)	1:17:A:THR:H	1:17:A:THR:HA	18	0.14
(2,103)	1:16:A:SEP:H	1:15:A:ALA:HA	15	0.14
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	9	0.14
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	14	0.14
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	5	0.14
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	6	0.14
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	10	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	1	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	2	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	5	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	6	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	7	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	8	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	9	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	10	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	11	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	12	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	13	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	16	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	17	0.14
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	18	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	2	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	3	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	4	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	5	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	10	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	11	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	14	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	15	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	17	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	18	0.14
(2,31)	1:7:A:LEU:H	1:6:A:TYR:HA	19	0.14
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	2	0.14
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	4	0.14
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	7	0.14
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	12	0.14
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	15	0.14
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	18	0.14
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	19	0.14
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	4	0.13
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	6	0.13
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	9	0.13
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	11	0.13
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	12	0.13
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	16	0.13
(2,2045)	1:50:E:MET:H	1:50:E:MET:HB3	2	0.13
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	14	0.13
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	14	0.13
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	14	0.13
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	14	0.13
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	6	0.13
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	6	0.13
(2,1906)	1:37:E:LEU:H	1:34:E:ASN:HA	9	0.13
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	16	0.13
(2,1891)	1:35:E:PHE:H	1:34:E:ASN:HA	20	0.13
(2,1863)	1:32:E:PHE:H	1:31:E:LEU:HA	10	0.13
(2,1813)	1:27:E:ASN:H	1:25:E:ARG:H	15	0.13
(2,1766)	1:17:E:THR:H	1:17:E:THR:HA	15	0.13
(2,1759)	1:16:E:SEP:H	1:15:E:ALA:HA	9	0.13
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	6	0.13
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	7	0.13
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	12	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	1	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	6	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	7	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	9	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	10	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	12	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	15	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	16	0.13
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	20	0.13
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	2	0.13
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	6	0.13
(2,1727)	1:12:E:ILE:H	1:11:E:ALA:HA	15	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	7	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	7	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	7	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	11	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	11	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	11	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	18	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	18	0.13
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	18	0.13
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	5	0.13
(2,1679)	1:6:E:TYR:H	1:5:E:GLN:HA	12	0.13
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	4	0.13
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	6	0.13
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	9	0.13
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	11	0.13
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	12	0.13
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	16	0.13
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	20	0.13
(2,1631)	1:50:D:MET:H	1:50:D:MET:HB3	2	0.13
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD11	14	0.13
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD12	14	0.13
(2,1603)	1:47:D:ILE:H	1:47:D:ILE:HD13	14	0.13
(2,1578)	1:45:D:ILE:H	1:42:D:LEU:HA	14	0.13
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB2	6	0.13
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB3	6	0.13
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB2	19	0.13
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB3	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1477)	1:35:D:PHE:H	1:34:D:ASN:HA	17	0.13
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	13	0.13
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	6	0.13
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	12	0.13
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	17	0.13
(2,1449)	1:32:D:PHE:H	1:31:D:LEU:HA	10	0.13
(2,1352)	1:17:D:THR:H	1:17:D:THR:HA	15	0.13
(2,1352)	1:17:D:THR:H	1:17:D:THR:HA	18	0.13
(2,1345)	1:16:D:SEP:H	1:15:D:ALA:HA	9	0.13
(2,1345)	1:16:D:SEP:H	1:15:D:ALA:HA	16	0.13
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	1	0.13
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	6	0.13
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	7	0.13
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	10	0.13
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	12	0.13
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	19	0.13
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	1	0.13
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	7	0.13
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	9	0.13
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	12	0.13
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	15	0.13
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	16	0.13
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	19	0.13
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	20	0.13
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	2	0.13
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	15	0.13
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	19	0.13
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	11	0.13
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	15	0.13
(2,1313)	1:12:D:ILE:H	1:11:D:ALA:HA	19	0.13
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	18	0.13
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	18	0.13
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	18	0.13
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	5	0.13
(2,1265)	1:6:D:TYR:H	1:5:D:GLN:HA	12	0.13
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	4	0.13
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	11	0.13
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	12	0.13
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	16	0.13
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	2	0.13
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	10	0.13
(2,1217)	1:50:C:MET:H	1:50:C:MET:HB3	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	11	0.13
(2,1113)	1:40:C:ILE:H	1:37:C:LEU:HA	6	0.13
(2,1098)	1:39:C:LEU:H	1:36:C:CYS:HA	7	0.13
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	6	0.13
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	16	0.13
(2,1063)	1:35:C:PHE:H	1:34:C:ASN:HA	20	0.13
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	6	0.13
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	6	0.13
(2,1035)	1:32:C:PHE:H	1:31:C:LEU:HA	10	0.13
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	2	0.13
(2,938)	1:17:C:THR:H	1:17:C:THR:HA	15	0.13
(2,938)	1:17:C:THR:H	1:17:C:THR:HA	18	0.13
(2,931)	1:16:C:SEP:H	1:15:C:ALA:HA	9	0.13
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	1	0.13
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	6	0.13
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	7	0.13
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	10	0.13
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	12	0.13
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	16	0.13
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	19	0.13
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	6	0.13
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	7	0.13
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	12	0.13
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	15	0.13
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	16	0.13
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	20	0.13
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	2	0.13
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	6	0.13
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	15	0.13
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	15	0.13
(2,899)	1:12:C:ILE:H	1:11:C:ALA:HA	17	0.13
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	7	0.13
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	7	0.13
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	7	0.13
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	14	0.13
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	14	0.13
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	14	0.13
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	12	0.13
(2,851)	1:6:C:TYR:H	1:5:C:GLN:HA	19	0.13
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	4	0.13
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	6	0.13
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	11	0.13
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	12	0.13
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	16	0.13
(2,803)	1:50:B:MET:H	1:50:B:MET:HB3	2	0.13
(2,738)	1:44:B:LEU:H	1:41:B:CYS:HB2	20	0.13
(2,738)	1:44:B:LEU:H	1:41:B:CYS:HB3	20	0.13
(2,699)	1:40:B:ILE:H	1:37:B:LEU:HA	14	0.13
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	6	0.13
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	13	0.13
(2,524)	1:17:B:THR:H	1:17:B:THR:HA	15	0.13
(2,524)	1:17:B:THR:H	1:17:B:THR:HA	18	0.13
(2,517)	1:16:B:SEP:H	1:15:B:ALA:HA	9	0.13
(2,517)	1:16:B:SEP:H	1:15:B:ALA:HA	16	0.13
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	1	0.13
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	6	0.13
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	7	0.13
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	10	0.13
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	11	0.13
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	12	0.13
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	19	0.13
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	1	0.13
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	7	0.13
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	15	0.13
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	16	0.13
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	15	0.13
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	6	0.13
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	15	0.13
(2,485)	1:12:B:ILE:H	1:11:B:ALA:HA	17	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	2	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	2	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	2	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	7	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	7	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	7	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	11	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	11	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	11	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	18	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	18	0.13
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	18	0.13
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	12	0.13
(2,437)	1:6:B:TYR:H	1:5:B:GLN:HA	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	4	0.13
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	9	0.13
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	11	0.13
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	12	0.13
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	13	0.13
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	18	0.13
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	4	0.13
(2,250)	1:37:A:LEU:H	1:34:A:ASN:HA	7	0.13
(2,250)	1:37:A:LEU:H	1:34:A:ASN:HA	15	0.13
(2,235)	1:35:A:PHE:H	1:34:A:ASN:HA	20	0.13
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	6	0.13
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	6	0.13
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	12	0.13
(2,207)	1:32:A:PHE:H	1:31:A:LEU:HA	10	0.13
(2,110)	1:17:A:THR:H	1:17:A:THR:HA	15	0.13
(2,103)	1:16:A:SEP:H	1:15:A:ALA:HA	9	0.13
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	1	0.13
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	6	0.13
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	7	0.13
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	12	0.13
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	16	0.13
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	19	0.13
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	1	0.13
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	6	0.13
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	7	0.13
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	15	0.13
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	16	0.13
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	20	0.13
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	2	0.13
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	15	0.13
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	18	0.13
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	15	0.13
(2,71)	1:12:A:ILE:H	1:11:A:ALA:HA	19	0.13
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	7	0.13
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	7	0.13
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	7	0.13
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	11	0.13
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	11	0.13
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	11	0.13
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	5	0.13
(2,23)	1:6:A:TYR:H	1:5:A:GLN:HA	14	0.13
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	20	0.12
(2,1992)	1:45:E:ILE:H	1:42:E:LEU:HA	8	0.12
(2,1965)	1:43:E:LEU:H	1:40:E:ILE:HA	8	0.12
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	4	0.12
(2,1953)	1:42:E:LEU:H	1:39:E:LEU:HB2	8	0.12
(2,1953)	1:42:E:LEU:H	1:39:E:LEU:HB3	8	0.12
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	6	0.12
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	13	0.12
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	17	0.12
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	5	0.12
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	6	0.12
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	7	0.12
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	10	0.12
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	15	0.12
(2,1769)	1:18:E:ILE:H	1:17:E:THR:H	11	0.12
(2,1766)	1:17:E:THR:H	1:17:E:THR:HA	11	0.12
(2,1759)	1:16:E:SEP:H	1:15:E:ALA:HA	16	0.12
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	3	0.12
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	5	0.12
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	13	0.12
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	15	0.12
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	18	0.12
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	19	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	2	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	3	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	5	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	8	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	11	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	13	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	14	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	17	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	18	0.12
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	19	0.12
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	7	0.12
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	11	0.12
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	18	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	2	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	2	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	2	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	5	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	5	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	10	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	10	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	10	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD11	19	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD12	19	0.12
(2,1704)	1:9:E:ARG:H	1:7:E:LEU:HD13	19	0.12
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	2	0.12
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	10	0.12
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	13	0.12
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	18	0.12
(2,1641)	1:51:D:LEU:H	1:51:D:LEU:HA	3	0.12
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB2	14	0.12
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB3	14	0.12
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	19	0.12
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	20	0.12
(2,1539)	1:42:D:LEU:H	1:39:D:LEU:HB2	8	0.12
(2,1539)	1:42:D:LEU:H	1:39:D:LEU:HB3	8	0.12
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	16	0.12
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	5	0.12
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	10	0.12
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	15	0.12
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	16	0.12
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	18	0.12
(2,1436)	1:31:D:LEU:H	1:28:D:LEU:HA	2	0.12
(2,1366)	1:19:D:GLU:H	1:19:D:GLU:HA	15	0.12
(2,1355)	1:18:D:ILE:H	1:17:D:THR:H	11	0.12
(2,1352)	1:17:D:THR:H	1:17:D:THR:HA	11	0.12
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	3	0.12
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	5	0.12
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	13	0.12
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	15	0.12
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	18	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	2	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	3	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	5	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	6	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	8	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	10	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	11	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	13	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	14	0.12
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	18	0.12
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	7	0.12
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	11	0.12
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	14	0.12
(2,1314)	1:12:D:ILE:H	1:9:D:ARG:HA	18	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	5	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	5	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	5	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	10	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	10	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	10	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	11	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	11	0.12
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	11	0.12
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	1	0.12
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	2	0.12
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	15	0.12
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	18	0.12
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	20	0.12
(2,1227)	1:51:C:LEU:H	1:51:C:LEU:HA	3	0.12
(2,1113)	1:40:C:ILE:H	1:37:C:LEU:HA	14	0.12
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	5	0.12
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	15	0.12
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	16	0.12
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	18	0.12
(2,985)	1:27:C:ASN:H	1:25:C:ARG:H	15	0.12
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	7	0.12
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	7	0.12
(2,952)	1:19:C:GLU:H	1:19:C:GLU:HA	15	0.12
(2,941)	1:18:C:ILE:H	1:17:C:THR:H	11	0.12
(2,938)	1:17:C:THR:H	1:17:C:THR:HA	11	0.12
(2,931)	1:16:C:SEP:H	1:15:C:ALA:HA	16	0.12
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	3	0.12
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	5	0.12
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	13	0.12
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	15	0.12
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	18	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	1	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	2	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	3	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	5	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	9	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	10	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	11	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	13	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	14	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	17	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	18	0.12
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	19	0.12
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	7	0.12
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	11	0.12
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	18	0.12
(2,900)	1:12:C:ILE:H	1:9:C:ARG:HA	19	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	2	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	2	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	2	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	5	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	5	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	5	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	11	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	11	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	11	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	15	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	15	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	15	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	19	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	19	0.12
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	19	0.12
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	2	0.12
(2,813)	1:51:B:LEU:H	1:51:B:LEU:HA	3	0.12
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	20	0.12
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	15	0.12
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	17	0.12
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	5	0.12
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	6	0.12
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	10	0.12
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	17	0.12
(2,621)	1:32:B:PHE:H	1:31:B:LEU:HA	10	0.12
(2,571)	1:27:B:ASN:H	1:25:B:ARG:H	15	0.12
(2,524)	1:17:B:THR:H	1:17:B:THR:HA	11	0.12
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	3	0.12
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	5	0.12
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	15	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	3	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	5	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	6	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	8	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	9	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	10	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	12	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	13	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	14	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	17	0.12
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	19	0.12
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	14	0.12
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	19	0.12
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	10	0.12
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	10	0.12
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	10	0.12
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	19	0.12
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	19	0.12
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	19	0.12
(2,410)	1:52:A:LEU:H	1:51:A:LEU:H	16	0.12
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	2	0.12
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	7	0.12
(2,408)	1:52:A:LEU:H	1:51:A:LEU:HA	20	0.12
(2,297)	1:42:A:LEU:H	1:39:A:LEU:HB2	8	0.12
(2,297)	1:42:A:LEU:H	1:39:A:LEU:HB3	8	0.12
(2,287)	1:39:A:LEU:H	1:35:A:PHE:HD1	11	0.12
(2,287)	1:39:A:LEU:H	1:35:A:PHE:HD2	11	0.12
(2,250)	1:37:A:LEU:H	1:34:A:ASN:HA	16	0.12
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	8	0.12
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	16	0.12
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	5	0.12
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	7	0.12
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	10	0.12
(2,157)	1:27:A:ASN:H	1:25:A:ARG:H	15	0.12
(2,128)	1:20:A:MET:H	1:19:A:GLU:HA	14	0.12
(2,103)	1:16:A:SEP:H	1:15:A:ALA:HA	16	0.12
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	3	0.12
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	5	0.12
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	10	0.12
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	11	0.12
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	15	0.12
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	18	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	2	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	3	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	5	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	8	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	9	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	10	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	11	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	12	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	13	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	14	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	17	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	18	0.12
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	19	0.12
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	7	0.12
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	11	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	6	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	6	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	6	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	14	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	14	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	14	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	15	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	15	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	15	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	18	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	18	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	18	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	19	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	19	0.12
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	19	0.12
(2,2127)	1:47:C:ILE:CG2	1:44:B:LEU:CD2	8	0.11
(2,2064)	1:52:E:LEU:H	1:51:E:LEU:HA	13	0.11
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	10	0.11
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	10	0.11
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	14	0.11
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	14	0.11
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	16	0.11
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	16	0.11
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB2	17	0.11
(2,1980)	1:44:E:LEU:H	1:41:E:CYS:HB3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	20	0.11
(2,1946)	1:41:E:CYS:H	1:38:E:ILE:HA	11	0.11
(2,1943)	1:39:E:LEU:H	1:35:E:PHE:HD1	11	0.11
(2,1943)	1:39:E:LEU:H	1:35:E:PHE:HD2	11	0.11
(2,1941)	1:40:E:ILE:H	1:37:E:LEU:HA	7	0.11
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	7	0.11
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	2	0.11
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	8	0.11
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	6	0.11
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	13	0.11
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	19	0.11
(2,1882)	1:27:E:ASN:HD22	1:27:E:ASN:HB3	18	0.11
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	1	0.11
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	4	0.11
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	8	0.11
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	14	0.11
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	19	0.11
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	20	0.11
(2,1780)	1:19:E:GLU:H	1:19:E:GLU:HA	15	0.11
(2,1766)	1:17:E:THR:H	1:17:E:THR:HA	2	0.11
(2,1759)	1:16:E:SEP:H	1:15:E:ALA:HA	10	0.11
(2,1754)	1:15:E:ALA:H	1:14:E:ARG:HA	8	0.11
(2,1741)	1:13:E:ARG:H	1:12:E:ILE:HA	4	0.11
(2,1728)	1:12:E:ILE:H	1:9:E:ARG:HA	19	0.11
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	15	0.11
(2,1544)	1:42:D:LEU:H	1:39:D:LEU:HA	5	0.11
(2,1527)	1:40:D:ILE:H	1:37:D:LEU:HA	6	0.11
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	1	0.11
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	2	0.11
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	15	0.11
(2,1474)	1:35:D:PHE:H	1:33:D:ILE:HB	20	0.11
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	3	0.11
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	5	0.11
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	6	0.11
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	13	0.11
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	19	0.11
(2,1468)	1:27:D:ASN:HD22	1:27:D:ASN:HB3	7	0.11
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	1	0.11
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	4	0.11
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	8	0.11
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	14	0.11
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	20	0.11
(2,1370)	1:20:D:MET:H	1:19:D:GLU:HA	14	0.11
(2,1352)	1:17:D:THR:H	1:17:D:THR:HA	2	0.11
(2,1345)	1:16:D:SEP:H	1:15:D:ALA:HA	10	0.11
(2,1340)	1:15:D:ALA:H	1:14:D:ARG:HA	8	0.11
(2,1327)	1:13:D:ARG:H	1:12:D:ILE:HA	4	0.11
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	2	0.11
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	2	0.11
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	2	0.11
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	10	0.11
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	13	0.11
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD11	2	0.11
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD12	2	0.11
(2,1189)	1:47:C:ILE:H	1:47:C:ILE:HD13	2	0.11
(2,1137)	1:43:C:LEU:H	1:40:C:ILE:HA	8	0.11
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	5	0.11
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	20	0.11
(2,1125)	1:42:C:LEU:H	1:39:C:LEU:HB2	8	0.11
(2,1125)	1:42:C:LEU:H	1:39:C:LEU:HB3	8	0.11
(2,1115)	1:39:C:LEU:H	1:35:C:PHE:HD1	11	0.11
(2,1115)	1:39:C:LEU:H	1:35:C:PHE:HD2	11	0.11
(2,1113)	1:40:C:ILE:H	1:37:C:LEU:HA	16	0.11
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	14	0.11
(2,1078)	1:37:C:LEU:H	1:34:C:ASN:HA	16	0.11
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	11	0.11
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	16	0.11
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	17	0.11
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	4	0.11
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	5	0.11
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	6	0.11
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	13	0.11
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	19	0.11
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	7	0.11
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	10	0.11
(2,1054)	1:27:C:ASN:HD22	1:27:C:ASN:HB3	17	0.11
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	1	0.11
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	4	0.11
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	8	0.11
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	14	0.11
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	19	0.11
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	20	0.11
(2,956)	1:20:C:MET:H	1:19:C:GLU:HA	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,938)	1:17:C:THR:H	1:17:C:THR:HA	2	0.11
(2,931)	1:16:C:SEP:H	1:15:C:ALA:HA	10	0.11
(2,926)	1:15:C:ALA:H	1:14:C:ARG:HA	8	0.11
(2,913)	1:13:C:ARG:H	1:12:C:ILE:HA	4	0.11
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	10	0.11
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	10	0.11
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	10	0.11
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	8	0.11
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	13	0.11
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	14	0.11
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	20	0.11
(2,738)	1:44:B:LEU:H	1:41:B:CYS:HB2	10	0.11
(2,738)	1:44:B:LEU:H	1:41:B:CYS:HB3	10	0.11
(2,716)	1:42:B:LEU:H	1:39:B:LEU:HA	5	0.11
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	9	0.11
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	20	0.11
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	5	0.11
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	6	0.11
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	10	0.11
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	13	0.11
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	7	0.11
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	15	0.11
(2,640)	1:27:B:ASN:HD22	1:27:B:ASN:HB3	18	0.11
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	1	0.11
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	8	0.11
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	11	0.11
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	19	0.11
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	20	0.11
(2,542)	1:20:B:MET:H	1:19:B:GLU:HA	14	0.11
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG12	7	0.11
(2,541)	1:20:B:MET:H	1:18:B:ILE:HG13	7	0.11
(2,538)	1:19:B:GLU:H	1:19:B:GLU:HA	15	0.11
(2,527)	1:18:B:ILE:H	1:17:B:THR:H	11	0.11
(2,524)	1:17:B:THR:H	1:17:B:THR:HA	2	0.11
(2,517)	1:16:B:SEP:H	1:15:B:ALA:HA	10	0.11
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	8	0.11
(2,512)	1:15:B:ALA:H	1:14:B:ARG:HA	18	0.11
(2,499)	1:13:B:ARG:H	1:12:B:ILE:HA	4	0.11
(2,486)	1:12:B:ILE:H	1:9:B:ARG:HA	7	0.11
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD11	5	0.11
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD12	5	0.11
(2,462)	1:9:B:ARG:H	1:7:B:LEU:HD13	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD11	2	0.11
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD12	2	0.11
(2,361)	1:47:A:ILE:H	1:47:A:ILE:HD13	2	0.11
(2,324)	1:44:A:LEU:H	1:41:A:CYS:HB2	16	0.11
(2,324)	1:44:A:LEU:H	1:41:A:CYS:HB3	16	0.11
(2,297)	1:42:A:LEU:H	1:39:A:LEU:HB2	7	0.11
(2,297)	1:42:A:LEU:H	1:39:A:LEU:HB3	7	0.11
(2,270)	1:39:A:LEU:H	1:36:A:CYS:HA	1	0.11
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	1	0.11
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	12	0.11
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	15	0.11
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	5	0.11
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	6	0.11
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	13	0.11
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	19	0.11
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	15	0.11
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	16	0.11
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	17	0.11
(2,226)	1:27:A:ASN:HD22	1:27:A:ASN:HB3	18	0.11
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	1	0.11
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	4	0.11
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	11	0.11
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	19	0.11
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	20	0.11
(2,124)	1:19:A:GLU:H	1:19:A:GLU:HA	15	0.11
(2,110)	1:17:A:THR:H	1:17:A:THR:HA	2	0.11
(2,98)	1:15:A:ALA:H	1:14:A:ARG:HA	8	0.11
(2,85)	1:13:A:ARG:H	1:12:A:ILE:HA	4	0.11
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	14	0.11
(2,72)	1:12:A:ILE:H	1:9:A:ARG:HA	19	0.11
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	2	0.11
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	2	0.11
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	2	0.11
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD11	5	0.11
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD12	5	0.11
(2,48)	1:9:A:ARG:H	1:7:A:LEU:HD13	5	0.11
(2,2127)	1:47:C:ILE:CG2	1:44:B:LEU:CD2	17	0.1
(2,2066)	1:52:E:LEU:H	1:51:E:LEU:H	3	0.1
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD11	1	0.1
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD12	1	0.1
(2,2017)	1:47:E:ILE:H	1:47:E:ILE:HD13	1	0.1
(2,1958)	1:42:E:LEU:H	1:39:E:LEU:HA	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1926)	1:39:E:LEU:H	1:36:E:CYS:HA	4	0.1
(2,1888)	1:35:E:PHE:H	1:33:E:ILE:HB	15	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	1	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	2	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	3	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	4	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	5	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	7	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	8	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	9	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	10	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	11	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	12	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	14	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	15	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	16	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	17	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	18	0.1
(2,1883)	1:27:E:ASN:HD21	1:27:E:ASN:HD22	20	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	2	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	3	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	5	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	6	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	7	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	9	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	10	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	11	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	12	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	13	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	15	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	16	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	17	0.1
(2,1830)	1:30:E:ASN:HD21	1:30:E:ASN:HD22	18	0.1
(2,1650)	1:52:D:LEU:H	1:51:D:LEU:HA	1	0.1
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB2	18	0.1
(2,1566)	1:44:D:LEU:H	1:41:D:CYS:HB3	18	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	1	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	2	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	4	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	7	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	8	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	10	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	11	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	12	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	14	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	15	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	16	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	17	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	18	0.1
(2,1469)	1:27:D:ASN:HD21	1:27:D:ASN:HD22	20	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	2	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	3	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	5	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	6	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	7	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	9	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	10	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	11	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	12	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	13	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	15	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	16	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	17	0.1
(2,1416)	1:30:D:ASN:HD21	1:30:D:ASN:HD22	18	0.1
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD11	3	0.1
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD12	3	0.1
(2,1290)	1:9:D:ARG:H	1:7:D:LEU:HD13	3	0.1
(2,1236)	1:52:C:LEU:H	1:51:C:LEU:HA	14	0.1
(2,1156)	1:44:C:LEU:H	1:44:C:LEU:HA	5	0.1
(2,1156)	1:44:C:LEU:H	1:44:C:LEU:HA	10	0.1
(2,1156)	1:44:C:LEU:H	1:44:C:LEU:HA	17	0.1
(2,1130)	1:42:C:LEU:H	1:39:C:LEU:HA	14	0.1
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	12	0.1
(2,1060)	1:35:C:PHE:H	1:33:C:ILE:HB	15	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	1	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	2	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	3	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	7	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	8	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	9	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	10	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	11	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	14	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	15	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	16	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	17	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	18	0.1
(2,1055)	1:27:C:ASN:HD21	1:27:C:ASN:HD22	20	0.1
(2,1022)	1:31:C:LEU:H	1:28:C:LEU:HA	4	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	2	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	3	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	5	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	6	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	7	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	9	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	10	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	11	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	12	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	13	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	15	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	16	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	17	0.1
(2,1002)	1:30:C:ASN:HD21	1:30:C:ASN:HD22	18	0.1
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG12	9	0.1
(2,955)	1:20:C:MET:H	1:18:C:ILE:HG13	9	0.1
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD11	6	0.1
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD12	6	0.1
(2,876)	1:9:C:ARG:H	1:7:C:LEU:HD13	6	0.1
(2,822)	1:52:B:LEU:H	1:51:B:LEU:HA	1	0.1
(2,813)	1:51:B:LEU:H	1:51:B:LEU:HA	14	0.1
(2,742)	1:44:B:LEU:H	1:44:B:LEU:HA	14	0.1
(2,684)	1:39:B:LEU:H	1:36:B:CYS:HA	18	0.1
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	11	0.1
(2,646)	1:35:B:PHE:H	1:33:B:ILE:HB	16	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	1	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	2	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	3	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	4	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	7	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	8	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	9	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	11	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	12	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	15	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	16	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	17	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	18	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	19	0.1
(2,641)	1:27:B:ASN:HD21	1:27:B:ASN:HD22	20	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	2	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	3	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	4	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	5	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	6	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	7	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	9	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	10	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	12	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	13	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	14	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	15	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	16	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	17	0.1
(2,588)	1:30:B:ASN:HD21	1:30:B:ASN:HD22	18	0.1
(2,309)	1:43:A:LEU:H	1:40:A:ILE:HA	8	0.1
(2,302)	1:42:A:LEU:H	1:39:A:LEU:HA	12	0.1
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	2	0.1
(2,232)	1:35:A:PHE:H	1:33:A:ILE:HB	20	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	1	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	2	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	3	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	4	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	7	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	8	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	9	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	10	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	11	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	12	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	14	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	15	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	16	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	17	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	18	0.1
(2,227)	1:27:A:ASN:HD21	1:27:A:ASN:HD22	20	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	3	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	5	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	6	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	7	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	8	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	9	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	10	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	12	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	13	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	14	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	15	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	16	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	17	0.1
(2,174)	1:30:A:ASN:HD21	1:30:A:ASN:HD22	18	0.1
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG12	7	0.1
(2,127)	1:20:A:MET:H	1:18:A:ILE:HG13	7	0.1
(2,110)	1:17:A:THR:H	1:17:A:THR:HA	11	0.1

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

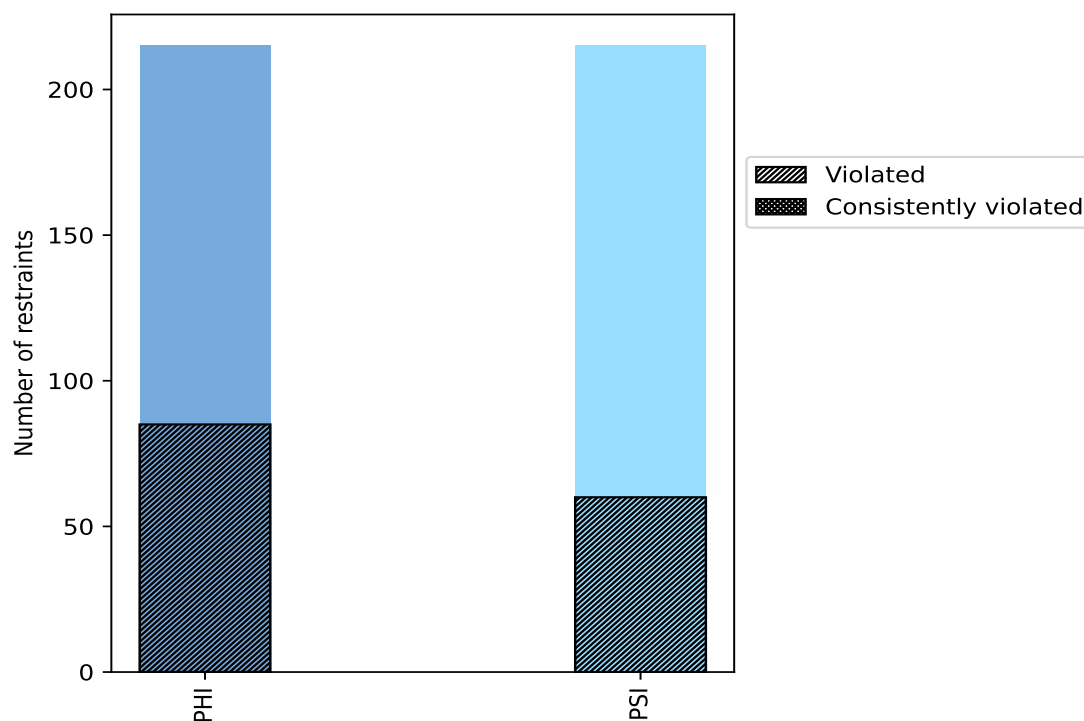
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	215	50.0	85	39.5	19.8	0	0.0	0.0
PSI	215	50.0	60	27.9	14.0	0	0.0	0.0
Total	430	100.0	145	33.7	33.7	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



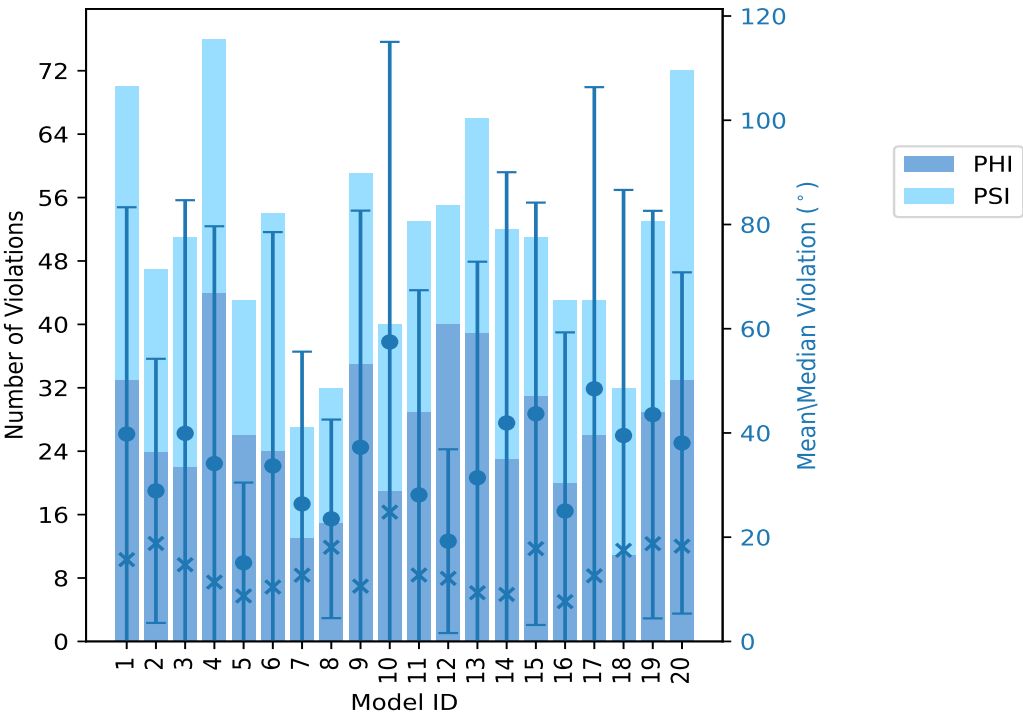
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	33	37	70	39.8	131.46	43.51	15.7
2	24	23	47	28.89	78.41	25.34	18.8
3	22	29	51	39.93	120.34	44.73	14.72
4	44	32	76	34.13	165.47	45.53	11.38
5	26	17	43	15.08	42.63	15.4	8.73
6	24	30	54	33.68	136.69	44.86	10.44
7	13	14	27	26.39	78.51	29.21	12.71
8	15	17	32	23.52	64.36	19.05	18.06
9	35	24	59	37.25	155.31	45.41	10.61
10	19	21	40	57.46	153.59	57.58	24.82
11	29	24	53	28.11	125.97	39.28	12.74
12	40	15	55	19.24	64.37	17.63	12.1
13	39	27	66	31.4	123.9	41.46	9.35
14	23	29	52	41.92	131.79	48.11	9.02
15	31	20	51	43.68	114.19	40.52	17.8
16	20	23	43	25.02	100.05	34.28	7.64
17	26	17	43	48.48	168.14	57.87	12.6
18	11	21	32	39.51	144.32	47.12	17.48
19	29	24	53	43.52	116.68	39.1	18.76
20	33	39	72	38.08	91.75	32.74	18.28

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
19	3	22	1	5.0
7	5	12	2	10.0
11	1	12	3	15.0
0	11	11	4	20.0
10	5	15	5	25.0
9	3	12	6	30.0
0	0	0	7	35.0
2	7	9	8	40.0
5	5	10	9	45.0
3	5	8	10	50.0
3	0	3	11	55.0

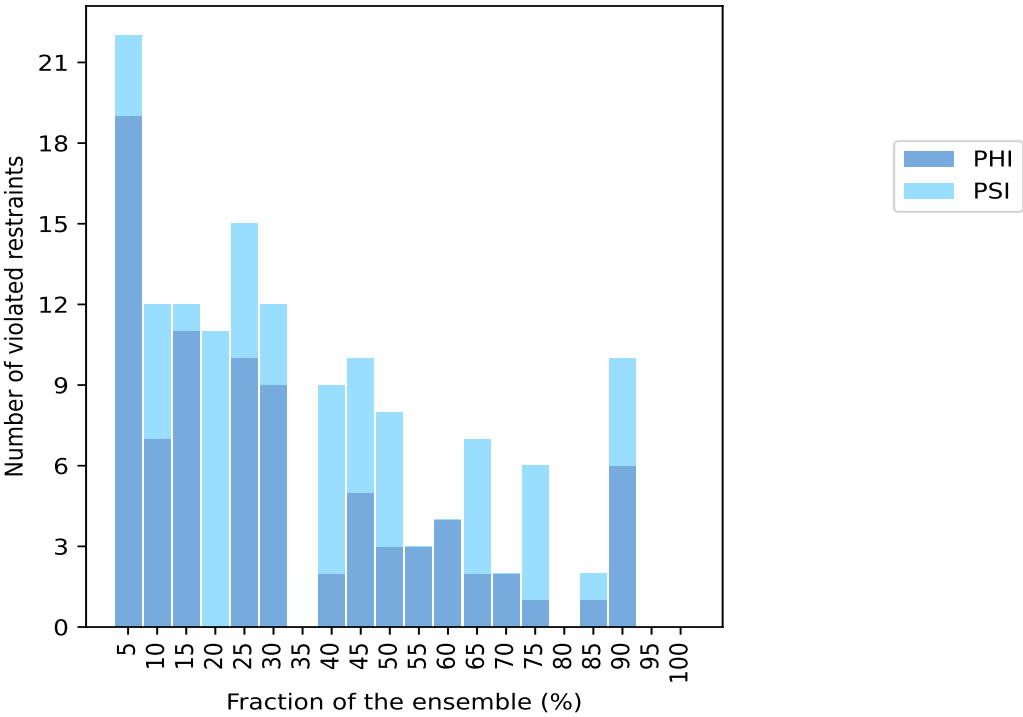
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
4	0	4	12	60.0
2	5	7	13	65.0
2	0	2	14	70.0
1	5	6	15	75.0
0	0	0	16	80.0
1	1	2	17	85.0
6	4	10	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

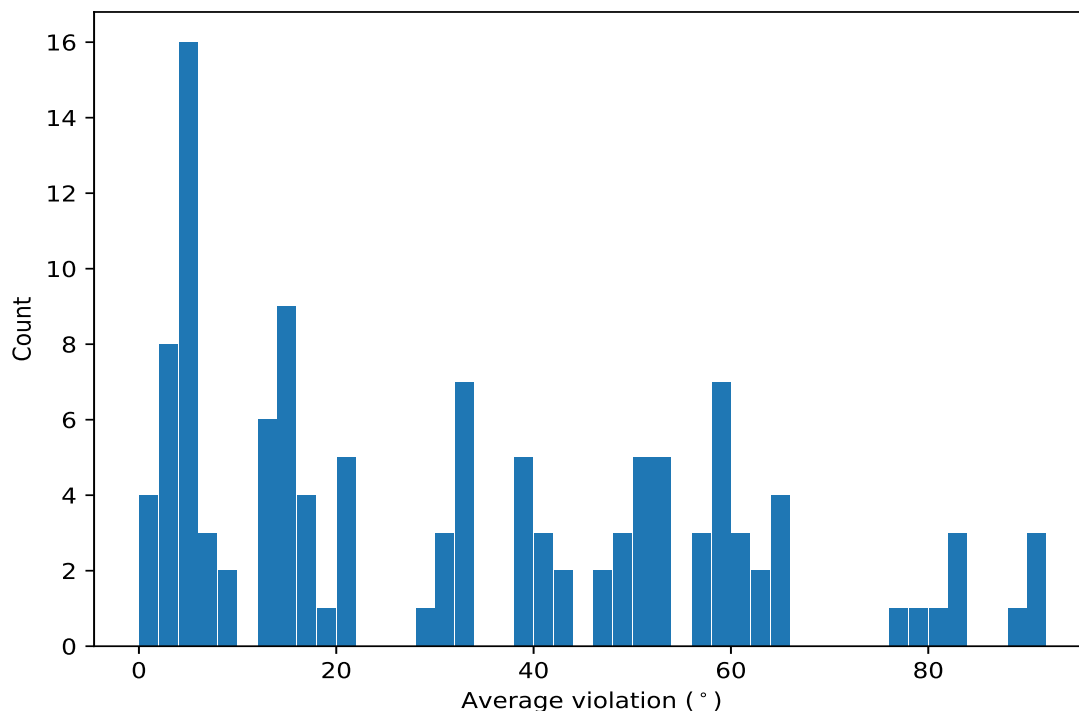


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	18	83.03	53.47	87.1
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	18	82.6	54.23	86.24
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	18	78.01	56.41	70.64
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	18	77.73	56.13	71.38
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	18	13.26	10.01	9.73
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	18	12.42	9.8	7.92
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	18	12.33	9.76	9.04
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	18	12.31	9.77	7.7
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	18	12.29	9.74	7.41
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	18	7.29	4.65	6.44
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	17	82.21	55.48	77.13
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	17	7.55	4.71	5.78
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	15	51.18	39.72	42.27
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	15	51.15	39.86	41.58
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	15	51.09	39.8	42.38
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	15	51.06	39.77	41.84
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	15	50.93	39.56	41.85
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	15	38.44	38.45	15.51
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	14	41.0	38.41	22.28
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	14	40.13	37.86	18.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	13	48.38	52.0	13.81
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	13	48.24	51.89	14.24
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	13	48.19	51.96	13.83
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	13	47.87	51.98	14.16
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	13	46.69	52.91	14.04
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	13	43.64	38.15	23.67
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	13	43.6	37.36	23.54
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	12	20.66	27.42	15.22
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	12	20.64	27.45	15.04
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	12	20.52	27.54	15.0
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	12	20.26	27.59	15.07
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	11	21.93	28.42	16.03
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	11	5.22	4.15	3.75
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	11	2.18	1.07	2.06
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	10	5.94	2.31	6.5
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	10	5.82	2.54	5.64
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	10	5.81	2.47	5.38
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	10	5.81	2.4	5.69
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	10	5.41	2.12	4.6
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	10	4.23	2.53	3.42
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	10	4.02	2.38	3.57
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	10	2.7	1.27	2.85
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	9	63.3	46.29	54.08
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	9	62.25	45.22	54.45
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	9	60.86	45.02	53.38
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	9	60.8	44.16	53.18
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	9	60.79	44.25	53.52
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	9	33.99	29.16	20.56
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	9	33.52	29.04	21.11
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	9	33.36	29.22	20.4
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	9	33.26	28.97	20.87
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	9	33.13	29.3	20.8
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	8	59.57	42.85	60.72
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	8	58.18	42.28	60.41
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	8	57.91	42.04	60.22
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	8	57.77	42.12	59.77
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	8	57.67	42.08	59.02
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	8	18.18	1.38	18.3
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	8	17.05	2.14	16.87
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	8	14.45	0.99	14.8
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	8	13.8	1.96	13.42
(1,57)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:SEP:N	6	80.41	24.87	82.07
(1,159)	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	1:38:B:ILE:N	6	16.81	2.05	16.82
(1,361)	1:17:E:THR:C	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	6	15.16	10.42	13.52
(1,117)	1:37:B:LEU:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	6	15.02	0.94	14.93
(1,17)	1:17:A:THR:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	6	14.97	10.27	13.04
(1,189)	1:17:C:THR:C	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	6	14.91	10.3	12.88
(1,103)	1:17:B:THR:C	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	6	14.9	10.38	12.64
(1,275)	1:17:D:THR:C	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	6	14.82	10.34	12.86
(1,374)	1:36:E:CYS:C	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	6	4.24	2.72	4.12
(1,247)	1:39:C:LEU:N	1:39:C:LEU:CA	1:39:C:LEU:C	1:40:C:ILE:N	6	2.55	1.02	2.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,122)	1:42:B:LEU:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	6	2.14	0.56	2.3
(1,294)	1:42:D:LEU:C	1:43:D:LEU:N	1:43:D:LEU:CA	1:43:D:LEU:C	6	1.81	0.62	1.56
(1,229)	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	1:16:C:SEP:N	5	90.89	12.64	87.17
(1,401)	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	1:16:E:SEP:N	5	90.67	12.89	86.49
(1,315)	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	1:16:D:SEP:N	5	90.15	13.41	85.88
(1,143)	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	1:16:B:SEP:N	5	89.68	13.98	87.69
(1,273)	1:15:D:ALA:C	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	5	65.03	38.73	74.16
(1,187)	1:15:C:ALA:C	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	5	64.96	38.84	74.21
(1,359)	1:15:E:ALA:C	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	5	64.91	38.84	74.25
(1,101)	1:15:B:ALA:C	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	5	64.71	38.56	74.42
(1,191)	1:21:C:PRO:C	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	5	40.2	37.33	12.88
(1,19)	1:21:A:PRO:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	5	39.66	39.27	11.9
(1,363)	1:21:E:PRO:C	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	5	39.54	40.07	11.47
(1,105)	1:21:B:PRO:C	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	5	39.32	39.51	11.9
(1,277)	1:21:D:PRO:C	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	5	38.82	40.32	9.83
(1,15)	1:15:A:ALA:C	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	5	28.27	24.48	13.62
(1,419)	1:39:E:LEU:N	1:39:E:LEU:CA	1:39:E:LEU:C	1:40:E:ILE:N	5	2.08	0.44	1.94
(1,232)	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	1:19:C:GLU:N	4	59.6	52.99	55.68
(1,404)	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	1:19:E:GLU:N	4	59.36	52.82	55.08
(1,60)	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	1:19:A:GLU:N	4	59.3	53.39	55.6
(1,146)	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	1:19:B:GLU:N	4	59.08	53.06	54.4
(1,318)	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	1:19:D:GLU:N	4	59.0	52.92	54.72
(1,406)	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	1:23:E:GLN:N	4	32.12	29.5	22.18
(1,320)	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	1:23:D:GLN:N	4	32.07	30.23	22.44
(1,148)	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	1:23:B:GLN:N	4	31.99	30.05	21.14
(1,62)	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	1:23:A:GLN:N	4	31.73	30.13	21.75
(1,234)	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	1:23:C:GLN:N	4	31.57	30.31	21.27
(1,161)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:ILE:N	4	4.21	0.8	4.22
(1,100)	1:14:B:ARG:C	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	3	53.11	12.74	51.12
(1,358)	1:14:E:ARG:C	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	3	53.06	14.17	51.25
(1,14)	1:14:A:ARG:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	3	53.02	13.98	51.31
(1,272)	1:14:D:ARG:C	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	3	53.0	13.85	51.53
(1,186)	1:14:C:ARG:C	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	3	52.19	13.73	49.88
(1,197)	1:31:C:LEU:C	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	3	6.0	0.86	6.39
(1,369)	1:31:E:LEU:C	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	3	5.82	1.1	6.32
(1,25)	1:31:A:LEU:C	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	3	5.74	1.68	6.07
(1,283)	1:31:D:LEU:C	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	3	5.66	0.48	5.94
(1,111)	1:31:B:LEU:C	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	3	5.53	0.68	5.7
(1,202)	1:36:C:CYS:C	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	3	5.47	2.99	7.1
(1,416)	1:36:E:CYS:N	1:36:E:CYS:CA	1:36:E:CYS:C	1:37:E:LEU:N	3	3.09	1.45	4.01
(1,331)	1:37:D:LEU:N	1:37:D:LEU:CA	1:37:D:LEU:C	1:38:D:ILE:N	2	17.9	0.02	17.9
(1,73)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:ILE:N	2	16.34	2.11	16.34
(1,31)	1:37:A:LEU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	2	15.56	0.55	15.56
(1,289)	1:37:D:LEU:C	1:38:D:ILE:N	1:38:D:ILE:CA	1:38:D:ILE:C	2	14.06	0.15	14.06
(1,429)	1:50:E:MET:N	1:50:E:MET:CA	1:50:E:MET:C	1:51:E:LEU:N	2	9.42	5.87	9.42
(1,85)	1:50:A:MET:N	1:50:A:MET:CA	1:50:A:MET:C	1:51:A:LEU:N	2	8.19	6.63	8.19
(1,288)	1:36:D:CYS:C	1:37:D:LEU:N	1:37:D:LEU:CA	1:37:D:LEU:C	2	4.77	2.43	4.77
(1,244)	1:36:C:CYS:N	1:36:C:CYS:CA	1:36:C:CYS:C	1:37:C:LEU:N	2	3.76	0.7	3.76
(1,262)	1:4:D:VAL:C	1:5:D:GLN:N	1:5:D:GLN:CA	1:5:D:GLN:C	2	2.83	0.9	2.83
(1,367)	1:29:E:GLN:C	1:30:E:ASN:N	1:30:E:ASN:CA	1:30:E:ASN:C	2	1.81	0.22	1.81
(1,4)	1:4:A:VAL:C	1:5:A:GLN:N	1:5:A:GLN:CA	1:5:A:GLN:C	2	1.77	0.58	1.77

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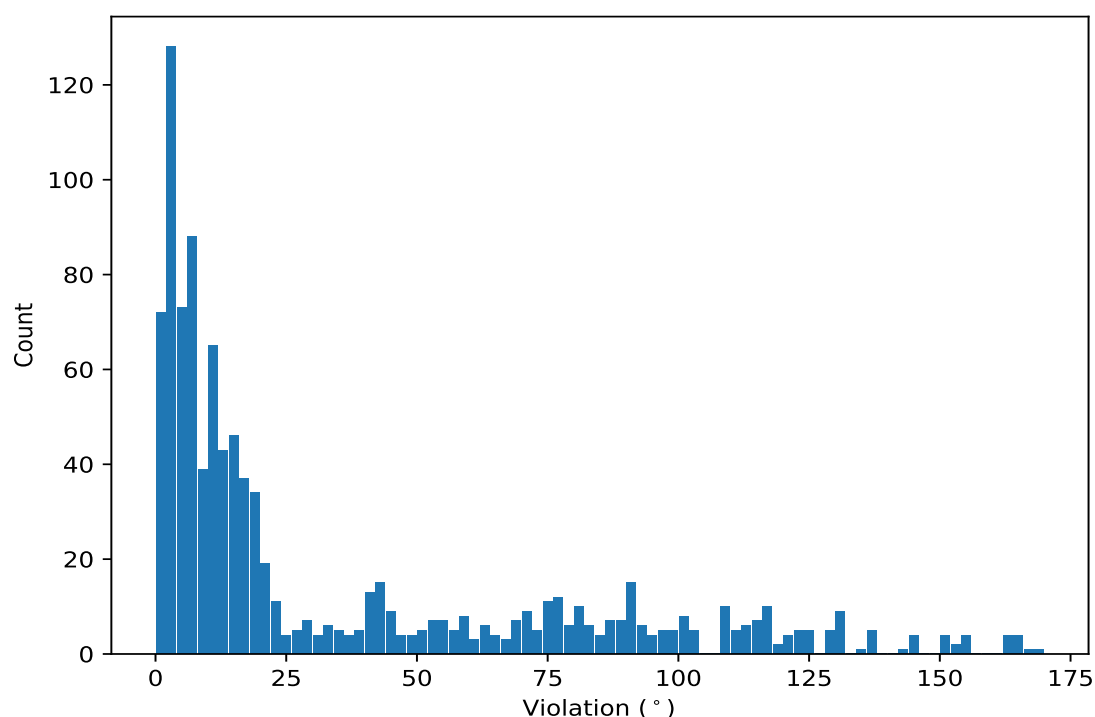
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,380)	1:42:E:LEU:C	1:43:E:LEU:N	1:43:E:LEU:CA	1:43:E:LEU:C	2	1.48	0.14	1.48

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 (°)
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	17	168.14
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	17	166.62
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	4	165.47
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	4	165.12
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	4	165.04
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	4	165.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	17	163.56
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	17	163.42
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	4	163.12
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	17	162.33
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	9	155.31
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	9	154.57
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	9	154.42
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	9	154.38
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	9	153.93
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	10	153.59
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	10	151.03
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	10	150.93
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	10	150.82
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	10	150.71
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	18	144.32
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	18	144.32
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	18	144.22
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	18	144.09
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	18	143.97
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	6	136.69
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	6	136.54
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	6	136.18
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	6	136.07
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	6	136.01
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	10	135.08
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	14	131.79
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	1	131.46
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	1	131.32
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	14	131.2
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	14	131.1
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	1	131.04
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	1	131.0
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	1	130.97
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	14	130.1
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	14	129.43
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	10	128.5
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	10	128.2
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	10	128.19
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	10	128.13
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	11	125.97
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	11	125.91
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	11	125.77
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	11	125.68
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	11	125.57
(1,318)	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	1:19:D:GLU:N	13	123.9
(1,146)	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	1:19:B:GLU:N	13	123.88
(1,60)	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	1:19:A:GLU:N	13	123.8
(1,404)	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	1:19:E:GLU:N	13	123.79
(1,232)	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	1:19:C:GLU:N	13	123.68
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	3	120.34
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	3	120.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	3	120.13
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	3	120.05
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	3	119.95
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	3	118.03
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	3	117.99
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	3	117.96
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	3	117.9
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	19	116.68
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	3	116.6
(1,187)	1:15:C:ALA:C	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	10	116.45
(1,273)	1:15:D:ALA:C	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	10	116.41
(1,359)	1:15:E:ALA:C	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	10	116.3
(1,101)	1:15:B:ALA:C	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	10	116.29
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	19	116.14
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	17	114.77
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	19	114.57
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	15	114.19
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	17	114.07
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	15	114.06
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	15	114.03
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	15	114.02
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	15	113.99
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	17	112.88
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	17	112.58
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	19	112.31
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	17	112.25
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	19	112.2
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	13	111.51
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	13	111.34
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	13	111.02
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	13	110.84
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	13	110.61
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	14	109.46
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	14	109.36
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	14	109.25
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	14	109.23
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	14	109.07
(1,143)	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	1:16:B:SEP:N	1	108.9
(1,57)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:SEP:N	1	108.78
(1,401)	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	1:16:E:SEP:N	1	108.74
(1,315)	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	1:16:D:SEP:N	1	108.73
(1,229)	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	1:16:C:SEP:N	1	108.61
(1,315)	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	1:16:D:SEP:N	4	102.97
(1,401)	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	1:16:E:SEP:N	4	102.82
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	15	102.81
(1,57)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:SEP:N	4	102.74
(1,229)	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	1:16:C:SEP:N	4	102.69
(1,143)	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	1:16:B:SEP:N	4	101.96
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	1	100.47
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	1	100.39
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	1	100.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	1	100.36
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	1	100.23
(1,60)	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	1:19:A:GLU:N	16	100.05
(1,232)	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	1:19:C:GLU:N	16	100.0
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	15	99.23
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	15	99.07
(1,404)	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	1:19:E:GLU:N	16	98.96
(1,146)	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	1:19:B:GLU:N	16	98.81
(1,318)	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	1:19:D:GLU:N	16	98.19
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	15	97.15
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	16	96.79
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	15	96.67
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	15	96.6
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	17	96.18
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	16	95.96
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	17	95.69
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	15	94.48
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	14	94.13
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	15	93.79
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	14	93.58
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	14	93.49
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	17	93.1
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	15	92.8
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	15	92.6
(1,273)	1:15:D:ALA:C	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	11	91.78
(1,187)	1:15:C:ALA:C	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	11	91.76
(1,359)	1:15:E:ALA:C	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	11	91.75
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	20	91.75
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	20	91.68
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	20	91.62
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	19	91.52
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	20	91.5
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	20	91.18
(1,363)	1:21:E:PRO:C	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	6	90.92
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	19	90.64
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	19	90.43
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	14	90.35
(1,101)	1:15:B:ALA:C	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	11	90.24
(1,277)	1:21:D:PRO:C	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	6	90.01
(1,191)	1:21:C:PRO:C	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	6	89.84
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	19	89.79
(1,105)	1:21:B:PRO:C	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	6	89.65
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	19	89.63
(1,19)	1:21:A:PRO:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	6	89.51
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	17	88.26
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	17	88.14
(1,143)	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	1:16:B:SEP:N	19	87.69
(1,229)	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	1:16:C:SEP:N	19	87.17
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	14	87.11
(1,401)	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	1:16:E:SEP:N	19	86.49
(1,57)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:SEP:N	19	86.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,277)	1:21:D:PRO:C	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	4	86.21
(1,363)	1:21:E:PRO:C	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	4	86.02
(1,315)	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	1:16:D:SEP:N	19	85.88
(1,19)	1:21:A:PRO:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	4	85.77
(1,105)	1:21:B:PRO:C	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	4	85.5
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	3	84.36
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	20	83.32
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	20	83.21
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	20	83.16
(1,148)	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	1:23:B:GLN:N	6	82.37
(1,234)	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	1:23:C:GLN:N	6	82.18
(1,320)	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	1:23:D:GLN:N	6	82.11
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	20	81.91
(1,62)	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	1:23:A:GLN:N	6	81.85
(1,191)	1:21:C:PRO:C	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	4	81.43
(1,406)	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	1:23:E:GLN:N	6	81.29
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	9	81.29
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	20	81.18
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	9	80.72
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	9	80.66
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	9	80.36
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	9	80.27
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	7	78.51
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	7	78.42
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	2	78.41
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	7	78.32
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	7	78.26
(1,229)	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	1:16:C:SEP:N	20	78.02
(1,229)	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	1:16:C:SEP:N	13	77.98
(1,315)	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	1:16:D:SEP:N	13	77.89
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	7	77.89
(1,143)	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	1:16:B:SEP:N	13	77.84
(1,401)	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	1:16:E:SEP:N	13	77.83
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	2	77.75
(1,57)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:SEP:N	13	77.71
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	2	77.61
(1,401)	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	1:16:E:SEP:N	20	77.47
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	2	77.13
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	20	76.95
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	2	76.52
(1,315)	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	1:16:D:SEP:N	20	75.27
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	20	75.21
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	20	75.21
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	20	75.01
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	20	74.86
(1,57)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:SEP:N	20	74.66
(1,101)	1:15:B:ALA:C	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1	74.42
(1,15)	1:15:A:ALA:C	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1	74.34
(1,359)	1:15:E:ALA:C	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1	74.25
(1,187)	1:15:C:ALA:C	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1	74.21
(1,273)	1:15:D:ALA:C	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1	74.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	9	73.45
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	9	73.25
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	9	72.66
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	9	72.24
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	3	72.16
(1,143)	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	1:16:B:SEP:N	20	71.99
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	3	71.93
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	3	71.91
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	9	71.88
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	3	71.8
(1,358)	1:14:E:ARG:C	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	19	71.25
(1,14)	1:14:A:ARG:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	19	70.94
(1,272)	1:14:D:ARG:C	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	19	70.64
(1,186)	1:14:C:ARG:C	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	19	70.04
(1,100)	1:14:B:ARG:C	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	19	69.62
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	20	69.18
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	20	68.83
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	20	68.73
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	20	68.18
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	14	68.1
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	14	68.08
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	14	67.88
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	14	67.55
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	20	67.45
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	14	65.67
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	12	64.37
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	8	64.36
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	12	64.11
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	12	63.93
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	8	63.52
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	8	63.44
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	12	63.04
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	8	62.93
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	8	62.39
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	9	61.12
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	12	60.32
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	20	60.27
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	15	59.52
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	9	59.04
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	20	58.89
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	20	58.84
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	9	58.74
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	9	58.48
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	20	58.36
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	20	58.35
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	15	57.79
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	15	57.6
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	9	57.03
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	15	56.73
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	15	56.63
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	2	55.83

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	2	55.78
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	2	55.64
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	2	55.62
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	2	54.49
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	1	54.45
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	1	54.08
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	1	53.52
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	1	53.38
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	2	53.33
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	1	53.18
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	2	52.74
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	2	52.56
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	2	52.37
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	2	51.99
(1,272)	1:14:D:ARG:C	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	4	51.53
(1,14)	1:14:A:ARG:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	4	51.31
(1,358)	1:14:E:ARG:C	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	4	51.25
(1,100)	1:14:B:ARG:C	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	4	51.12
(1,186)	1:14:C:ARG:C	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	4	49.88
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	3	49.0
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	3	48.35
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	3	48.08
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	3	47.77
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	3	47.53
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	18	47.19
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	18	47.13
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	7	45.67
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	7	45.16
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	7	45.0
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	18	44.74
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	7	44.58
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	7	44.56
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	18	44.55
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	12	44.14
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	12	44.09
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	12	43.85
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	10	42.7
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	5	42.63
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	10	42.58
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	5	42.56
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	5	42.56
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	10	42.54
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	5	42.48
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	5	42.44
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	5	42.38
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	5	42.27
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	11	42.19
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	11	42.13
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	10	42.06
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	11	42.04
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	5	41.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	5	41.84
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	18	41.8
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	16	41.78
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	16	41.72
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	5	41.58
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	19	41.1
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	12	41.07
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	11	40.76
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	19	40.69
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	19	40.62
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	12	40.41
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	19	40.28
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	19	39.79
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	16	39.62
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	16	39.31
(1,100)	1:14:B:ARG:C	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	2	38.6
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	16	38.44
(1,272)	1:14:D:ARG:C	1:15:D:ALA:N	1:15:D:ALA:CA	1:15:D:ALA:C	2	36.82
(1,14)	1:14:A:ARG:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	2	36.82
(1,358)	1:14:E:ARG:C	1:15:E:ALA:N	1:15:E:ALA:CA	1:15:E:ALA:C	2	36.67
(1,186)	1:14:C:ARG:C	1:15:C:ALA:N	1:15:C:ALA:CA	1:15:C:ALA:C	2	36.64
(1,361)	1:17:E:THR:C	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	9	35.43
(1,103)	1:17:B:THR:C	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	9	35.37
(1,189)	1:17:C:THR:C	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	9	35.25
(1,275)	1:17:D:THR:C	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	9	35.1
(1,17)	1:17:A:THR:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	9	35.08
(1,273)	1:15:D:ALA:C	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	13	32.74
(1,101)	1:15:B:ALA:C	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	13	32.71
(1,15)	1:15:A:ALA:C	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	13	32.64
(1,359)	1:15:E:ALA:C	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	13	32.56
(1,187)	1:15:C:ALA:C	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	13	32.51
(1,57)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:SEP:N	10	32.12
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	18	31.07
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	10	30.93
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	18	30.34
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	18	30.16
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	18	29.45
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	18	29.28
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	8	28.29
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	8	28.28
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	8	28.2
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	8	28.14
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	8	28.03
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	20	27.77
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	20	27.59
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	20	27.42
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	20	27.22
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	20	26.86
(1,320)	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	1:23:D:GLN:N	4	25.57
(1,406)	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	1:23:E:GLN:N	4	24.26
(1,62)	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	1:23:A:GLN:N	4	24.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,148)	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	1:23:B:GLN:N	4	24.04
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	8	23.91
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	11	23.86
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	8	23.67
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	8	23.54
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	8	23.5
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	8	22.82
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	4	22.21
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	12	22.18
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	4	22.12
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	4	22.11
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	4	22.06
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	4	21.91
(1,357)	1:13:E:ARG:C	1:14:E:ARG:N	1:14:E:ARG:CA	1:14:E:ARG:C	13	21.83
(1,185)	1:13:C:ARG:C	1:14:C:ARG:N	1:14:C:ARG:CA	1:14:C:ARG:C	13	21.76
(1,271)	1:13:D:ARG:C	1:14:D:ARG:N	1:14:D:ARG:CA	1:14:D:ARG:C	13	21.73
(1,234)	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	1:23:C:GLN:N	12	21.71
(1,13)	1:13:A:ARG:C	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	13	21.7
(1,99)	1:13:B:ARG:C	1:14:B:ARG:N	1:14:B:ARG:CA	1:14:B:ARG:C	13	21.57
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	12	21.47
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1	21.11
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	12	21.08
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1	20.87
(1,234)	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	1:23:C:GLN:N	4	20.83
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1	20.8
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	15	20.66
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1	20.56
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1	20.4
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	13	20.38
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	12	20.24
(1,406)	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	1:23:E:GLN:N	12	20.11
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	12	19.86
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	17	19.73
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	12	19.69
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	12	19.66
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	1	19.57
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	6	19.56
(1,159)	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	1:38:B:ILE:N	7	19.5
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	12	19.45
(1,62)	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	1:23:A:GLN:N	12	19.41
(1,320)	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	1:23:D:GLN:N	12	19.3
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	12	19.3
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	6	19.28
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	15	19.16
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	19	19.01
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	12	18.89
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	2	18.84
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	2	18.83
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	2	18.81
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	2	18.8
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	19	18.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	1:38:B:ILE:N	14	18.74
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	10	18.72
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	10	18.67
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	10	18.6
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	10	18.59
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	15	18.5
(1,73)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:ILE:N	19	18.45
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	19	18.31
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	19	18.29
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	20	18.29
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	20	18.27
(1,148)	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	1:23:B:GLN:N	12	18.25
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	8	18.18
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	11	18.04
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	8	17.94
(1,331)	1:37:D:LEU:N	1:37:D:LEU:CA	1:37:D:LEU:C	1:38:D:ILE:N	19	17.92
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	2	17.91
(1,331)	1:37:D:LEU:N	1:37:D:LEU:CA	1:37:D:LEU:C	1:38:D:ILE:N	11	17.88
(1,103)	1:17:B:THR:C	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	15	17.88
(1,361)	1:17:E:THR:C	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	15	17.87
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	8	17.87
(1,17)	1:17:A:THR:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	15	17.8
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	8	17.79
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	8	17.76
(1,275)	1:17:D:THR:C	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	15	17.73
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	18	17.71
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	16	17.65
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	2	17.51
(1,189)	1:17:C:THR:C	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	15	17.51
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	10	17.41
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	18	17.26
(1,159)	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	1:38:B:ILE:N	19	17.17
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	15	17.14
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	18	17.12
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	15	17.11
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	18	17.09
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	19	17.04
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	13	16.96
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	14	16.92
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	15	16.9
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	15	16.78
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	15	16.78
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	3	16.73
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	11	16.61
(1,159)	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	1:38:B:ILE:N	4	16.46
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	2	16.42
(1,117)	1:37:B:LEU:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	19	16.23
(1,117)	1:37:B:LEU:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	7	16.14
(1,31)	1:37:A:LEU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	19	16.1
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	16	16.08
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1	16.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1	15.93
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	5	15.83
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1	15.79
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1	15.75
(1,159)	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	1:38:B:ILE:N	8	15.74
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1	15.66
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	18	15.63
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	19	15.62
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	5	15.56
(1,245)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:ILE:N	9	15.55
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	3	15.51
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	1	15.42
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	20	15.39
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	10	15.33
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	17	15.3
(1,429)	1:50:E:MET:N	1:50:E:MET:CA	1:50:E:MET:C	1:51:E:LEU:N	3	15.29
(1,117)	1:37:B:LEU:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	8	15.26
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	20	15.18
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	18	15.17
(1,31)	1:37:A:LEU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	5	15.01
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	3	14.91
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	17	14.85
(1,361)	1:17:E:THR:C	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	20	14.82
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	19	14.82
(1,85)	1:50:A:MET:N	1:50:A:MET:CA	1:50:A:MET:C	1:51:A:LEU:N	3	14.82
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	6	14.78
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	15	14.78
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	3	14.72
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	11	14.68
(1,117)	1:37:B:LEU:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	14	14.61
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	3	14.57
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	11	14.48
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	11	14.33
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	11	14.28
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	15	14.24
(1,73)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:ILE:N	5	14.22
(1,289)	1:37:D:LEU:C	1:38:D:ILE:N	1:38:D:ILE:CA	1:38:D:ILE:C	11	14.21
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	11	14.21
(1,117)	1:37:B:LEU:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	4	14.2
(1,17)	1:17:A:THR:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	20	14.2
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	15	14.16
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	13	14.11
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	20	14.1
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	15	14.04
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	2	14.03
(1,189)	1:17:C:THR:C	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	20	14.01
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	17	13.93
(1,289)	1:37:D:LEU:C	1:38:D:ILE:N	1:38:D:ILE:CA	1:38:D:ILE:C	19	13.91
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	18	13.86
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	15	13.83
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	15	13.81

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	18	13.77
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	18	13.73
(1,117)	1:37:B:LEU:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	9	13.71
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	11	13.68
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	11	13.64
(1,275)	1:17:D:THR:C	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	20	13.63
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	11	13.63
(1,103)	1:17:B:THR:C	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	20	13.62
(1,15)	1:15:A:ALA:C	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	10	13.62
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	9	13.34
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	20	13.32
(1,159)	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	1:38:B:ILE:N	9	13.24
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	6	13.11
(1,417)	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	1:38:E:ILE:N	3	13.07
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	15	12.88
(1,191)	1:21:C:PRO:C	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	15	12.88
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	17	12.79
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	11	12.74
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	17	12.74
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	7	12.72
(1,191)	1:21:C:PRO:C	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	12	12.72
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	7	12.71
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	11	12.61
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	17	12.6
(1,203)	1:37:C:LEU:C	1:38:C:ILE:N	1:38:C:ILE:CA	1:38:C:ILE:C	14	12.53
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	13	12.5
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	6	12.49
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	13	12.45
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	6	12.39
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	20	12.38
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	16	12.3
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	20	12.23
(1,361)	1:17:E:THR:C	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	12	12.23
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	20	12.2
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	13	12.19
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	13	12.11
(1,275)	1:17:D:THR:C	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	12	12.1
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	4	12.08
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	20	11.91
(1,105)	1:21:B:PRO:C	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	12	11.9
(1,19)	1:21:A:PRO:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	12	11.9
(1,17)	1:17:A:THR:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	12	11.89
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	6	11.88
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	20	11.85
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	6	11.82
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	13	11.82
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	6	11.78
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	12	11.76
(1,189)	1:17:C:THR:C	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	12	11.74
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	4	11.71
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	4	11.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	4	11.69
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	4	11.65
(1,103)	1:17:B:THR:C	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	12	11.65
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	12	11.59
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	6	11.53
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	6	11.51
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	12	11.5
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	12	11.48
(1,363)	1:21:E:PRO:C	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	12	11.47
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	2	11.47
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	12	11.45
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	4	11.38
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	4	11.37
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	4	11.36
(1,232)	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	1:19:C:GLU:N	19	11.35
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	10	11.27
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	10	11.25
(1,318)	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	1:19:D:GLU:N	19	11.25
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	20	11.25
(1,404)	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	1:19:E:GLU:N	19	11.21
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	4	11.19
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	4	11.18
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	1	11.15
(1,60)	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	1:19:A:GLU:N	19	11.14
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	20	11.13
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	4	11.13
(1,15)	1:15:A:ALA:C	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	11	10.9
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	1	10.79
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	4	10.73
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	4	10.72
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	20	10.7
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	4	10.62
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	9	10.61
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	9	10.61
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	14	10.6
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	9	10.52
(1,375)	1:37:E:LEU:C	1:38:E:ILE:N	1:38:E:ILE:CA	1:38:E:ILE:C	3	10.51
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	1	10.51
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	6	10.47
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	6	10.41
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	1	10.39
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	9	10.32
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	9	10.31
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	8	10.25
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	1	10.25
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	4	10.24
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	15	10.21
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	6	10.16
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	15	10.14
(1,273)	1:15:D:ALA:C	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	5	10.08
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	8	10.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	15	10.01
(1,146)	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	1:19:B:GLU:N	19	9.98
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1	9.95
(1,101)	1:15:B:ALA:C	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	5	9.91
(1,187)	1:15:C:ALA:C	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	5	9.87
(1,15)	1:15:A:ALA:C	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	5	9.87
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	8	9.83
(1,277)	1:21:D:PRO:C	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	12	9.83
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	1	9.8
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	2	9.79
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	2	9.77
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	2	9.76
(1,359)	1:15:E:ALA:C	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	5	9.69
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	2	9.68
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	14	9.59
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	3	9.58
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	8	9.27
(1,361)	1:17:E:THR:C	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	1	9.25
(1,103)	1:17:B:THR:C	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	1	9.14
(1,189)	1:17:C:THR:C	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	1	9.11
(1,17)	1:17:A:THR:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	1	9.11
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	6	8.9
(1,275)	1:17:D:THR:C	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	1	8.87
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	5	8.83
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	5	8.81
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	5	8.73
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	5	8.71
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	6	8.6
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	16	8.51
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	5	8.49
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	14	8.46
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	6	8.44
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	16	8.44
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	17	8.44
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	16	8.24
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	6	8.17
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	4	8.14
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	17	8.07
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	17	8.05
(1,202)	1:36:C:CYS:C	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	14	8.04
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	17	7.89
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	16	7.84
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	20	7.78
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	16	7.75
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	16	7.69
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	16	7.64
(1,25)	1:31:A:LEU:C	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1	7.61
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	3	7.55
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	14	7.55
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	6	7.54
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	1	7.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,374)	1:36:E:CYS:C	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	5	7.53
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	20	7.52
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	4	7.48
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	12	7.41
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	20	7.37
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	16	7.35
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	4	7.25
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	3	7.23
(1,374)	1:36:E:CYS:C	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	11	7.22
(1,288)	1:36:D:CYS:C	1:37:D:LEU:N	1:37:D:LEU:CA	1:37:D:LEU:C	11	7.19
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	4	7.19
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	12	7.17
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	3	7.16
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	3	7.13
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	4	7.11
(1,202)	1:36:C:CYS:C	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	20	7.1
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	4	7.07
(1,19)	1:21:A:PRO:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	15	7.07
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	12	7.06
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	1	7.05
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	11	7.05
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	16	7.05
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	4	7.04
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	17	7.03
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	4	6.96
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	20	6.95
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	11	6.95
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	14	6.94
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	1	6.93
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	17	6.89
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	12	6.88
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	12	6.88
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	13	6.87
(1,369)	1:31:E:LEU:C	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1	6.85
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	20	6.82
(1,197)	1:31:C:LEU:C	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1	6.8
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	17	6.79
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	13	6.75
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	13	6.75
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	1	6.74
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	16	6.72
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	17	6.67
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	11	6.66
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	13	6.65
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	11	6.64
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	13	6.64
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	4	6.62
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	17	6.62
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	10	6.59
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	10	6.53
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	17	6.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	10	6.47
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	14	6.46
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	10	6.45
(1,197)	1:31:C:LEU:C	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	4	6.39
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	2	6.38
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	17	6.37
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	17	6.35
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	2	6.35
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	3	6.34
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	2	6.33
(1,369)	1:31:E:LEU:C	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	4	6.32
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	2	6.31
(1,111)	1:31:B:LEU:C	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	4	6.27
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	17	6.26
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	1	6.23
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	3	6.16
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	11	6.16
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	2	6.09
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	3	6.09
(1,363)	1:21:E:PRO:C	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	15	6.08
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	13	6.08
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	13	6.08
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	5	6.07
(1,25)	1:31:A:LEU:C	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	4	6.07
(1,283)	1:31:D:LEU:C	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1	6.05
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	9	6.02
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	5	5.98
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	13	5.98
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	13	5.96
(1,283)	1:31:D:LEU:C	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	4	5.94
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	13	5.94
(1,374)	1:36:E:CYS:C	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	20	5.9
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	9	5.9
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	9	5.85
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	9	5.78
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	17	5.78
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	5	5.76
(1,111)	1:31:B:LEU:C	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1	5.7
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	3	5.68
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	5	5.6
(1,231)	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1:18:C:ILE:N	16	5.6
(1,403)	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1:18:E:ILE:N	16	5.59
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	17	5.57
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	17	5.55
(1,317)	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1:18:D:ILE:N	16	5.47
(1,59)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:ILE:N	16	5.47
(1,145)	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1:18:B:ILE:N	16	5.46
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	5	5.46
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	9	5.39
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	4	5.37
(1,161)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:ILE:N	7	5.33

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	1	5.26
(1,105)	1:21:B:PRO:C	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	15	5.23
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	2	5.12
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	1	5.11
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	1	5.07
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	10	5.07
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	1	5.05
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	17	5.05
(1,283)	1:31:D:LEU:C	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	20	4.99
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	1	4.98
(1,63)	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	1:24:A:ALA:N	18	4.91
(1,197)	1:31:C:LEU:C	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	20	4.8
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	16	4.78
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	14	4.77
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	17	4.74
(1,407)	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	1:24:E:ALA:N	18	4.73
(1,277)	1:21:D:PRO:C	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	15	4.67
(1,111)	1:31:B:LEU:C	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	20	4.62
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	2	4.54
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	3	4.5
(1,244)	1:36:C:CYS:N	1:36:C:CYS:CA	1:36:C:CYS:C	1:37:C:LEU:N	14	4.45
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	17	4.43
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	3	4.4
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	3	4.35
(1,161)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:ILE:N	8	4.35
(1,105)	1:21:B:PRO:C	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	14	4.32
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	17	4.31
(1,369)	1:31:E:LEU:C	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	20	4.3
(1,194)	1:28:C:LEU:C	1:29:C:GLN:N	1:29:C:GLN:CA	1:29:C:GLN:C	7	4.3
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	13	4.3
(1,149)	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	1:24:B:ALA:N	18	4.28
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	13	4.27
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	3	4.26
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	3	4.26
(1,416)	1:36:E:CYS:N	1:36:E:CYS:CA	1:36:E:CYS:C	1:37:E:LEU:N	11	4.22
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	13	4.22
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	16	4.17
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	10	4.13
(1,247)	1:39:C:LEU:N	1:39:C:LEU:CA	1:39:C:LEU:C	1:40:C:ILE:N	9	4.12
(1,191)	1:21:C:PRO:C	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	14	4.12
(1,161)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:ILE:N	9	4.09
(1,108)	1:28:B:LEU:C	1:29:B:GLN:N	1:29:B:GLN:CA	1:29:B:GLN:C	7	4.07
(1,19)	1:21:A:PRO:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	14	4.07
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	13	4.06
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	16	4.03
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	3	4.02
(1,416)	1:36:E:CYS:N	1:36:E:CYS:CA	1:36:E:CYS:C	1:37:E:LEU:N	5	4.01
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	10	4.01
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	16	3.99
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	13	3.96
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	4	3.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	16	3.9
(1,321)	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	1:24:D:ALA:N	18	3.88
(1,116)	1:36:B:CYS:C	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	14	3.87
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	4	3.85
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	6	3.83
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	4	3.82
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	9	3.77
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	9	3.75
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	4	3.74
(1,262)	1:4:D:VAL:C	1:5:D:GLN:N	1:5:D:GLN:CA	1:5:D:GLN:C	13	3.73
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	6	3.73
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	9	3.69
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	6	3.69
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	6	3.69
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	4	3.67
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	9	3.67
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	3	3.66
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	6	3.64
(1,146)	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	1:19:B:GLU:N	11	3.63
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	4	3.62
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	14	3.61
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	10	3.6
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	9	3.6
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	4	3.6
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	6	3.59
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	6	3.58
(1,429)	1:50:E:MET:N	1:50:E:MET:CA	1:50:E:MET:C	1:51:E:LEU:N	2	3.55
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	6	3.54
(1,25)	1:31:A:LEU:C	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	20	3.53
(1,366)	1:28:E:LEU:C	1:29:E:GLN:N	1:29:E:GLN:CA	1:29:E:GLN:C	7	3.51
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	14	3.51
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	6	3.5
(1,22)	1:28:A:LEU:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	7	3.5
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	14	3.5
(1,404)	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	1:19:E:GLU:N	11	3.49
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	4	3.48
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	14	3.44
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	4	3.42
(1,277)	1:21:D:PRO:C	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	14	3.39
(1,232)	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	1:19:C:GLU:N	11	3.35
(1,148)	1:22:B:GLN:N	1:22:B:GLN:CA	1:22:B:GLN:C	1:23:B:GLN:N	14	3.32
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	4	3.31
(1,330)	1:36:D:CYS:N	1:36:D:CYS:CA	1:36:D:CYS:C	1:37:D:LEU:N	11	3.29
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	10	3.29
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	14	3.25
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	6	3.23
(1,154)	1:32:B:PHE:N	1:32:B:PHE:CA	1:32:B:PHE:C	1:33:B:ILE:N	9	3.22
(1,363)	1:21:E:PRO:C	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	14	3.19
(1,280)	1:28:D:LEU:C	1:29:D:GLN:N	1:29:D:GLN:CA	1:29:D:GLN:C	7	3.19
(1,247)	1:39:C:LEU:N	1:39:C:LEU:CA	1:39:C:LEU:C	1:40:C:ILE:N	17	3.19
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	10	3.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	5	3.14
(1,176)	1:4:C:VAL:C	1:5:C:GLN:N	1:5:C:GLN:CA	1:5:C:GLN:C	13	3.14
(1,106)	1:22:B:GLN:C	1:23:B:GLN:N	1:23:B:GLN:CA	1:23:B:GLN:C	5	3.1
(1,161)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:ILE:N	4	3.07
(1,244)	1:36:C:CYS:N	1:36:C:CYS:CA	1:36:C:CYS:C	1:37:C:LEU:N	20	3.06
(1,235)	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	1:24:C:ALA:N	18	3.03
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	5	3.03
(1,192)	1:22:C:GLN:C	1:23:C:GLN:N	1:23:C:GLN:CA	1:23:C:GLN:C	5	2.98
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	5	2.93
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	4	2.91
(1,188)	1:16:C:SEP:C	1:17:C:THR:N	1:17:C:THR:CA	1:17:C:THR:C	1	2.9
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	15	2.87
(1,406)	1:22:E:GLN:N	1:22:E:GLN:CA	1:22:E:GLN:C	1:23:E:GLN:N	14	2.83
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	20	2.83
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	5	2.83
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	8	2.82
(1,360)	1:16:E:SEP:C	1:17:E:THR:N	1:17:E:THR:CA	1:17:E:THR:C	1	2.79
(1,294)	1:42:D:LEU:C	1:43:D:LEU:N	1:43:D:LEU:CA	1:43:D:LEU:C	15	2.79
(1,122)	1:42:B:LEU:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	4	2.77
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	8	2.76
(1,240)	1:32:C:PHE:N	1:32:C:PHE:CA	1:32:C:PHE:C	1:33:C:ILE:N	9	2.75
(1,419)	1:39:E:LEU:N	1:39:E:LEU:CA	1:39:E:LEU:C	1:40:E:ILE:N	6	2.71
(1,247)	1:39:C:LEU:N	1:39:C:LEU:CA	1:39:C:LEU:C	1:40:C:ILE:N	1	2.71
(1,20)	1:22:A:GLN:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	5	2.71
(1,247)	1:39:C:LEU:N	1:39:C:LEU:CA	1:39:C:LEU:C	1:40:C:ILE:N	6	2.7
(1,318)	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	1:19:D:GLU:N	11	2.67
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	8	2.64
(1,23)	1:29:A:GLN:C	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	13	2.64
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	8	2.6
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	3	2.6
(1,122)	1:42:B:LEU:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	15	2.58
(1,68)	1:32:A:PHE:N	1:32:A:PHE:CA	1:32:A:PHE:C	1:33:A:ILE:N	9	2.56
(1,144)	1:16:B:SEP:N	1:16:B:SEP:CA	1:16:B:SEP:C	1:17:B:THR:N	13	2.52
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	18	2.51
(1,294)	1:42:D:LEU:C	1:43:D:LEU:N	1:43:D:LEU:CA	1:43:D:LEU:C	20	2.5
(1,122)	1:42:B:LEU:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	3	2.5
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	5	2.47
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	16	2.45
(1,419)	1:39:E:LEU:N	1:39:E:LEU:CA	1:39:E:LEU:C	1:40:E:ILE:N	16	2.42
(1,16)	1:16:A:SEP:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1	2.4
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	8	2.39
(1,326)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:ILE:N	9	2.37
(1,58)	1:16:A:SEP:N	1:16:A:SEP:CA	1:16:A:SEP:C	1:17:A:THR:N	13	2.37
(1,374)	1:36:E:CYS:C	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	6	2.35
(1,90)	1:4:B:VAL:C	1:5:B:GLN:N	1:5:B:GLN:CA	1:5:B:GLN:C	13	2.35
(1,4)	1:4:A:VAL:C	1:5:A:GLN:N	1:5:A:GLN:CA	1:5:A:GLN:C	13	2.35
(1,288)	1:36:D:CYS:C	1:37:D:LEU:N	1:37:D:LEU:CA	1:37:D:LEU:C	19	2.34
(1,109)	1:29:B:GLN:C	1:30:B:ASN:N	1:30:B:ASN:CA	1:30:B:ASN:C	13	2.34
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	19	2.34
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	5	2.33
(1,348)	1:4:E:VAL:C	1:5:E:GLN:N	1:5:E:GLN:CA	1:5:E:GLN:C	13	2.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	12	2.27
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	12	2.25
(1,278)	1:22:D:GLN:C	1:23:D:GLN:N	1:23:D:GLN:CA	1:23:D:GLN:C	5	2.24
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	11	2.21
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	12	2.21
(1,102)	1:16:B:SEP:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1	2.2
(1,60)	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	1:19:A:GLU:N	11	2.2
(1,316)	1:16:D:SEP:N	1:16:D:SEP:CA	1:16:D:SEP:C	1:17:D:THR:N	13	2.19
(1,274)	1:16:D:SEP:C	1:17:D:THR:N	1:17:D:THR:CA	1:17:D:THR:C	1	2.19
(1,230)	1:16:C:SEP:N	1:16:C:SEP:CA	1:16:C:SEP:C	1:17:C:THR:N	13	2.19
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	19	2.14
(1,402)	1:16:E:SEP:N	1:16:E:SEP:CA	1:16:E:SEP:C	1:17:E:THR:N	13	2.13
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	16	2.13
(1,412)	1:32:E:PHE:N	1:32:E:PHE:CA	1:32:E:PHE:C	1:33:E:ILE:N	9	2.12
(1,364)	1:22:E:GLN:C	1:23:E:GLN:N	1:23:E:GLN:CA	1:23:E:GLN:C	5	2.11
(1,122)	1:42:B:LEU:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	5	2.11
(1,195)	1:29:C:GLN:C	1:30:C:ASN:N	1:30:C:ASN:CA	1:30:C:ASN:C	13	2.07
(1,236)	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	1:25:C:ARG:N	11	2.06
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	10	2.06
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	12	2.05
(1,367)	1:29:E:GLN:C	1:30:E:ASN:N	1:30:E:ASN:CA	1:30:E:ASN:C	13	2.03
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	20	2.03
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	12	2.01
(1,408)	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	1:25:E:ARG:N	11	1.99
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	16	1.98
(1,281)	1:29:D:GLN:C	1:30:D:ASN:N	1:30:D:ASN:CA	1:30:D:ASN:C	13	1.96
(1,387)	1:50:E:MET:C	1:51:E:LEU:N	1:51:E:LEU:CA	1:51:E:LEU:C	11	1.95
(1,419)	1:39:E:LEU:N	1:39:E:LEU:CA	1:39:E:LEU:C	1:40:E:ILE:N	3	1.94
(1,262)	1:4:D:VAL:C	1:5:D:GLN:N	1:5:D:GLN:CA	1:5:D:GLN:C	3	1.93
(1,301)	1:50:D:MET:C	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	19	1.9
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	11	1.89
(1,419)	1:39:E:LEU:N	1:39:E:LEU:CA	1:39:E:LEU:C	1:40:E:ILE:N	7	1.85
(1,362)	1:18:E:ILE:C	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	9	1.85
(1,75)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:ILE:N	6	1.85
(1,189)	1:17:C:THR:C	1:18:C:ILE:N	1:18:C:ILE:CA	1:18:C:ILE:C	7	1.82
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	3	1.8
(1,322)	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	1:25:D:ARG:N	11	1.78
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	2	1.73
(1,122)	1:42:B:LEU:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	18	1.73
(1,103)	1:17:B:THR:C	1:18:B:ILE:N	1:18:B:ILE:CA	1:18:B:ILE:C	7	1.73
(1,17)	1:17:A:THR:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	7	1.71
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	19	1.68
(1,61)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:MET:N	6	1.66
(1,107)	1:23:B:GLN:C	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	2	1.65
(1,380)	1:42:E:LEU:C	1:43:E:LEU:N	1:43:E:LEU:CA	1:43:E:LEU:C	12	1.63
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	11	1.63
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	11	1.62
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	4	1.61
(1,294)	1:42:D:LEU:C	1:43:D:LEU:N	1:43:D:LEU:CA	1:43:D:LEU:C	12	1.6
(1,233)	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	1:20:C:MET:N	6	1.6
(1,104)	1:18:B:ILE:C	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	9	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,367)	1:29:E:GLN:C	1:30:E:ASN:N	1:30:E:ASN:CA	1:30:E:ASN:C	12	1.59
(1,62)	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	1:23:A:GLN:N	14	1.58
(1,43)	1:50:A:MET:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	19	1.57
(1,85)	1:50:A:MET:N	1:50:A:MET:CA	1:50:A:MET:C	1:51:A:LEU:N	16	1.56
(1,234)	1:22:C:GLN:N	1:22:C:GLN:CA	1:22:C:GLN:C	1:23:C:GLN:N	14	1.55
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	19	1.55
(1,319)	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	1:20:D:MET:N	6	1.53
(1,294)	1:42:D:LEU:C	1:43:D:LEU:N	1:43:D:LEU:CA	1:43:D:LEU:C	16	1.53
(1,405)	1:19:E:GLU:N	1:19:E:GLU:CA	1:19:E:GLU:C	1:20:E:MET:N	6	1.52
(1,275)	1:17:D:THR:C	1:18:D:ILE:N	1:18:D:ILE:CA	1:18:D:ILE:C	7	1.49
(1,147)	1:19:B:GLU:N	1:19:B:GLU:CA	1:19:B:GLU:C	1:20:B:MET:N	6	1.47
(1,419)	1:39:E:LEU:N	1:39:E:LEU:CA	1:39:E:LEU:C	1:40:E:ILE:N	13	1.46
(1,247)	1:39:C:LEU:N	1:39:C:LEU:CA	1:39:C:LEU:C	1:40:C:ILE:N	2	1.45
(1,129)	1:50:B:MET:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	16	1.44
(1,64)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:ARG:N	11	1.4
(1,215)	1:50:C:MET:C	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	19	1.39
(1,361)	1:17:E:THR:C	1:18:E:ILE:N	1:18:E:ILE:CA	1:18:E:ILE:C	7	1.38
(1,190)	1:18:C:ILE:C	1:19:C:GLU:N	1:19:C:GLU:CA	1:19:C:GLU:C	9	1.38
(1,380)	1:42:E:LEU:C	1:43:E:LEU:N	1:43:E:LEU:CA	1:43:E:LEU:C	20	1.34
(1,30)	1:36:A:CYS:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	19	1.34
(1,294)	1:42:D:LEU:C	1:43:D:LEU:N	1:43:D:LEU:CA	1:43:D:LEU:C	13	1.32
(1,320)	1:22:D:GLN:N	1:22:D:GLN:CA	1:22:D:GLN:C	1:23:D:GLN:N	14	1.31
(1,276)	1:18:D:ILE:C	1:19:D:GLU:N	1:19:D:GLU:CA	1:19:D:GLU:C	9	1.29
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	2	1.29
(1,202)	1:36:C:CYS:C	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	19	1.28
(1,374)	1:36:E:CYS:C	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	18	1.24
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	9	1.24
(1,18)	1:18:A:ILE:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	9	1.21
(1,374)	1:36:E:CYS:C	1:37:E:LEU:N	1:37:E:LEU:CA	1:37:E:LEU:C	13	1.2
(1,279)	1:23:D:GLN:C	1:24:D:ALA:N	1:24:D:ALA:CA	1:24:D:ALA:C	14	1.2
(1,150)	1:24:B:ALA:N	1:24:B:ALA:CA	1:24:B:ALA:C	1:25:B:ARG:N	11	1.2
(1,4)	1:4:A:VAL:C	1:5:A:GLN:N	1:5:A:GLN:CA	1:5:A:GLN:C	3	1.19
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	9	1.18
(1,21)	1:23:A:GLN:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	14	1.17
(1,365)	1:23:E:GLN:C	1:24:E:ALA:N	1:24:E:ALA:CA	1:24:E:ALA:C	2	1.15
(1,122)	1:42:B:LEU:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	16	1.14
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	6	1.13
(1,294)	1:42:D:LEU:C	1:43:D:LEU:N	1:43:D:LEU:CA	1:43:D:LEU:C	9	1.11
(1,247)	1:39:C:LEU:N	1:39:C:LEU:CA	1:39:C:LEU:C	1:40:C:ILE:N	14	1.11
(1,333)	1:39:D:LEU:N	1:39:D:LEU:CA	1:39:D:LEU:C	1:40:D:ILE:N	7	1.1
(1,208)	1:42:C:LEU:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	12	1.07
(1,36)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	12	1.05
(1,416)	1:36:E:CYS:N	1:36:E:CYS:CA	1:36:E:CYS:C	1:37:E:LEU:N	20	1.04
(1,193)	1:23:C:GLN:C	1:24:C:ALA:N	1:24:C:ALA:CA	1:24:C:ALA:C	2	1.03