



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 09:34 PM UTC

PDB ID : 6IJQ / pdb_00006ijq
Title : Solution structure of BCL-XL bound to P73-TAD peptide
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Deposited on : 2018-10-11

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

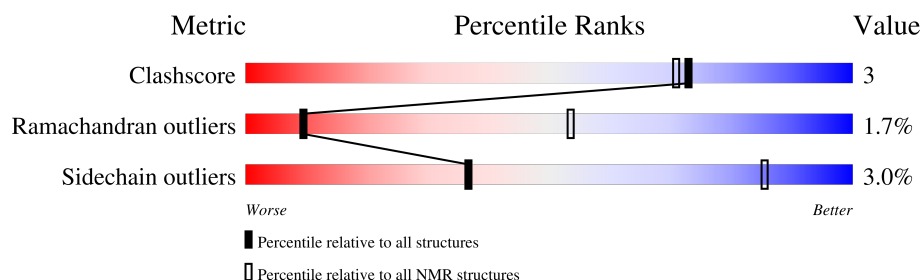
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 61%.

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	16	
2	B	181	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:314-A:325, B:1-B:24, B:42-B:156 (151)	1.29	1

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2910 atoms, of which 1404 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor protein p73.

Mol	Chain	Residues	Atoms					Trace
1	A	16	Total	C	H	N	O	0
			235	79	108	19	29	

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

Mol	Chain	Residues	Atoms						Trace
2	B	171	Total	C	H	N	O	S	0
			2675	866	1296	236	273	4	

There are 12 discrepancies between the modelled and reference sequences:

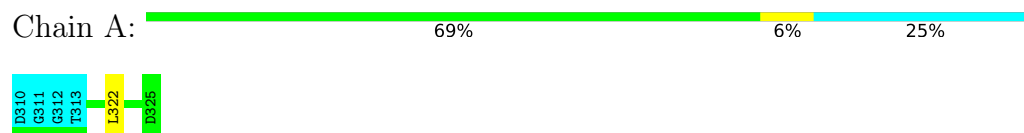
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	expression tag	UNP Q07817
B	-2	SER	-	expression tag	UNP Q07817
B	-1	MET	-	expression tag	UNP Q07817
B	0	ALA	-	expression tag	UNP Q07817
B	170	LEU	-	expression tag	UNP Q07817
B	171	GLU	-	expression tag	UNP Q07817
B	172	HIS	-	expression tag	UNP Q07817
B	173	HIS	-	expression tag	UNP Q07817
B	174	HIS	-	expression tag	UNP Q07817
B	175	HIS	-	expression tag	UNP Q07817
B	176	HIS	-	expression tag	UNP Q07817
B	177	HIS	-	expression tag	UNP Q07817

4 Residue-property plots [i](#)

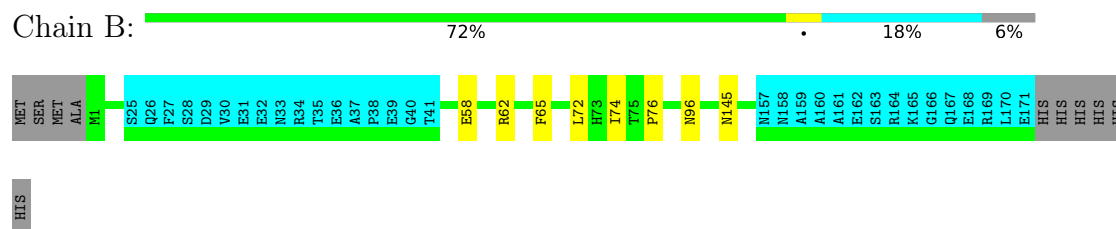
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Tumor protein p73



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

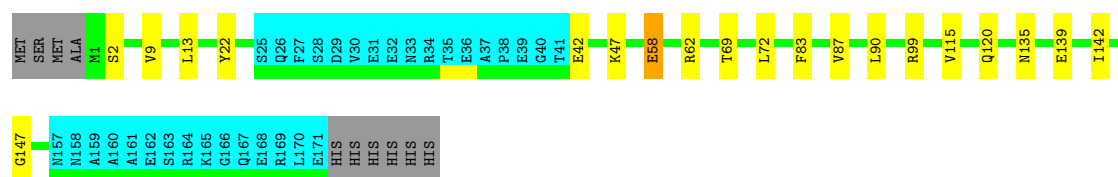
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Tumor protein p73



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1



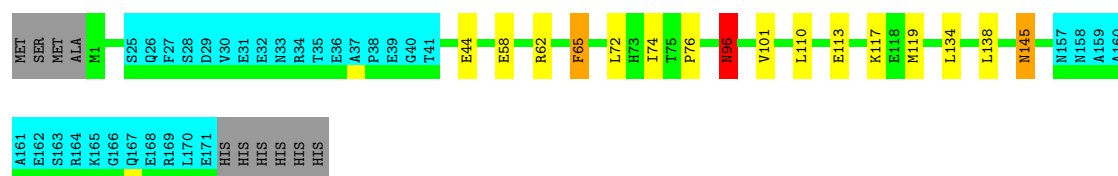


4.2.2 Score per residue for model 2

- Molecule 1: Tumor protein p73

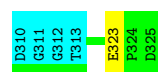


- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

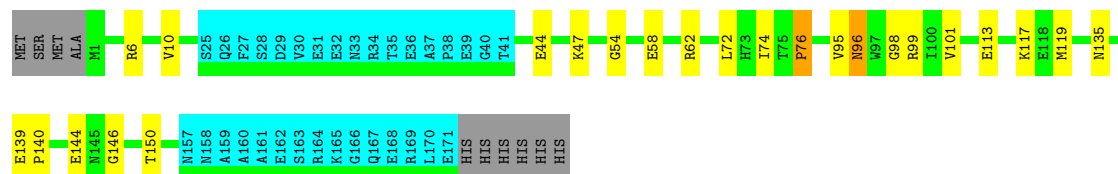


4.2.3 Score per residue for model 3

- Molecule 1: Tumor protein p73



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1



4.2.4 Score per residue for model 4

- Molecule 1: Tumor protein p73

Chain A: 



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

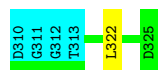
Chain B: 



4.2.5 Score per residue for model 5

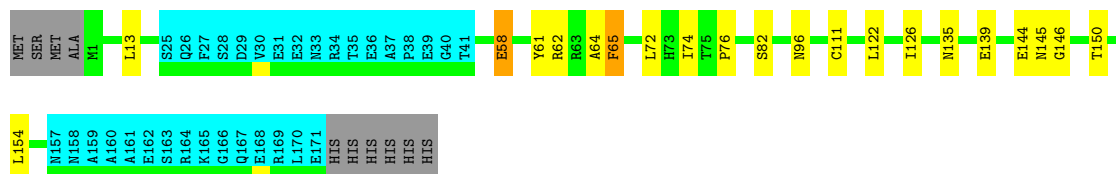
- Molecule 1: Tumor protein p73

Chain A: 



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

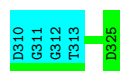
Chain B: 



4.2.6 Score per residue for model 6

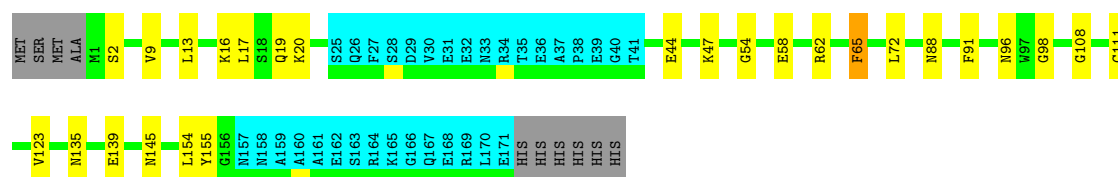
- Molecule 1: Tumor protein p73

Chain A: 



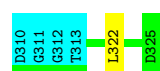
- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

Chain B: 

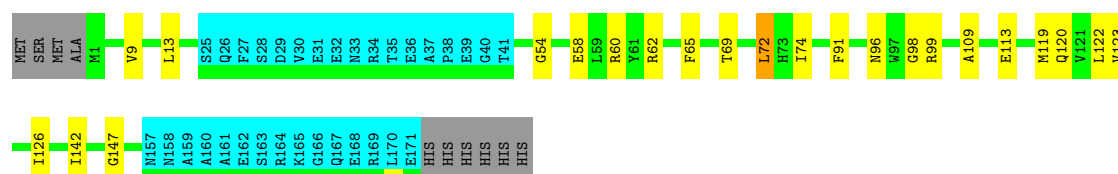


4.2.7 Score per residue for model 7

- Molecule 1: Tumor protein p73



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

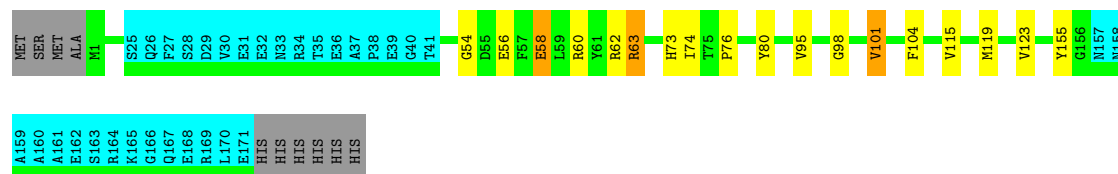


4.2.8 Score per residue for model 8

- Molecule 1: Tumor protein p73



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

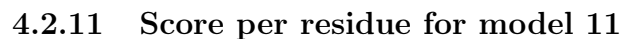


4.2.9 Score per residue for model 9

- Molecule 1: Tumor protein p73

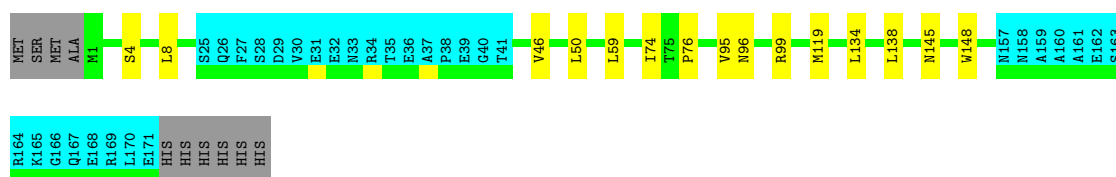


- Molecule 1: Tumor protein p73



- Molecule 1: Tumor protein p73



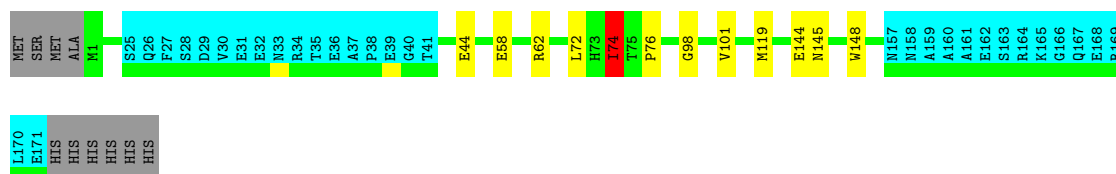


4.2.12 Score per residue for model 12

- Molecule 1: Tumor protein p73

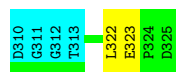


- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

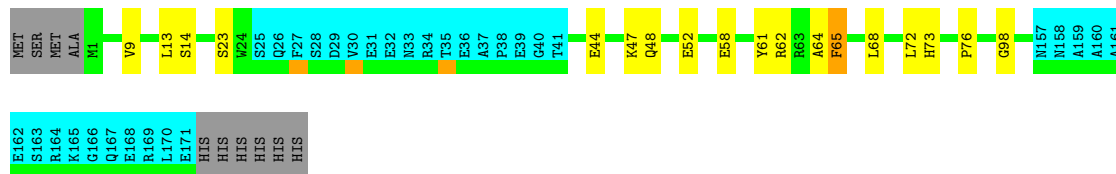


4.2.13 Score per residue for model 13

- Molecule 1: Tumor protein p73



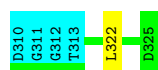
- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1



4.2.14 Score per residue for model 14

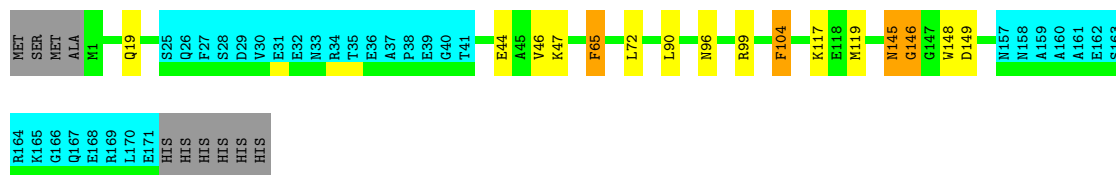
- Molecule 1: Tumor protein p73

Chain A:  69% 6% 25%



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

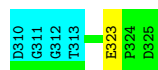
Chain B:  68% 7% 18% 6%



4.2.15 Score per residue for model 15

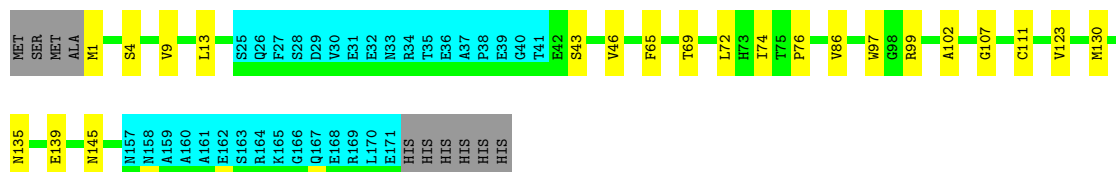
- Molecule 1: Tumor protein p73

Chain A:  69% 6% 25%



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

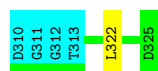
Chain B:  65% 12% 18% 6%



4.2.16 Score per residue for model 16

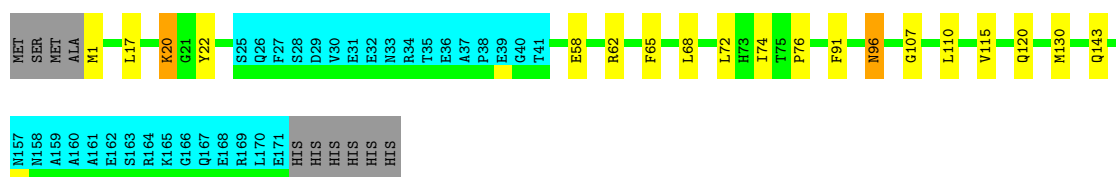
- Molecule 1: Tumor protein p73

Chain A:  69% 6% 25%



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

Chain B:  66% 9% 18% 6%



4.2.17 Score per residue for model 17

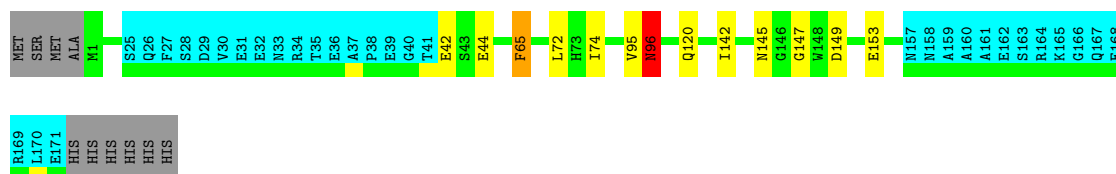
- Molecule 1: Tumor protein p73

Chain A: 69% 6% 25%



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

Chain B: 70% 6% 18% 6%



4.2.18 Score per residue for model 18

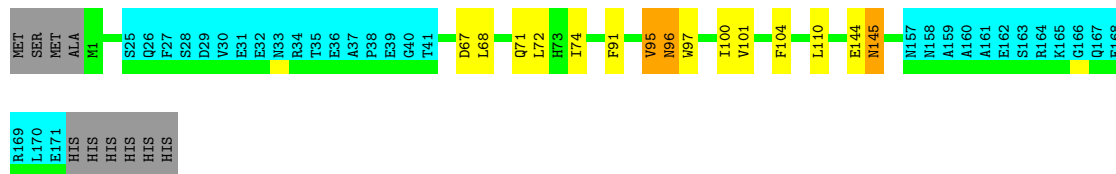
- Molecule 1: Tumor protein p73

Chain A: 75% 25%



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

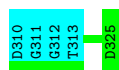
Chain B: 69% 7% 18% 6%



4.2.19 Score per residue for model 19

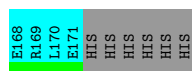
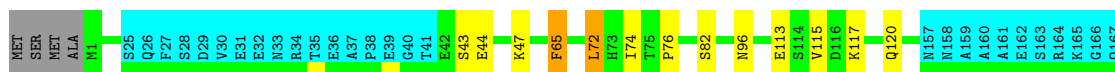
- Molecule 1: Tumor protein p73

Chain A:  75% 25%



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

Chain B:  70% 6% 18% 6%



4.2.20 Score per residue for model 20

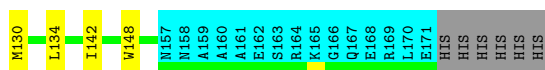
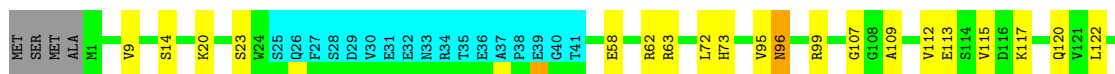
- Molecule 1: Tumor protein p73

Chain A:  69% 6% 25%



- Molecule 2: Bcl-2-like protein 1, Bcl-2-like protein 1

Chain B:  64% 13% 18% 6%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
CNS	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	1531
Number of shifts mapped to atoms	1531
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	61%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.13±0.07	0±0/108 (0.3± 0.4%)	1.04±0.06	0±0/146 (0.0± 0.0%)
2	B	1.19±0.02	0±0/1160 (0.0± 0.0%)	1.09±0.02	1±1/1572 (0.0± 0.0%)
All	All	1.19	12/25360 (0.0%)	1.09	11/34360 (0.0%)

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

Mol	Chain	Chirality	Planarity
2	B	0.0±0.0	0.1±0.3
All	All	0	2

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	323	GLU	C-N	6.63	1.39	1.33	12	7
2	B	58	GLU	C-O	-6.45	1.16	1.24	8	3
2	B	74	ILE	CA-CB	6.00	1.62	1.54	12	1
2	B	139	GLU	C-N	5.11	1.40	1.33	4	1

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
2	B	65	PHE	CA-CB-CG	8.17	121.97	113.80	14	10
2	B	104	PHE	CA-CB-CG	5.76	119.56	113.80	14	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	95	VAL	Peptide	2

6.2 Too-close contacts

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	104	89	88	0±0
2	B	1131	1073	1073	8±3
All	All	24700	23240	23220	157

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:95:VAL:HA	2:B:99:ARG:HB3	0.70	1.63	3	1
2:B:95:VAL:HA	2:B:99:ARG:HB2	0.65	1.68	20	2
2:B:96:ASN:HB3	2:B:99:ARG:HB2	0.64	1.68	14	2
2:B:135:ASN:HA	2:B:139:GLU:HG3	0.60	1.73	3	1
2:B:72:LEU:HD21	2:B:86:VAL:HG21	0.58	1.75	15	2
2:B:76:PRO:HA	2:B:119:MET:SD	0.57	2.39	8	2
2:B:61:TYR:HA	2:B:64:ALA:HB3	0.57	1.76	13	2
1:A:322:LEU:HD11	2:B:98:GLY:HA3	0.56	1.76	7	1
2:B:142:ILE:HG23	2:B:148:TRP:HB3	0.55	1.78	20	1
2:B:111:CYS:SG	2:B:123:VAL:HG23	0.55	2.42	15	1
2:B:58:GLU:HB3	2:B:62:ARG:HB2	0.54	1.80	12	1
2:B:58:GLU:HG2	2:B:62:ARG:HB2	0.53	1.78	20	5
2:B:142:ILE:HB	2:B:147:GLY:HA3	0.52	1.82	1	2
2:B:17:LEU:O	2:B:20:LYS:HG2	0.52	2.03	4	3
2:B:142:ILE:HA	2:B:147:GLY:HA3	0.52	1.82	7	1
2:B:76:PRO:HB3	2:B:119:MET:SD	0.52	2.45	2	1
2:B:91:PHE:HA	2:B:96:ASN:HD21	0.51	1.65	6	5
2:B:135:ASN:HA	2:B:139:GLU:HB2	0.51	1.83	6	4
2:B:96:ASN:HD22	2:B:96:ASN:N	0.51	2.04	20	4
2:B:107:GLY:HA3	2:B:130:MET:HE1	0.51	1.83	15	3
2:B:13:LEU:HD13	2:B:111:CYS:SG	0.50	2.46	6	2
2:B:58:GLU:HG2	2:B:62:ARG:HB3	0.50	1.83	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:69:THR:HA	2:B:72:LEU:HG	0.50	1.83	7	1
2:B:90:LEU:HA	2:B:99:ARG:HH21	0.50	1.67	1	1
2:B:74:ILE:HG23	2:B:119:MET:SD	0.50	2.46	12	1
2:B:44:GLU:HA	2:B:47:LYS:HD2	0.49	1.83	19	2
2:B:115:VAL:HG22	2:B:120:GLN:HG3	0.49	1.83	20	1
2:B:113:GLU:O	2:B:117:LYS:HG2	0.49	2.08	3	4
2:B:22:TYR:CE2	2:B:115:VAL:HG11	0.48	2.43	1	1
1:A:318:LEU:HD22	2:B:155:TYR:OH	0.48	2.09	4	1
2:B:72:LEU:HD12	2:B:110:LEU:HD21	0.48	1.85	2	3
2:B:20:LYS:HE3	2:B:112:VAL:HG11	0.48	1.84	10	1
2:B:58:GLU:O	2:B:62:ARG:N	0.47	2.47	8	6
2:B:107:GLY:O	2:B:111:CYS:SG	0.47	2.68	15	1
2:B:134:LEU:HA	2:B:138:LEU:HB2	0.47	1.85	2	1
2:B:54:GLY:O	2:B:58:GLU:HB3	0.47	2.09	6	1
2:B:14:SER:HB3	2:B:23:SER:HB2	0.47	1.85	13	1
2:B:68:LEU:O	2:B:72:LEU:HG	0.47	2.10	13	2
1:A:315:PHE:HB3	2:B:56:GLU:HG2	0.47	1.87	8	1
2:B:44:GLU:O	2:B:47:LYS:HG2	0.47	2.10	14	1
2:B:20:LYS:HE2	2:B:112:VAL:HG13	0.46	1.87	20	1
2:B:96:ASN:HB3	2:B:100:ILE:N	0.46	2.25	18	3
2:B:72:LEU:HG	2:B:82:SER:HB3	0.46	1.88	5	2
2:B:117:LYS:HB3	2:B:119:MET:SD	0.46	2.51	14	1
2:B:119:MET:HB3	2:B:122:LEU:HD13	0.46	1.87	7	1
2:B:111:CYS:SG	2:B:123:VAL:HG13	0.46	2.50	10	1
2:B:65:PHE:O	2:B:69:THR:HG22	0.45	2.11	15	2
2:B:1:MET:HB2	2:B:143:GLN:HG2	0.45	1.87	16	1
2:B:74:ILE:O	2:B:117:LYS:HG2	0.45	2.12	10	1
2:B:44:GLU:HA	2:B:47:LYS:HE2	0.44	1.88	13	2
2:B:137:HIS:HB2	2:B:138:LEU:HD12	0.44	1.89	10	1
2:B:62:ARG:HA	2:B:65:PHE:CD1	0.44	2.48	13	1
2:B:115:VAL:HG13	2:B:120:GLN:HE22	0.44	1.72	16	1
2:B:4:SER:O	2:B:8:LEU:HG	0.44	2.13	11	1
2:B:142:ILE:HD12	2:B:143:GLN:N	0.44	2.27	9	1
2:B:83:PHE:O	2:B:87:VAL:HG23	0.44	2.12	10	2
2:B:43:SER:O	2:B:47:LYS:HG3	0.44	2.13	9	2
2:B:98:GLY:O	2:B:101:VAL:HG12	0.44	2.13	8	3
2:B:76:PRO:HD3	2:B:119:MET:SD	0.44	2.52	11	1
2:B:146:GLY:HA2	2:B:149:ASP:HB3	0.43	1.89	14	1
2:B:6:ARG:O	2:B:10:VAL:HG23	0.43	2.13	3	1
2:B:115:VAL:HG23	2:B:123:VAL:HG11	0.43	1.89	8	1
2:B:54:GLY:HA2	2:B:57:PHE:CE2	0.43	2.49	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:46:VAL:HG21	2:B:148:TRP:HB2	0.43	1.91	14	1
2:B:115:VAL:HG22	2:B:120:GLN:HB3	0.43	1.90	19	1
1:A:322:LEU:HD21	2:B:98:GLY:HA3	0.43	1.89	9	2
2:B:90:LEU:HD11	2:B:99:ARG:HB3	0.43	1.89	14	1
2:B:115:VAL:HG23	2:B:123:VAL:HG21	0.43	1.89	4	1
2:B:149:ASP:O	2:B:153:GLU:HG3	0.43	2.13	17	1
2:B:62:ARG:NH2	2:B:109:ALA:HA	0.43	2.29	20	1
2:B:1:MET:HA	2:B:4:SER:HB2	0.43	1.91	15	1
2:B:96:ASN:N	2:B:96:ASN:ND2	0.43	2.67	17	1
2:B:9:VAL:O	2:B:13:LEU:HG	0.43	2.14	15	5
2:B:132:THR:HA	2:B:135:ASN:ND2	0.42	2.29	4	1
2:B:74:ILE:HG23	2:B:78:THR:HB	0.42	1.91	4	1
2:B:43:SER:O	2:B:46:VAL:HG12	0.42	2.14	15	1
2:B:146:GLY:HA2	2:B:150:THR:HG23	0.42	1.92	3	1
2:B:69:THR:HA	2:B:72:LEU:HB2	0.42	1.92	1	1
2:B:122:LEU:O	2:B:126:ILE:HG13	0.42	2.14	10	3
2:B:14:SER:OG	2:B:23:SER:HB2	0.42	2.15	20	1
2:B:54:GLY:O	2:B:58:GLU:HB2	0.42	2.14	8	3
2:B:13:LEU:HD22	2:B:111:CYS:SG	0.42	2.55	5	1
2:B:46:VAL:HB	2:B:148:TRP:HB3	0.42	1.91	11	1
2:B:60:ARG:O	2:B:63:ARG:HG3	0.41	2.15	8	1
2:B:101:VAL:HA	2:B:104:PHE:CE2	0.41	2.49	18	1
2:B:134:LEU:HD12	2:B:138:LEU:HD12	0.41	1.91	11	1
2:B:108:GLY:HA2	2:B:111:CYS:SG	0.41	2.56	4	1
2:B:150:THR:O	2:B:154:LEU:HG	0.41	2.16	5	1
2:B:16:LYS:HG3	2:B:108:GLY:HA3	0.41	1.92	6	1
2:B:59:LEU:O	2:B:62:ARG:HG2	0.41	2.16	10	1
1:A:318:LEU:O	1:A:322:LEU:HB2	0.41	2.15	10	2
2:B:119:MET:HA	2:B:119:MET:HE3	0.41	1.92	10	1
2:B:109:ALA:O	2:B:113:GLU:HG2	0.41	2.16	7	1
2:B:48:GLN:O	2:B:52:GLU:HG2	0.41	2.16	13	1
2:B:99:ARG:HA	2:B:102:ALA:HB3	0.41	1.91	15	1
2:B:115:VAL:HG22	2:B:120:GLN:HG2	0.41	1.93	1	1
2:B:22:TYR:CE2	2:B:115:VAL:HG21	0.41	2.51	16	1
2:B:46:VAL:O	2:B:50:LEU:HG	0.40	2.17	11	1
2:B:67:ASP:O	2:B:71:GLN:HG2	0.40	2.16	18	1
2:B:9:VAL:HG13	2:B:130:MET:SD	0.40	2.56	20	1
2:B:140:PRO:O	2:B:144:GLU:HG2	0.40	2.16	3	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	11/16 (69%)	10±1 (92±6%)	1±1 (7±6%)	0±0 (1±3%)	11	58
2	B	138/181 (76%)	125±2 (91±2%)	10±3 (7±2%)	2±1 (2±1%)	9	52
All	All	2980/3940 (76%)	2710 (91%)	218 (7%)	52 (2%)	9	53

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

Mol	Chain	Res	Type	Models (Total)
2	B	74	ILE	12
2	B	145	ASN	9
2	B	76	PRO	9
2	B	73	HIS	4
1	A	314	THR	3
2	B	42	GLU	3
2	B	2	SER	2
2	B	96	ASN	2
2	B	146	GLY	2
2	B	97	TRP	2
2	B	98	GLY	1
2	B	59	LEU	1
2	B	148	TRP	1
2	B	95	VAL	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	12/14 (86%)	12±1 (96±5%)	0±1 (4±5%)	28	78
2	B	119/154 (77%)	116±2 (97±2%)	3±2 (3±2%)	38	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2620/3360 (78%)	2542 (97%)	78 (3%)	37 85

All 28 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)
2	B	96	ASN	11
2	B	65	PHE	8
2	B	72	LEU	8
1	A	322	LEU	7
2	B	145	ASN	6
2	B	144	GLU	3
2	B	19	GLN	3
2	B	155	TYR	3
2	B	104	PHE	3
1	A	314	THR	2
2	B	101	VAL	2
2	B	123	VAL	2
2	B	120	GLN	2
2	B	63	ARG	2
2	B	95	VAL	2
2	B	20	LYS	2
2	B	97	TRP	1
2	B	88	ASN	1
2	B	60	ARG	1
2	B	80	TYR	1
2	B	15	TYR	1
2	B	83	PHE	1
1	A	323	GLU	1
2	B	44	GLU	1
2	B	74	ILE	1
2	B	68	LEU	1
2	B	122	LEU	1
2	B	134	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 61% for the well-defined parts and 61% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `final.str`

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	1531
Number of shifts mapped to atoms	1531
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	158	-0.13 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	145	0.58 ± 0.06	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	164	0.33 ± 0.16	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 61%, i.e. 1260 atoms were assigned a chemical shift out of a possible 2077. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	563/759 (74%)	303/309 (98%)	127/302 (42%)	133/148 (90%)
Sidechain	670/1068 (63%)	475/692 (69%)	195/335 (58%)	0/41 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	27/250 (11%)	27/122 (22%)	0/116 (0%)	0/12 (0%)
Overall	1260/2077 (61%)	805/1123 (72%)	322/753 (43%)	133/201 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 61%, i.e. 1522 atoms were assigned a chemical shift out of a possible 2512. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	698/941 (74%)	376/384 (98%)	158/374 (42%)	164/183 (90%)
Sidechain	797/1311 (61%)	561/843 (67%)	236/412 (57%)	0/56 (0%)
Aromatic	27/260 (10%)	27/127 (21%)	0/121 (0%)	0/12 (0%)
Overall	1522/2512 (61%)	964/1354 (71%)	394/907 (43%)	164/251 (65%)

7.1.4 Statistically unusual chemical shifts ⓘ

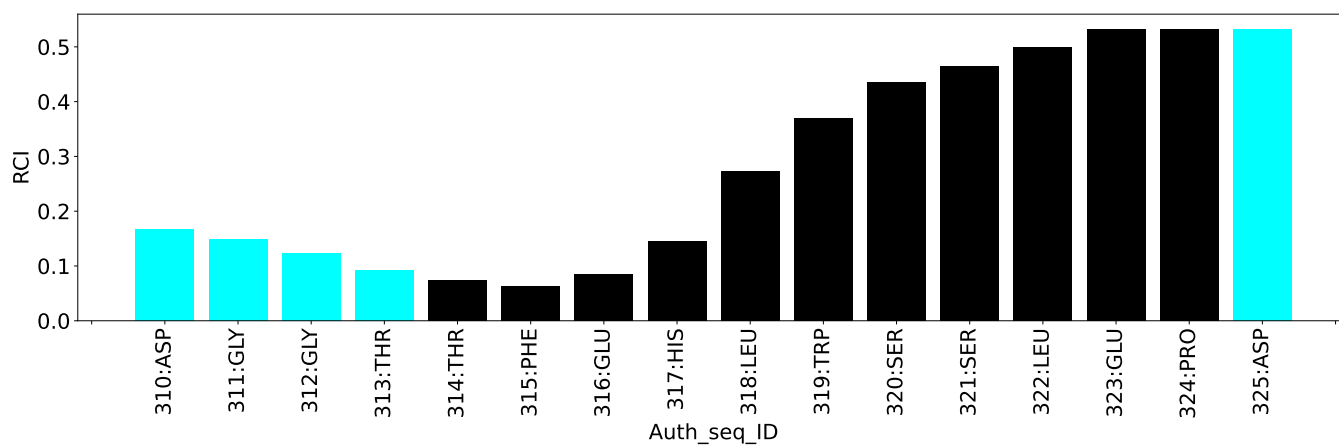
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	35	THR	HG1	4.75	0.08 – 2.19	17.1
1	B	41	THR	HG1	4.75	0.08 – 2.19	17.1
1	B	132	THR	HG1	4.75	0.08 – 2.19	17.1
1	B	150	THR	HG1	4.74	0.08 – 2.19	17.1
1	B	69	THR	HG1	4.73	0.08 – 2.19	17.0
1	B	95	VAL	HB	0.22	0.43 – 3.54	-5.7
1	B	145	ASN	HB3	0.94	1.12 – 4.38	-5.5
1	B	95	VAL	HG21	-0.70	-0.58 – 2.19	-5.4
1	B	95	VAL	HG22	-0.70	-0.58 – 2.19	-5.4
1	B	95	VAL	HG23	-0.70	-0.58 – 2.19	-5.4

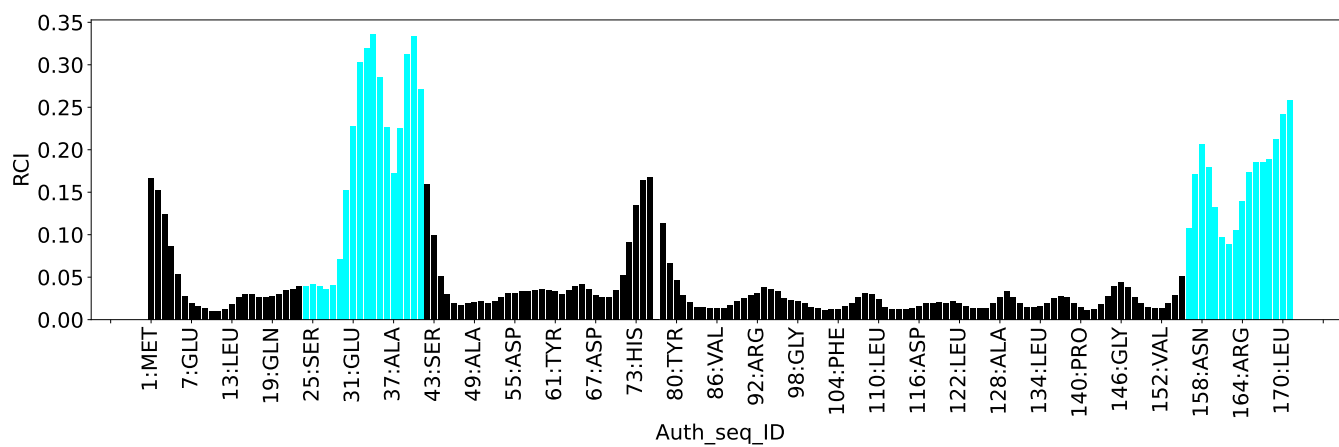
7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2159
Intra-residue ($ i-j =0$)	623
Sequential ($ i-j =1$)	783
Medium range ($ i-j >1$ and $ i-j <5$)	510
Long range ($ i-j \geq 5$)	218
Inter-chain	25
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	273
Number of unmapped restraints	0
Number of restraints per residue	12.3
Number of long range restraints per residue ¹	1.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	77.7	0.2
0.2-0.5 (Medium)	47.3	0.5
>0.5 (Large)	7.6	6.8

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)	18.2	8.84
10.0-20.0 (Medium)	0.1	10.87
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

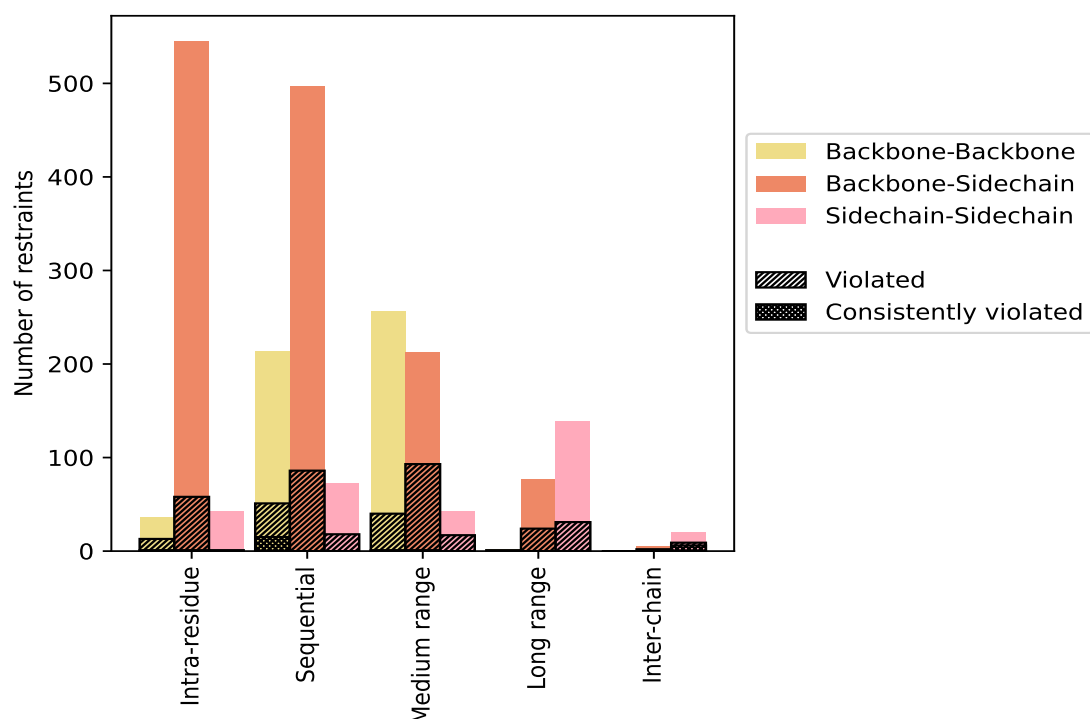
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	623	28.9	72	11.6	3.3	2	0.3	0.1
Backbone-Backbone	36	1.7	13	36.1	0.6	1	2.8	0.0
Backbone-Sidechain	545	25.2	58	10.6	2.7	1	0.2	0.0
Sidechain-Sidechain	42	1.9	1	2.4	0.0	0	0.0	0.0
Sequential ($i-j =1$)	783	36.3	155	19.8	7.2	15	1.9	0.7
Backbone-Backbone	214	9.9	51	23.8	2.4	15	7.0	0.7
Backbone-Sidechain	497	23.0	86	17.3	4.0	0	0.0	0.0
Sidechain-Sidechain	72	3.3	18	25.0	0.8	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	510	23.6	150	29.4	6.9	2	0.4	0.1
Backbone-Backbone	256	11.9	40	15.6	1.9	1	0.4	0.0
Backbone-Sidechain	212	9.8	93	43.9	4.3	1	0.5	0.0
Sidechain-Sidechain	42	1.9	17	40.5	0.8	0	0.0	0.0
Long range ($i-j \geq 5$)	218	10.1	56	25.7	2.6	0	0.0	0.0
Backbone-Backbone	2	0.1	1	50.0	0.0	0	0.0	0.0
Backbone-Sidechain	77	3.6	24	31.2	1.1	0	0.0	0.0
Sidechain-Sidechain	139	6.4	31	22.3	1.4	0	0.0	0.0
Inter-chain	25	1.2	11	44.0	0.5	6	24.0	0.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	5	0.2	2	40.0	0.1	0	0.0	0.0
Sidechain-Sidechain	20	0.9	9	45.0	0.4	6	30.0	0.3
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	2159	100.0	444	20.6	20.6	25	1.2	1.2
Backbone-Backbone	508	23.5	105	20.7	4.9	17	3.3	0.8
Backbone-Sidechain	1336	61.9	263	19.7	12.2	2	0.1	0.1
Sidechain-Sidechain	315	14.6	76	24.1	3.5	6	1.9	0.3

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	21	52	43	13	6	135	0.29	3.98	0.53	0.18
2	29	56	39	20	7	151	0.29	4.77	0.56	0.18
3	24	43	42	16	7	132	0.32	4.8	0.63	0.18
4	25	58	31	11	6	131	0.28	3.13	0.42	0.21
5	24	51	52	10	8	145	0.31	4.54	0.6	0.17
6	24	50	43	13	7	137	0.36	5.78	0.81	0.19
7	22	49	33	12	7	123	0.32	4.74	0.59	0.18
8	21	59	34	12	6	132	0.28	3.66	0.42	0.2
9	26	60	38	10	7	141	0.31	3.16	0.5	0.19
10	25	57	41	9	7	139	0.31	5.15	0.62	0.18

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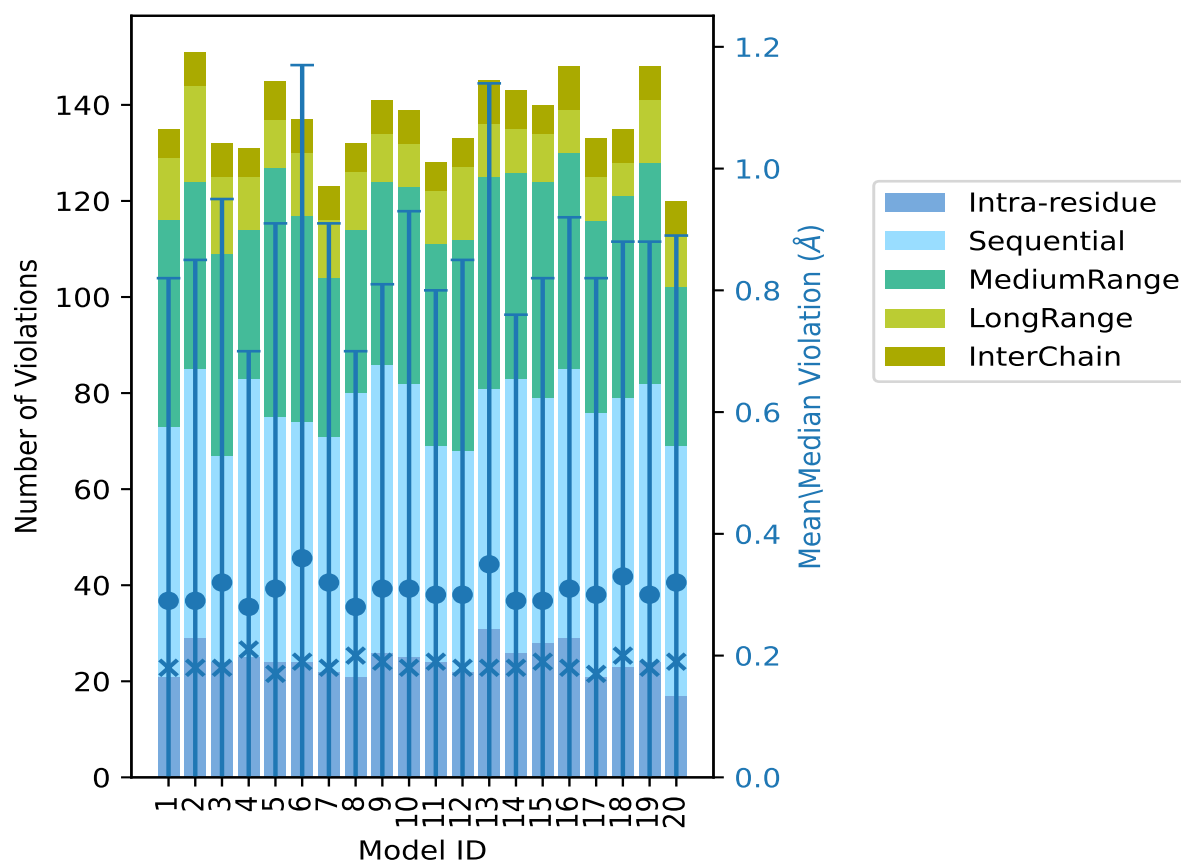
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	24	45	42	11	6	128	0.3	3.45	0.5	0.19
12	22	46	44	15	6	133	0.3	4.12	0.55	0.18
13	31	50	44	11	9	145	0.35	6.8	0.79	0.18
14	26	57	43	9	8	143	0.29	3.33	0.47	0.18
15	28	51	45	10	6	140	0.29	4.17	0.53	0.19
16	29	56	45	9	9	148	0.31	4.42	0.61	0.18
17	21	55	40	9	8	133	0.3	3.38	0.52	0.17
18	23	56	42	7	7	135	0.33	3.82	0.55	0.2
19	24	58	46	13	7	148	0.3	4.47	0.58	0.18
20	17	52	33	11	7	120	0.32	3.96	0.57	0.19

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

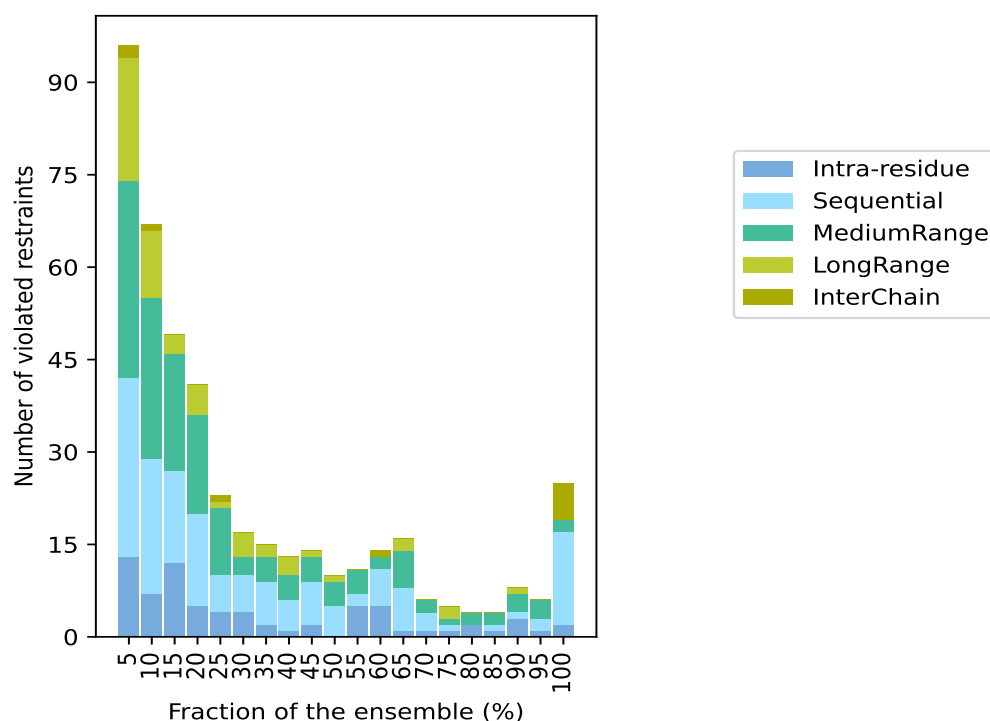
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1715(IR:551, SQ:628, MR:360, LR:162, IC:14) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
13	29	32	20	2	96	1	5.0
7	22	26	11	1	67	2	10.0
12	15	19	3	0	49	3	15.0
5	15	16	5	0	41	4	20.0
4	6	11	1	1	23	5	25.0
4	6	3	4	0	17	6	30.0
2	7	4	2	0	15	7	35.0
1	5	4	3	0	13	8	40.0
2	7	4	1	0	14	9	45.0
0	5	4	1	0	10	10	50.0
5	2	4	0	0	11	11	55.0
5	6	2	0	1	14	12	60.0
1	7	6	2	0	16	13	65.0
1	3	2	0	0	6	14	70.0
1	1	1	2	0	5	15	75.0
2	0	2	0	0	4	16	80.0
1	1	2	0	0	4	17	85.0
3	1	3	1	0	8	18	90.0
1	2	3	0	0	6	19	95.0
2	15	2	0	6	25	20	100.0

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

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

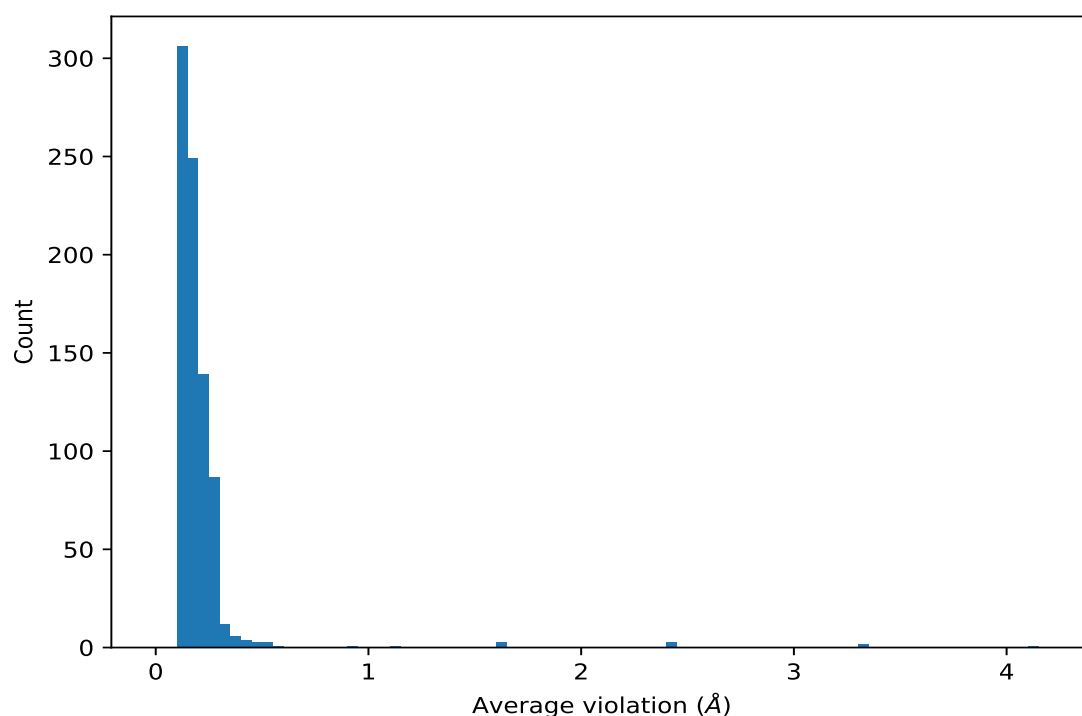
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	20	4.12	1.03	4.05
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	20	3.33	0.5	3.3
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	20	3.31	0.47	3.22
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	20	2.41	0.81	2.27
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	20	2.41	0.81	2.27
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	20	2.41	0.81	2.27
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	20	1.65	0.88	1.5
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	20	1.65	0.88	1.5
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	20	1.65	0.88	1.5
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	20	1.13	0.29	1.15
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	20	0.29	0.06	0.29
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	20	0.29	0.07	0.3
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	20	0.29	0.07	0.3
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	20	0.29	0.07	0.3
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	20	0.26	0.02	0.26
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	20	0.23	0.02	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	20	0.22	0.02	0.22
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	20	0.21	0.04	0.2
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	20	0.21	0.05	0.22
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	20	0.21	0.01	0.2
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	20	0.2	0.03	0.21
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	20	0.2	0.02	0.2
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	20	0.2	0.03	0.2
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	20	0.2	0.02	0.2
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	20	0.2	0.02	0.2
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	20	0.2	0.03	0.2
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	20	0.19	0.03	0.2
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	20	0.18	0.01	0.18
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	20	0.18	0.02	0.18
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	20	0.15	0.02	0.16
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	20	0.14	0.03	0.14
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	19	0.29	0.06	0.29
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	19	0.21	0.04	0.21
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	19	0.21	0.04	0.21
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	19	0.21	0.04	0.21
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	19	0.2	0.02	0.21
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	19	0.19	0.02	0.19
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	19	0.18	0.07	0.16
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	19	0.13	0.02	0.13
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	18	0.3	0.22	0.26
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	18	0.3	0.22	0.26
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	18	0.3	0.22	0.26
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	18	0.3	0.22	0.26
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	18	0.3	0.22	0.26
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	18	0.3	0.22	0.26
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	18	0.24	0.07	0.25
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	18	0.24	0.07	0.25
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	18	0.24	0.07	0.25
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	18	0.24	0.03	0.24
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	18	0.24	0.03	0.24
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	18	0.23	0.05	0.23
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	18	0.2	0.06	0.2
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	18	0.2	0.06	0.2
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	18	0.16	0.03	0.16
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	18	0.14	0.02	0.14
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	18	0.13	0.03	0.13
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	17	0.21	0.05	0.21
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	17	0.21	0.05	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	17	0.19	0.06	0.19
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	17	0.14	0.03	0.15
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	17	0.14	0.02	0.14
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	16	0.4	0.11	0.41
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	16	0.37	0.19	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	16	0.27	0.06	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	16	0.27	0.06	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	16	0.27	0.06	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	16	0.27	0.06	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	16	0.27	0.06	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	16	0.27	0.06	0.29
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	16	0.26	0.01	0.26
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	15	0.25	0.02	0.25
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	15	0.21	0.05	0.22
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	15	0.21	0.05	0.22
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	15	0.21	0.05	0.22
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	15	0.17	0.05	0.17
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	15	0.17	0.05	0.17
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	15	0.17	0.05	0.17
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	15	0.17	0.04	0.15
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	15	0.15	0.04	0.14
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	15	0.15	0.04	0.14
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	15	0.15	0.04	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	15	0.15	0.04	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	15	0.15	0.04	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	15	0.15	0.04	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	15	0.15	0.04	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	15	0.15	0.04	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	15	0.15	0.04	0.14
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	14	0.38	0.1	0.41
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	14	0.25	0.07	0.26
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	14	0.25	0.07	0.26
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	14	0.25	0.07	0.26
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	14	0.19	0.04	0.2
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	14	0.19	0.04	0.2
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	14	0.19	0.04	0.2
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	14	0.19	0.04	0.2
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	14	0.19	0.04	0.2
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	14	0.19	0.04	0.2
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	14	0.17	0.05	0.16
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	14	0.14	0.04	0.14
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	14	0.14	0.04	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	13	0.31	0.07	0.32
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	13	0.31	0.07	0.32
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	13	0.31	0.07	0.32
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	13	0.28	0.08	0.3
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	13	0.28	0.08	0.3
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	13	0.24	0.1	0.23
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	13	0.24	0.1	0.23
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	13	0.24	0.1	0.23
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	13	0.24	0.1	0.23
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	13	0.24	0.1	0.23
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	13	0.24	0.1	0.23
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	13	0.24	0.07	0.27
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	13	0.24	0.07	0.27
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	13	0.24	0.07	0.27
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	13	0.22	0.05	0.22
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	13	0.22	0.08	0.2
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	13	0.22	0.08	0.2
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	13	0.21	0.13	0.18
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	13	0.21	0.13	0.18
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	13	0.21	0.13	0.18
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	13	0.2	0.05	0.22
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	13	0.2	0.05	0.22
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	13	0.2	0.05	0.22
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	13	0.2	0.04	0.2
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	13	0.2	0.04	0.2
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	13	0.19	0.06	0.17
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	13	0.19	0.06	0.17
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	13	0.19	0.06	0.17
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	13	0.19	0.06	0.17
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	13	0.18	0.05	0.17
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	13	0.18	0.05	0.17
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	13	0.17	0.05	0.15
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	13	0.17	0.05	0.15
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	13	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	13	0.16	0.04	0.15
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	13	0.15	0.03	0.15
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	13	0.15	0.03	0.15
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	13	0.12	0.01	0.12
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	13	0.12	0.01	0.12
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	12	0.92	0.52	0.91
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	12	0.47	0.06	0.46
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	12	0.47	0.06	0.46
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	12	0.47	0.06	0.46
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	12	0.38	0.14	0.42
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	12	0.28	0.1	0.32
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	12	0.26	0.03	0.25
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	12	0.25	0.08	0.22
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	12	0.22	0.06	0.22
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	12	0.18	0.06	0.17
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	12	0.18	0.06	0.17
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	12	0.18	0.06	0.17
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	12	0.18	0.06	0.17
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	12	0.18	0.06	0.17
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	12	0.18	0.06	0.17
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	12	0.18	0.06	0.16
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	12	0.16	0.03	0.16
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	12	0.16	0.03	0.16
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	12	0.16	0.04	0.16
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	12	0.16	0.04	0.16
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	12	0.14	0.02	0.14
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	12	0.14	0.02	0.13
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	12	0.14	0.02	0.13
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	11	0.23	0.05	0.24
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	11	0.18	0.07	0.15
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	11	0.18	0.07	0.15
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	11	0.17	0.04	0.18
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	11	0.17	0.03	0.17
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	11	0.17	0.04	0.16
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	11	0.17	0.05	0.16
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	11	0.16	0.05	0.14
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	11	0.16	0.05	0.14
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	11	0.16	0.05	0.14
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	11	0.16	0.05	0.14
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	11	0.16	0.05	0.14
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	11	0.16	0.05	0.14
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	11	0.16	0.05	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	11	0.16	0.05	0.14
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	11	0.16	0.04	0.15
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	11	0.15	0.03	0.16
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	11	0.13	0.01	0.14
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	10	0.35	0.27	0.28
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	10	0.24	0.09	0.22
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	10	0.24	0.09	0.22
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	10	0.22	0.09	0.2
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	10	0.22	0.09	0.2
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	10	0.22	0.09	0.2
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	10	0.22	0.09	0.2
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	10	0.22	0.09	0.2
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	10	0.22	0.09	0.2
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	10	0.22	0.09	0.2
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	10	0.22	0.09	0.2
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	10	0.22	0.09	0.2
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	10	0.18	0.05	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	10	0.18	0.05	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	10	0.18	0.05	0.18
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	10	0.17	0.07	0.14
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	10	0.17	0.07	0.14
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	10	0.16	0.04	0.15
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	10	0.16	0.05	0.15
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	10	0.16	0.05	0.15
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	10	0.16	0.04	0.14
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	10	0.16	0.04	0.14
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	10	0.13	0.03	0.12
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	10	0.13	0.03	0.13
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	10	0.13	0.03	0.13
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	9	0.26	0.08	0.27
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	9	0.26	0.08	0.27
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	9	0.26	0.08	0.27
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	9	0.26	0.08	0.27
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	9	0.26	0.08	0.27
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	9	0.26	0.08	0.27
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	9	0.26	0.07	0.28
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	9	0.26	0.07	0.28
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	9	0.21	0.03	0.21
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	9	0.19	0.04	0.19
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	9	0.19	0.04	0.19
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	9	0.19	0.07	0.15
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	9	0.19	0.07	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	9	0.19	0.07	0.15
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	9	0.19	0.07	0.15
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	9	0.19	0.07	0.15
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	9	0.19	0.07	0.15
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	9	0.19	0.07	0.16
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	9	0.17	0.03	0.16
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	9	0.15	0.04	0.13
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	9	0.15	0.03	0.14
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	9	0.15	0.02	0.14
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	9	0.14	0.02	0.14
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	9	0.13	0.03	0.12
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	9	0.13	0.03	0.12
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	9	0.12	0.03	0.11
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	9	0.12	0.01	0.12
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	8	0.51	0.27	0.5
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	8	0.28	0.11	0.27
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	8	0.28	0.11	0.27
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	8	0.28	0.11	0.27
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	8	0.25	0.02	0.24
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	8	0.22	0.06	0.21
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	8	0.22	0.06	0.21
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	8	0.21	0.09	0.18
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	8	0.21	0.09	0.18
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	8	0.21	0.09	0.18
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	8	0.18	0.05	0.2
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	8	0.18	0.05	0.2
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	8	0.18	0.05	0.2
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	8	0.18	0.05	0.2
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	8	0.18	0.05	0.18
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	8	0.18	0.05	0.18
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	8	0.18	0.05	0.18
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	8	0.18	0.03	0.16
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	8	0.17	0.04	0.18
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	8	0.17	0.07	0.14
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	8	0.17	0.07	0.14
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	8	0.17	0.07	0.14
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	8	0.16	0.02	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	8	0.15	0.02	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	8	0.15	0.02	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	8	0.15	0.02	0.15
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	8	0.13	0.03	0.12
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD11	7	0.33	0.09	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD12	7	0.33	0.09	0.37
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD13	7	0.33	0.09	0.37
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD11	7	0.29	0.06	0.31
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD12	7	0.29	0.06	0.31
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD13	7	0.29	0.06	0.31
(1,1847)	2:164:B:ARG:H	2:164:B:ARG:HB3	7	0.27	0.04	0.27
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE1	7	0.24	0.08	0.2
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE2	7	0.24	0.08	0.2
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE1	7	0.24	0.08	0.2
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE2	7	0.24	0.08	0.2
(1,1113)	2:96:B:ASN:H	2:99:B:ARG:H	7	0.23	0.09	0.2
(1,1809)	2:158:B:ASN:H	2:161:B:ALA:H	7	0.23	0.08	0.22
(1,867)	2:74:B:ILE:HG21	2:117:B:LYS:HB3	7	0.21	0.08	0.16
(1,867)	2:74:B:ILE:HG22	2:117:B:LYS:HB3	7	0.21	0.08	0.16
(1,867)	2:74:B:ILE:HG23	2:117:B:LYS:HB3	7	0.21	0.08	0.16
(1,155)	2:13:B:LEU:HG	2:14:B:SER:H	7	0.18	0.04	0.18
(1,486)	2:37:B:ALA:H	2:39:B:GLU:H	7	0.17	0.09	0.13
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB1	7	0.16	0.03	0.18
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB2	7	0.16	0.03	0.18
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB3	7	0.16	0.03	0.18
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD21	7	0.14	0.04	0.13
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD22	7	0.14	0.04	0.13
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD23	7	0.14	0.04	0.13
(1,809)	2:69:B:THR:HG1	2:110:B:LEU:H	7	0.14	0.03	0.13
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG2	7	0.13	0.03	0.14
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG3	7	0.13	0.03	0.14
(1,1908)	2:169:B:ARG:HA	2:170:B:LEU:H	7	0.13	0.02	0.12
(1,1923)	2:170:B:LEU:HG	2:171:B:GLU:H	7	0.13	0.02	0.12
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG21	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG22	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG23	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG21	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG22	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG23	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG21	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG22	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG23	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG21	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG22	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG23	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG21	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG22	6	0.3	0.14	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG23	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG21	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG22	6	0.3	0.14	0.3
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG23	6	0.3	0.14	0.3
(1,425)	2:33:B:ASN:H	2:33:B:ASN:HB2	6	0.28	0.02	0.28
(1,333)	2:25:B:SER:HB2	2:26:B:GLN:H	6	0.22	0.09	0.19
(1,333)	2:25:B:SER:HB3	2:26:B:GLN:H	6	0.22	0.09	0.19
(1,404)	2:31:B:GLU:H	2:31:B:GLU:HB2	6	0.21	0.03	0.22
(1,775)	2:63:B:ARG:HD2	2:64:B:ALA:H	6	0.2	0.08	0.16
(1,627)	2:47:B:LYS:H	2:47:B:LYS:HE3	6	0.18	0.04	0.18
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD11	6	0.18	0.07	0.16
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD12	6	0.18	0.07	0.16
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD13	6	0.18	0.07	0.16
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG21	6	0.18	0.05	0.19
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG22	6	0.18	0.05	0.19
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG23	6	0.18	0.05	0.19
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG21	6	0.18	0.05	0.19
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG22	6	0.18	0.05	0.19
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG23	6	0.18	0.05	0.19
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG21	6	0.18	0.05	0.19
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG22	6	0.18	0.05	0.19
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG23	6	0.18	0.05	0.19
(1,1979)	1:315:A:PHE:H	1:314:A:THR:HA	6	0.18	0.03	0.18
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG11	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG12	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG13	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG21	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG22	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG23	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG11	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG12	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG13	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG21	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG22	6	0.17	0.02	0.17
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG23	6	0.17	0.02	0.17
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD1	6	0.16	0.02	0.16
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD2	6	0.16	0.02	0.16
(1,1119)	2:97:B:TRP:H	2:97:B:TRP:HZ3	6	0.16	0.06	0.14
(1,410)	2:32:B:GLU:HG2	2:34:B:ARG:H	6	0.15	0.02	0.16
(1,410)	2:32:B:GLU:HG3	2:34:B:ARG:H	6	0.15	0.02	0.16
(1,211)	2:17:B:LEU:HD11	2:22:B:TYR:H	6	0.15	0.07	0.12
(1,211)	2:17:B:LEU:HD12	2:22:B:TYR:H	6	0.15	0.07	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,211)	2:17:B:LEU:HD13	2:22:B:TYR:H	6	0.15	0.07	0.12
(1,211)	2:17:B:LEU:HD21	2:22:B:TYR:H	6	0.15	0.07	0.12
(1,211)	2:17:B:LEU:HD22	2:22:B:TYR:H	6	0.15	0.07	0.12
(1,211)	2:17:B:LEU:HD23	2:22:B:TYR:H	6	0.15	0.07	0.12
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD1	6	0.14	0.04	0.14
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD2	6	0.14	0.04	0.14
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG2	6	0.14	0.02	0.14
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG3	6	0.14	0.02	0.14
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG2	6	0.14	0.02	0.14
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG3	6	0.14	0.02	0.14
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG2	6	0.14	0.02	0.14
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG3	6	0.14	0.02	0.14
(1,612)	2:47:B:LYS:HB2	2:51:B:ARG:HA	6	0.12	0.02	0.11
(1,612)	2:47:B:LYS:HB3	2:51:B:ARG:HA	6	0.12	0.02	0.11
(1,1030)	2:92:B:ARG:HB3	2:94:B:GLY:H	5	0.25	0.05	0.27
(1,774)	2:63:B:ARG:HD3	2:64:B:ALA:H	5	0.25	0.09	0.25
(1,1116)	2:97:B:TRP:H	2:97:B:TRP:HE1	5	0.23	0.12	0.14
(1,1787)	2:157:B:ASN:HB3	2:159:B:ALA:HA	5	0.21	0.12	0.15
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB2	5	0.21	0.07	0.2
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB3	5	0.21	0.07	0.2
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB2	5	0.2	0.05	0.22
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB3	5	0.2	0.05	0.22
(1,1861)	2:165:B:LYS:HD2	2:166:B:GLY:H	5	0.19	0.02	0.2
(1,1861)	2:165:B:LYS:HD3	2:166:B:GLY:H	5	0.19	0.02	0.2
(1,74)	2:8:B:LEU:HG	2:10:B:VAL:H	5	0.19	0.06	0.16
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD1	5	0.19	0.05	0.22
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD2	5	0.19	0.05	0.22
(1,1916)	2:169:B:ARG:H	2:169:B:ARG:HG3	5	0.19	0.03	0.18
(1,1786)	2:156:B:GLY:H	2:158:B:ASN:H	5	0.19	0.05	0.2
(1,1655)	2:145:B:ASN:H	2:146:B:GLY:H	5	0.18	0.04	0.17
(1,1735)	2:152:B:VAL:HG21	2:156:B:GLY:H	5	0.18	0.04	0.17
(1,1735)	2:152:B:VAL:HG22	2:156:B:GLY:H	5	0.18	0.04	0.17
(1,1735)	2:152:B:VAL:HG23	2:156:B:GLY:H	5	0.18	0.04	0.17
(1,2101)	1:323:A:GLU:H	1:321:A:SER:HB3	5	0.15	0.04	0.17
(1,1598)	2:142:B:ILE:HD11	2:146:B:GLY:H	5	0.15	0.04	0.14
(1,1598)	2:142:B:ILE:HD12	2:146:B:GLY:H	5	0.15	0.04	0.14
(1,1598)	2:142:B:ILE:HD13	2:146:B:GLY:H	5	0.15	0.04	0.14
(1,387)	2:30:B:VAL:HG11	2:32:B:GLU:H	5	0.14	0.03	0.12
(1,387)	2:30:B:VAL:HG12	2:32:B:GLU:H	5	0.14	0.03	0.12
(1,387)	2:30:B:VAL:HG13	2:32:B:GLU:H	5	0.14	0.03	0.12
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD21	5	0.14	0.04	0.12
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD22	5	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD23	5	0.14	0.04	0.12
(1,1661)	2:146:B:GLY:H	2:149:B:ASP:H	5	0.14	0.02	0.14
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD11	5	0.14	0.04	0.12
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD12	5	0.14	0.04	0.12
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD13	5	0.14	0.04	0.12
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD11	5	0.14	0.04	0.12
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD12	5	0.14	0.04	0.12
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD13	5	0.14	0.04	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG11	5	0.13	0.03	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG12	5	0.13	0.03	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG13	5	0.13	0.03	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG21	5	0.13	0.03	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG22	5	0.13	0.03	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG23	5	0.13	0.03	0.12
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD11	5	0.13	0.03	0.11
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD12	5	0.13	0.03	0.11
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD13	5	0.13	0.03	0.11
(1,628)	2:47:B:LYS:H	2:47:B:LYS:HE2	5	0.13	0.03	0.12
(1,1361)	2:116:B:ASP:H	2:119:B:MET:H	5	0.12	0.01	0.13
(1,1807)	2:158:B:ASN:H	2:159:B:ALA:H	4	0.3	0.18	0.24
(1,1911)	2:169:B:ARG:HD2	2:170:B:LEU:H	4	0.28	0.1	0.3
(1,1911)	2:169:B:ARG:HD3	2:170:B:LEU:H	4	0.28	0.1	0.3
(1,1109)	2:96:B:ASN:H	2:97:B:TRP:HE1	4	0.26	0.08	0.29
(1,507)	2:39:B:GLU:HG2	2:41:B:THR:HA	4	0.26	0.03	0.26
(1,507)	2:39:B:GLU:HG3	2:41:B:THR:HA	4	0.26	0.03	0.26
(1,1044)	2:92:B:ARG:H	2:92:B:ARG:HB2	4	0.26	0.03	0.25
(1,530)	2:40:B:GLY:H	2:42:B:GLU:H	4	0.24	0.03	0.23
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG2	4	0.23	0.08	0.22
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG3	4	0.23	0.08	0.22
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG2	4	0.23	0.05	0.24
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG3	4	0.23	0.05	0.24
(1,542)	2:41:B:THR:H	2:42:B:GLU:H	4	0.23	0.07	0.24
(1,1076)	2:95:B:VAL:HG11	2:96:B:ASN:HD22	4	0.22	0.1	0.22
(1,1076)	2:95:B:VAL:HG12	2:96:B:ASN:HD22	4	0.22	0.1	0.22
(1,1076)	2:95:B:VAL:HG13	2:96:B:ASN:HD22	4	0.22	0.1	0.22
(1,1601)	2:142:B:ILE:HD11	2:147:B:GLY:H	4	0.22	0.06	0.21
(1,1601)	2:142:B:ILE:HD12	2:147:B:GLY:H	4	0.22	0.06	0.21
(1,1601)	2:142:B:ILE:HD13	2:147:B:GLY:H	4	0.22	0.06	0.21
(1,1793)	2:157:B:ASN:H	2:159:B:ALA:H	4	0.21	0.09	0.2
(1,275)	2:20:B:LYS:HG2	2:22:B:TYR:H	4	0.2	0.04	0.2
(1,275)	2:20:B:LYS:HG3	2:22:B:TYR:H	4	0.2	0.04	0.2
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG12	4	0.2	0.06	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG13	4	0.2	0.06	0.22
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG12	4	0.2	0.06	0.22
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG13	4	0.2	0.06	0.22
(1,1507)	2:134:B:LEU:HD11	2:136:B:ASP:H	4	0.19	0.08	0.16
(1,1507)	2:134:B:LEU:HD12	2:136:B:ASP:H	4	0.19	0.08	0.16
(1,1507)	2:134:B:LEU:HD13	2:136:B:ASP:H	4	0.19	0.08	0.16
(1,1507)	2:134:B:LEU:HD21	2:136:B:ASP:H	4	0.19	0.08	0.16
(1,1507)	2:134:B:LEU:HD22	2:136:B:ASP:H	4	0.19	0.08	0.16
(1,1507)	2:134:B:LEU:HD23	2:136:B:ASP:H	4	0.19	0.08	0.16
(1,449)	2:35:B:THR:HA	2:36:B:GLU:H	4	0.18	0.03	0.18
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB2	4	0.18	0.03	0.18
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB3	4	0.18	0.03	0.18
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD11	4	0.18	0.06	0.16
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD12	4	0.18	0.06	0.16
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD13	4	0.18	0.06	0.16
(1,2102)	1:323:A:GLU:H	1:321:A:SER:HB2	4	0.18	0.05	0.16
(1,272)	2:20:B:LYS:HD2	2:22:B:TYR:H	4	0.18	0.06	0.16
(1,272)	2:20:B:LYS:HD3	2:22:B:TYR:H	4	0.18	0.06	0.16
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA2	4	0.18	0.07	0.15
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA3	4	0.18	0.07	0.15
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA2	4	0.18	0.07	0.15
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA3	4	0.18	0.07	0.15
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA2	4	0.18	0.07	0.15
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA3	4	0.18	0.07	0.15
(1,1788)	2:157:B:ASN:HB2	2:159:B:ALA:HA	4	0.18	0.06	0.18
(1,1106)	2:96:B:ASN:H	2:97:B:TRP:HB3	4	0.17	0.03	0.18
(1,465)	2:36:B:GLU:HB2	2:37:B:ALA:H	4	0.16	0.03	0.16
(1,465)	2:36:B:GLU:HB3	2:37:B:ALA:H	4	0.16	0.03	0.16
(1,451)	2:35:B:THR:HG1	2:36:B:GLU:H	4	0.16	0.06	0.14
(1,527)	2:40:B:GLY:H	2:41:B:THR:HG1	4	0.16	0.03	0.16
(1,1389)	2:119:B:MET:H	2:120:B:GLN:HE22	4	0.16	0.04	0.17
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG11	4	0.16	0.03	0.16
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG12	4	0.16	0.03	0.16
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG13	4	0.16	0.03	0.16
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG21	4	0.16	0.03	0.16
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG22	4	0.16	0.03	0.16
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG23	4	0.16	0.03	0.16
(1,536)	2:41:B:THR:HG1	2:45:B:ALA:H	4	0.16	0.06	0.14
(1,1657)	2:145:B:ASN:H	2:148:B:TRP:H	4	0.16	0.02	0.16
(1,526)	2:40:B:GLY:H	2:40:B:GLY:HA2	4	0.16	0.02	0.16
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD11	4	0.15	0.02	0.15
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD12	4	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD13	4	0.15	0.02	0.15
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD21	4	0.15	0.02	0.15
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD22	4	0.15	0.02	0.15
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD23	4	0.15	0.02	0.15
(1,550)	2:42:B:GLU:H	2:42:B:GLU:HG3	4	0.15	0.04	0.14
(1,1590)	2:141:B:TRP:H	2:142:B:ILE:HB	4	0.15	0.02	0.16
(1,502)	2:39:B:GLU:HB2	2:41:B:THR:HA	4	0.15	0.03	0.14
(1,502)	2:39:B:GLU:HB3	2:41:B:THR:HA	4	0.15	0.03	0.14
(1,1292)	2:112:B:VAL:HG11	2:113:B:GLU:H	4	0.15	0.02	0.15
(1,1292)	2:112:B:VAL:HG12	2:113:B:GLU:H	4	0.15	0.02	0.15
(1,1292)	2:112:B:VAL:HG13	2:113:B:GLU:H	4	0.15	0.02	0.15
(1,1367)	2:117:B:LYS:H	2:117:B:LYS:HD3	4	0.15	0.03	0.14
(1,910)	2:81:B:GLN:H	2:85:B:GLN:H	4	0.14	0.03	0.15
(1,1898)	2:168:B:GLU:HG2	2:170:B:LEU:H	4	0.14	0.01	0.14
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD1	4	0.13	0.02	0.14
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD2	4	0.13	0.02	0.14
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD1	4	0.13	0.02	0.14
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD2	4	0.13	0.02	0.14
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD1	4	0.13	0.02	0.14
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD2	4	0.13	0.02	0.14
(1,1919)	2:169:B:ARG:H	2:170:B:LEU:HA	4	0.12	0.02	0.12
(1,427)	2:33:B:ASN:H	2:33:B:ASN:HD22	3	0.58	0.11	0.53
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG21	3	0.4	0.08	0.43
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG22	3	0.4	0.08	0.43
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG23	3	0.4	0.08	0.43
(1,1917)	2:169:B:ARG:H	2:169:B:ARG:HG2	3	0.35	0.31	0.14
(1,1836)	2:162:B:GLU:H	2:162:B:GLU:HB2	3	0.3	0.02	0.29
(1,1808)	2:158:B:ASN:H	2:160:B:ALA:H	3	0.29	0.06	0.25
(1,453)	2:35:B:THR:HG21	2:36:B:GLU:HB3	3	0.27	0.09	0.22
(1,453)	2:35:B:THR:HG22	2:36:B:GLU:HB3	3	0.27	0.09	0.22
(1,453)	2:35:B:THR:HG23	2:36:B:GLU:HB3	3	0.27	0.09	0.22
(1,1402)	2:121:B:VAL:H	2:121:B:VAL:HB	3	0.27	0.02	0.28
(1,1382)	2:119:B:MET:HA	2:120:B:GLN:H	3	0.24	0.02	0.24
(1,458)	2:35:B:THR:H	2:35:B:THR:HB	3	0.23	0.03	0.21
(1,127)	2:11:B:ASP:HB2	2:47:B:LYS:HD2	3	0.22	0.03	0.2
(1,376)	2:29:B:ASP:HA	2:30:B:VAL:H	3	0.22	0.03	0.23
(1,1108)	2:96:B:ASN:H	2:97:B:TRP:HB2	3	0.2	0.05	0.18
(1,1108)	2:96:B:ASN:H	2:97:B:TRP:HB3	3	0.2	0.05	0.18
(1,703)	2:51:B:ARG:H	2:51:B:ARG:HD2	3	0.2	0.02	0.2
(1,931)	2:85:B:GLN:HB2	2:86:B:VAL:HB	3	0.2	0.02	0.19
(1,931)	2:85:B:GLN:HB3	2:86:B:VAL:HB	3	0.2	0.02	0.19
(1,266)	2:20:B:LYS:HB3	2:22:B:TYR:H	3	0.19	0.07	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1670)	2:148:B:TRP:HB2	2:150:B:THR:H	3	0.19	0.05	0.19
(1,1670)	2:148:B:TRP:HB3	2:150:B:THR:H	3	0.19	0.05	0.19
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD11	3	0.18	0.01	0.17
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD12	3	0.18	0.01	0.17
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD13	3	0.18	0.01	0.17
(1,1551)	2:138:B:LEU:HD11	2:139:B:GLU:H	3	0.18	0.04	0.15
(1,1551)	2:138:B:LEU:HD12	2:139:B:GLU:H	3	0.18	0.04	0.15
(1,1551)	2:138:B:LEU:HD13	2:139:B:GLU:H	3	0.18	0.04	0.15
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG21	3	0.17	0.01	0.16
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG22	3	0.17	0.01	0.16
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG23	3	0.17	0.01	0.16
(1,1071)	2:94:B:GLY:H	2:96:B:ASN:HD22	3	0.17	0.02	0.16
(1,1877)	2:166:B:GLY:H	2:167:B:GLN:HB2	3	0.17	0.04	0.19
(1,1877)	2:166:B:GLY:H	2:167:B:GLN:HB3	3	0.17	0.04	0.19
(1,551)	2:42:B:GLU:H	2:42:B:GLU:HG2	3	0.17	0.05	0.15
(1,1660)	2:146:B:GLY:H	2:148:B:TRP:H	3	0.17	0.04	0.18
(1,385)	2:30:B:VAL:HA	2:31:B:GLU:H	3	0.16	0.02	0.17
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD11	3	0.16	0.05	0.17
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD12	3	0.16	0.05	0.17
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD13	3	0.16	0.05	0.17
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD11	3	0.16	0.04	0.18
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD12	3	0.16	0.04	0.18
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD13	3	0.16	0.04	0.18
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG11	3	0.16	0.05	0.14
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG12	3	0.16	0.05	0.14
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG13	3	0.16	0.05	0.14
(1,375)	2:28:B:SER:H	2:30:B:VAL:H	3	0.16	0.03	0.17
(1,2003)	1:317:A:HIS:H	1:314:A:THR:HA	3	0.15	0.02	0.16
(1,104)	2:10:B:VAL:HG11	2:12:B:PHE:H	3	0.15	0.01	0.14
(1,104)	2:10:B:VAL:HG12	2:12:B:PHE:H	3	0.15	0.01	0.14
(1,104)	2:10:B:VAL:HG13	2:12:B:PHE:H	3	0.15	0.01	0.14
(1,861)	2:74:B:ILE:HD11	2:119:B:MET:HB2	3	0.15	0.04	0.15
(1,861)	2:74:B:ILE:HD11	2:119:B:MET:HB3	3	0.15	0.04	0.15
(1,861)	2:74:B:ILE:HD12	2:119:B:MET:HB2	3	0.15	0.04	0.15
(1,861)	2:74:B:ILE:HD12	2:119:B:MET:HB3	3	0.15	0.04	0.15
(1,861)	2:74:B:ILE:HD13	2:119:B:MET:HB2	3	0.15	0.04	0.15
(1,861)	2:74:B:ILE:HD13	2:119:B:MET:HB3	3	0.15	0.04	0.15
(1,1614)	2:143:B:GLN:HA	2:147:B:GLY:H	3	0.15	0.01	0.14
(1,480)	2:37:B:ALA:H	2:37:B:ALA:HA	3	0.15	0.03	0.15
(1,430)	2:33:B:ASN:H	2:35:B:THR:HG1	3	0.14	0.04	0.11
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG21	3	0.14	0.05	0.11
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG22	3	0.14	0.05	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG23	3	0.14	0.05	0.11
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG11	3	0.13	0.02	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG12	3	0.13	0.02	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG13	3	0.13	0.02	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG21	3	0.13	0.02	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG22	3	0.13	0.02	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG23	3	0.13	0.02	0.13
(1,1060)	2:93:B:ASP:H	2:94:B:GLY:HA2	3	0.13	0.02	0.13
(1,1531)	2:135:B:ASN:H	2:137:B:HIS:H	3	0.13	0.02	0.14
(1,2048)	1:319:A:TRP:H	1:319:A:TRP:HD1	3	0.13	0.02	0.13
(1,422)	2:33:B:ASN:HD22	2:34:B:ARG:H	3	0.13	0.01	0.13
(1,1640)	2:144:B:GLU:H	2:145:B:ASN:HD22	3	0.13	0.02	0.13
(1,1192)	2:104:B:PHE:HD1	2:106:B:PHE:H	3	0.12	0.03	0.11
(1,1192)	2:104:B:PHE:HD2	2:106:B:PHE:H	3	0.12	0.03	0.11
(1,1394)	2:120:B:GLN:H	2:120:B:GLN:HB2	3	0.12	0.03	0.11
(1,1394)	2:120:B:GLN:H	2:120:B:GLN:HB3	3	0.12	0.03	0.11
(1,1862)	2:165:B:LYS:HD2	2:167:B:GLN:H	3	0.12	0.02	0.13
(1,1862)	2:165:B:LYS:HD3	2:167:B:GLN:H	3	0.12	0.02	0.13
(1,1895)	2:168:B:GLU:HG3	2:169:B:ARG:H	3	0.12	0.01	0.13
(1,457)	2:35:B:THR:HG21	2:37:B:ALA:H	3	0.12	0.01	0.12
(1,457)	2:35:B:THR:HG22	2:37:B:ALA:H	3	0.12	0.01	0.12
(1,457)	2:35:B:THR:HG23	2:37:B:ALA:H	3	0.12	0.01	0.12
(1,1997)	1:317:A:HIS:HD1	1:317:A:HIS:HA	3	0.12	0.0	0.12
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD11	3	0.11	0.0	0.11
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD12	3	0.11	0.0	0.11
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD13	3	0.11	0.0	0.11
(1,1615)	2:143:B:GLN:HB3	2:144:B:GLU:HA	3	0.11	0.01	0.11
(1,1867)	2:165:B:LYS:H	2:165:B:LYS:HB2	2	0.5	0.07	0.5
(1,1867)	2:165:B:LYS:H	2:165:B:LYS:HB3	2	0.5	0.07	0.5
(1,1606)	2:142:B:ILE:HG21	2:144:B:GLU:HG2	2	0.36	0.06	0.36
(1,1606)	2:142:B:ILE:HG22	2:144:B:GLU:HG2	2	0.36	0.06	0.36
(1,1606)	2:142:B:ILE:HG23	2:144:B:GLU:HG2	2	0.36	0.06	0.36
(1,1605)	2:142:B:ILE:HG21	2:144:B:GLU:HG3	2	0.32	0.04	0.32
(1,1605)	2:142:B:ILE:HG22	2:144:B:GLU:HG3	2	0.32	0.04	0.32
(1,1605)	2:142:B:ILE:HG23	2:144:B:GLU:HG3	2	0.32	0.04	0.32
(1,1634)	2:144:B:GLU:HG2	2:146:B:GLY:H	2	0.32	0.08	0.32
(1,1198)	2:104:B:PHE:H	2:104:B:PHE:HE1	2	0.3	0.14	0.3
(1,1198)	2:104:B:PHE:H	2:104:B:PHE:HE2	2	0.3	0.14	0.3
(1,215)	2:17:B:LEU:HG	2:18:B:SER:H	2	0.29	0.0	0.29
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD21	2	0.26	0.03	0.26
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD22	2	0.26	0.03	0.26
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD23	2	0.26	0.03	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG21	2	0.26	0.12	0.26
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG22	2	0.26	0.12	0.26
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG23	2	0.26	0.12	0.26
(1,1)	2:1:B:MET:HA	2:3:B:GLN:H	2	0.24	0.11	0.24
(1,445)	2:35:B:THR:HA	2:36:B:GLU:HB3	2	0.23	0.02	0.23
(1,1095)	2:96:B:ASN:HD21	2:100:B:ILE:H	2	0.22	0.02	0.22
(1,1096)	2:96:B:ASN:HD21	2:99:B:ARG:H	2	0.22	0.08	0.22
(1,250)	2:19:B:GLN:HB2	2:21:B:GLY:H	2	0.22	0.02	0.22
(1,902)	2:81:B:GLN:HA	2:85:B:GLN:HB2	2	0.22	0.1	0.22
(1,902)	2:81:B:GLN:HA	2:85:B:GLN:HB3	2	0.22	0.1	0.22
(1,1738)	2:152:B:VAL:HG11	2:155:B:TYR:HE1	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG11	2:155:B:TYR:HE2	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG12	2:155:B:TYR:HE1	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG12	2:155:B:TYR:HE2	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG13	2:155:B:TYR:HE1	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG13	2:155:B:TYR:HE2	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG21	2:155:B:TYR:HE1	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG21	2:155:B:TYR:HE2	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG22	2:155:B:TYR:HE1	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG22	2:155:B:TYR:HE2	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG23	2:155:B:TYR:HE1	2	0.21	0.04	0.21
(1,1738)	2:152:B:VAL:HG23	2:155:B:TYR:HE2	2	0.21	0.04	0.21
(1,1183)	2:103:B:PHE:HB2	2:105:B:SER:HB2	2	0.2	0.03	0.2
(1,1183)	2:103:B:PHE:HB2	2:105:B:SER:HB3	2	0.2	0.03	0.2
(1,1183)	2:103:B:PHE:HB3	2:105:B:SER:HB2	2	0.2	0.03	0.2
(1,1183)	2:103:B:PHE:HB3	2:105:B:SER:HB3	2	0.2	0.03	0.2
(1,444)	2:34:B:ARG:H	2:35:B:THR:H	2	0.2	0.04	0.2
(1,1866)	2:165:B:LYS:H	2:165:B:LYS:HB2	2	0.2	0.05	0.2
(1,894)	2:80:B:TYR:H	2:129:B:TRP:HD1	2	0.19	0.0	0.19
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD11	2	0.19	0.02	0.19
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD12	2	0.19	0.02	0.19
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD13	2	0.19	0.02	0.19
(1,484)	2:37:B:ALA:H	2:38:B:PRO:HD2	2	0.18	0.04	0.18
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD11	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD12	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD13	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD21	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD22	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD23	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD11	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD12	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD13	2	0.18	0.06	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD21	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD22	2	0.18	0.06	0.18
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD23	2	0.18	0.06	0.18
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG11	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG12	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG13	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG21	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG22	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG23	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG11	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG12	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG13	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG21	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG22	2	0.18	0.04	0.18
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG23	2	0.18	0.04	0.18
(1,29)	2:4:B:SER:H	2:8:B:LEU:H	2	0.17	0.06	0.17
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG21	2	0.17	0.05	0.17
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG22	2	0.17	0.05	0.17
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG23	2	0.17	0.05	0.17
(1,1794)	2:158:B:ASN:HA	2:159:B:ALA:H	2	0.17	0.01	0.17
(1,187)	2:16:B:LYS:H	2:16:B:LYS:HE2	2	0.16	0.01	0.16
(1,187)	2:16:B:LYS:H	2:16:B:LYS:HE3	2	0.16	0.01	0.16
(1,442)	2:34:B:ARG:H	2:35:B:THR:HB	2	0.16	0.02	0.16
(1,3)	2:1:B:MET:HG2	2:2:B:SER:HA	2	0.16	0.02	0.16
(1,3)	2:1:B:MET:HG3	2:2:B:SER:HA	2	0.16	0.02	0.16
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG11	2	0.16	0.01	0.16
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG12	2	0.16	0.01	0.16
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG13	2	0.16	0.01	0.16
(1,1860)	2:165:B:LYS:HB2	2:168:B:GLU:H	2	0.16	0.02	0.16
(1,1695)	2:150:B:THR:HB	2:153:B:GLU:HG2	2	0.16	0.05	0.16
(1,345)	2:26:B:GLN:HG2	2:27:B:PHE:H	2	0.15	0.01	0.15
(1,401)	2:30:B:VAL:H	2:33:B:ASN:H	2	0.15	0.02	0.15
(1,436)	2:34:B:ARG:HD2	2:35:B:THR:H	2	0.15	0.02	0.15
(1,436)	2:34:B:ARG:HD3	2:35:B:THR:H	2	0.15	0.02	0.15
(1,321)	2:24:B:TRP:HB2	2:26:B:GLN:H	2	0.15	0.0	0.15
(1,321)	2:24:B:TRP:HB3	2:26:B:GLN:H	2	0.15	0.0	0.15
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG11	2	0.15	0.0	0.15
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG12	2	0.15	0.0	0.15
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG13	2	0.15	0.0	0.15
(1,1144)	2:100:B:ILE:HG21	2:138:B:LEU:HG	2	0.15	0.0	0.15
(1,1144)	2:100:B:ILE:HG22	2:138:B:LEU:HG	2	0.15	0.0	0.15
(1,1144)	2:100:B:ILE:HG23	2:138:B:LEU:HG	2	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,173)	2:14:B:SER:H	2:24:B:TRP:HE1	2	0.14	0.0	0.14
(1,446)	2:35:B:THR:HA	2:36:B:GLU:HB2	2	0.14	0.01	0.14
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG21	2	0.14	0.02	0.14
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG22	2	0.14	0.02	0.14
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG23	2	0.14	0.02	0.14
(1,812)	2:69:B:THR:HG21	2:106:B:PHE:HE1	2	0.14	0.02	0.14
(1,812)	2:69:B:THR:HG21	2:106:B:PHE:HE2	2	0.14	0.02	0.14
(1,812)	2:69:B:THR:HG22	2:106:B:PHE:HE1	2	0.14	0.02	0.14
(1,812)	2:69:B:THR:HG22	2:106:B:PHE:HE2	2	0.14	0.02	0.14
(1,812)	2:69:B:THR:HG23	2:106:B:PHE:HE1	2	0.14	0.02	0.14
(1,812)	2:69:B:THR:HG23	2:106:B:PHE:HE2	2	0.14	0.02	0.14
(1,1946)	1:313:A:THR:H	1:312:A:GLY:HA3	2	0.14	0.02	0.14
(1,334)	2:25:B:SER:HB2	2:29:B:ASP:H	2	0.13	0.01	0.13
(1,334)	2:25:B:SER:HB3	2:29:B:ASP:H	2	0.13	0.01	0.13
(1,1338)	2:115:B:VAL:HG11	2:119:B:MET:H	2	0.13	0.02	0.13
(1,1338)	2:115:B:VAL:HG12	2:119:B:MET:H	2	0.13	0.02	0.13
(1,1338)	2:115:B:VAL:HG13	2:119:B:MET:H	2	0.13	0.02	0.13
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG11	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG12	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG13	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG21	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG22	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG23	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG11	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG12	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG13	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG21	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG22	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG23	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG11	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG12	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG13	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG21	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG22	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG23	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG11	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG12	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG13	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG21	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG22	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG23	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG11	2	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG12	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG13	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG21	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG22	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG23	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG11	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG12	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG13	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG21	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG22	2	0.13	0.01	0.13
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG23	2	0.13	0.01	0.13
(1,1541)	2:137:B:HIS:H	2:137:B:HIS:HD2	2	0.13	0.01	0.13
(1,1628)	2:143:B:GLN:H	2:145:B:ASN:H	2	0.13	0.01	0.13
(1,415)	2:32:B:GLU:H	2:33:B:ASN:H	2	0.12	0.01	0.12
(1,492)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	2	0.12	0.02	0.12
(1,492)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	2	0.12	0.02	0.12
(1,492)	2:38:B:PRO:HD3	2:39:B:GLU:HG2	2	0.12	0.02	0.12
(1,492)	2:38:B:PRO:HD3	2:39:B:GLU:HG3	2	0.12	0.02	0.12
(1,1107)	2:96:B:ASN:H	2:97:B:TRP:HB2	2	0.12	0.02	0.12
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD11	2	0.12	0.01	0.12
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD12	2	0.12	0.01	0.12
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD13	2	0.12	0.01	0.12
(1,1552)	2:138:B:LEU:HD21	2:139:B:GLU:H	2	0.12	0.02	0.12
(1,1552)	2:138:B:LEU:HD22	2:139:B:GLU:H	2	0.12	0.02	0.12
(1,1552)	2:138:B:LEU:HD23	2:139:B:GLU:H	2	0.12	0.02	0.12
(1,1874)	2:166:B:GLY:HA2	2:167:B:GLN:H	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD11	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD12	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD13	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD21	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD22	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD23	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD11	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD12	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD13	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD21	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD22	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD23	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD11	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD12	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD13	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD21	2	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD22	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD23	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD11	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD12	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD13	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD21	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD22	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD23	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD11	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD12	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD13	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD21	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD22	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD23	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD11	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD12	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD13	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD21	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD22	2	0.12	0.02	0.12
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD23	2	0.12	0.02	0.12
(1,234)	2:18:B:SER:HB2	2:21:B:GLY:H	2	0.12	0.0	0.12
(1,468)	2:36:B:GLU:H	2:36:B:GLU:HB2	2	0.12	0.0	0.12
(1,468)	2:36:B:GLU:H	2:36:B:GLU:HB3	2	0.12	0.0	0.12
(1,1085)	2:95:B:VAL:HG11	2:141:B:TRP:H	2	0.12	0.01	0.12
(1,1085)	2:95:B:VAL:HG12	2:141:B:TRP:H	2	0.12	0.01	0.12
(1,1085)	2:95:B:VAL:HG13	2:141:B:TRP:H	2	0.12	0.01	0.12
(1,1085)	2:95:B:VAL:HG21	2:141:B:TRP:H	2	0.12	0.01	0.12
(1,1085)	2:95:B:VAL:HG22	2:141:B:TRP:H	2	0.12	0.01	0.12
(1,1085)	2:95:B:VAL:HG23	2:141:B:TRP:H	2	0.12	0.01	0.12
(1,2151)	2:155:B:TYR:HD1	1:315:A:PHE:HA	2	0.12	0.0	0.12
(1,2151)	2:155:B:TYR:HD2	1:315:A:PHE:HA	2	0.12	0.0	0.12
(1,666)	2:49:B:ALA:H	2:53:B:ALA:H	2	0.12	0.02	0.12
(1,614)	2:47:B:LYS:HD2	2:48:B:GLN:H	2	0.12	0.0	0.12
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB1	2	0.12	0.0	0.12
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB2	2	0.12	0.0	0.12
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB3	2	0.12	0.0	0.12
(1,508)	2:39:B:GLU:HG2	2:41:B:THR:HB	2	0.11	0.0	0.11
(1,508)	2:39:B:GLU:HG3	2:41:B:THR:HB	2	0.11	0.0	0.11
(1,842)	2:72:B:LEU:HD21	2:86:B:VAL:HB	2	0.11	0.01	0.11
(1,842)	2:72:B:LEU:HD22	2:86:B:VAL:HB	2	0.11	0.01	0.11
(1,842)	2:72:B:LEU:HD23	2:86:B:VAL:HB	2	0.11	0.01	0.11
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG11	2	0.11	0.01	0.11

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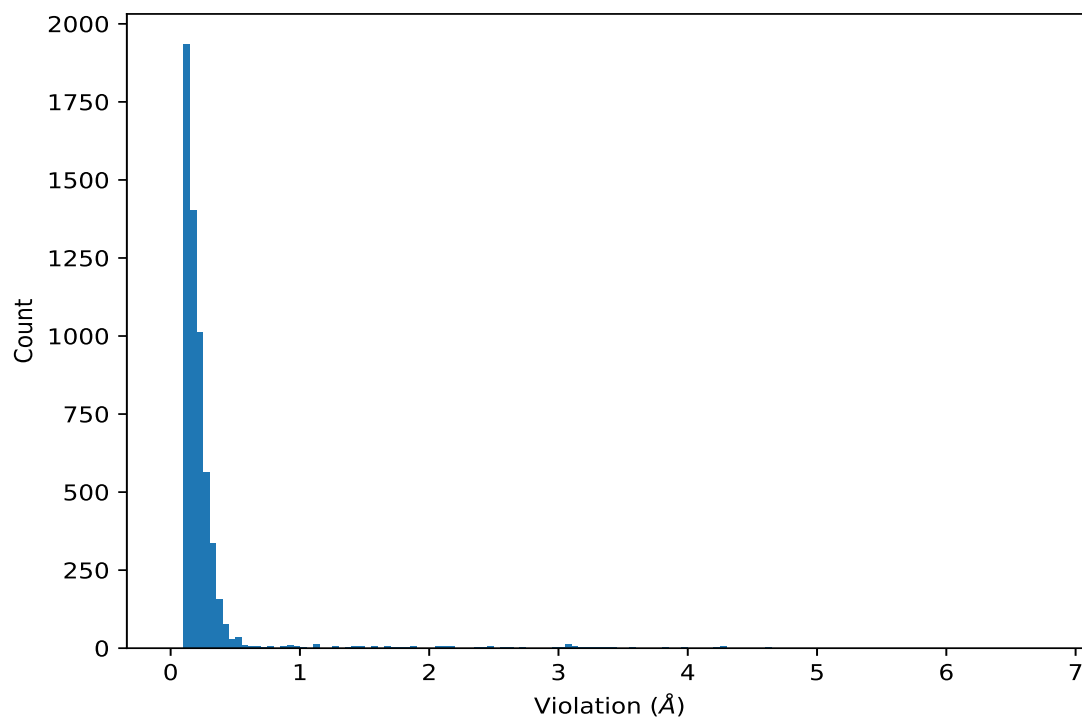
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG12	2	0.11	0.01	0.11
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG13	2	0.11	0.01	0.11
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG21	2	0.11	0.01	0.11
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG22	2	0.11	0.01	0.11
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG23	2	0.11	0.01	0.11
(1,1863)	2:165:B:LYS:HG3	2:166:B:GLY:H	2	0.11	0.0	0.11
(1,2027)	1:318:A:LEU:H	1:318:A:LEU:HA	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)
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	13	6.8
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	6	5.78
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	10	5.15
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	3	4.8
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	2	4.77
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	7	4.74
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	13	4.64
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	13	4.64
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	13	4.64
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	5	4.54
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	19	4.47
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	16	4.42
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	6	4.29
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	6	4.29
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	6	4.29
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	16	4.27
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	19	4.25
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	6	4.24
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	6	4.24
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	6	4.24
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	16	4.22
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	15	4.17
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	12	4.12
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	1	3.98
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	20	3.96
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	6	3.93
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	18	3.82
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	5	3.8
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	3	3.7
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	8	3.66
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	6	3.64
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	5	3.59
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	3	3.58
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	11	3.45
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	10	3.44
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	11	3.44
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	1	3.38
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	17	3.38
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	15	3.36
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	14	3.33
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	12	3.31
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	15	3.28
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	2	3.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	1	3.24
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	12	3.24
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	18	3.21
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	17	3.2
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	13	3.18
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	9	3.16
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	4	3.13
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	7	3.11
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	20	3.11
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	9	3.11
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	19	3.11
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	18	3.1
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	7	3.09
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	10	3.09
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	10	3.09
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	10	3.09
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	17	3.09
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	4	3.08
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	10	3.08
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	2	3.06
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	2	3.06
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	2	3.06
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	9	3.05
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	14	3.05
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	13	3.03
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	13	3.03
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	13	3.03
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	20	2.98
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	11	2.98
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	2	2.97
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	13	2.75
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	3	2.7
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	3	2.7
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	3	2.7
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	14	2.69
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	18	2.6
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	18	2.6
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	18	2.6
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	20	2.59
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	20	2.59
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	20	2.59
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	5	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	5	2.49
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	5	2.49
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	9	2.47
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	9	2.47
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	9	2.47
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	17	2.41
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	17	2.41
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	17	2.41
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	12	2.36
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	12	2.36
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	12	2.36
(1,2137)	2:101:B:VAL:HB	1:319:A:TRP:HD1	4	2.31
(1,2142)	2:154:B:LEU:HB3	1:319:A:TRP:HD1	8	2.21
(1,2148)	2:154:B:LEU:HB2	1:319:A:TRP:HD1	8	2.18
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	19	2.18
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	19	2.18
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	19	2.18
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	16	2.15
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	16	2.15
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	16	2.15
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	1	2.14
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	1	2.14
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	1	2.14
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	18	2.12
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	18	2.12
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	18	2.12
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	7	2.09
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	7	2.09
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	7	2.09
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	15	2.06
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	15	2.06
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	15	2.06
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	13	2.01
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	17	1.87
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	17	1.87
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	17	1.87
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	19	1.87
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	19	1.87
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	19	1.87
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	20	1.81
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	20	1.81
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	20	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	14	1.78
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	14	1.78
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	14	1.78
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	9	1.77
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	11	1.71
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	11	1.71
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	11	1.71
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	9	1.66
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	9	1.66
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	9	1.66
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	8	1.65
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	8	1.65
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	8	1.65
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	14	1.57
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	14	1.57
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	14	1.57
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	10	1.55
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	10	1.55
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	10	1.55
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	13	1.53
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	4	1.48
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	4	1.48
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	4	1.48
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	5	1.47
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	7	1.45
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	7	1.45
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	7	1.45
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	3	1.44
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	3	1.44
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	3	1.44
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	14	1.43
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	6	1.4
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	14	1.39
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	11	1.37
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	18	1.29
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	12	1.28
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	7	1.26
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	9	1.26
(1,2141)	2:101:B:VAL:HG21	1:319:A:TRP:HD1	2	1.25
(1,2141)	2:101:B:VAL:HG22	1:319:A:TRP:HD1	2	1.25
(1,2141)	2:101:B:VAL:HG23	1:319:A:TRP:HD1	2	1.25
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	16	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	17	1.16
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	5	1.14
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	5	1.14
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	5	1.14
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	3	1.14
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	5	1.14
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	12	1.12
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	12	1.12
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	12	1.12
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	12	1.12
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	12	1.12
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	12	1.12
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	5	1.11
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	11	1.02
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	11	1.02
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	11	1.02
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	19	0.97
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	12	0.96
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	12	0.96
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	12	0.96
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	1	0.96
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	20	0.96
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	15	0.94
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	15	0.94
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	15	0.94
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	7	0.94
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	1	0.92
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	1	0.92
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	1	0.92
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	15	0.92
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	8	0.91
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	5	0.9
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	18	0.88
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	2	0.86
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	17	0.86
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	16	0.85
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	16	0.85
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	16	0.85
(1,1917)	2:169:B:ARG:H	2:169:B:ARG:HG2	7	0.79
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	10	0.78
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	4	0.77
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	4	0.77
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	20	0.76
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	6	0.75
(1,427)	2:33:B:ASN:H	2:33:B:ASN:HD22	18	0.73
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	13	0.71
(1,2136)	2:57:B:PHE:HB3	1:322:A:LEU:HG	4	0.7
(1,2139)	2:101:B:VAL:HG11	1:319:A:TRP:HD1	8	0.68
(1,2139)	2:101:B:VAL:HG12	1:319:A:TRP:HD1	8	0.68
(1,2139)	2:101:B:VAL:HG13	1:319:A:TRP:HD1	8	0.68
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	2	0.65
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	2	0.65
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	2	0.65
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	16	0.63
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	13	0.6
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	13	0.6
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	13	0.6
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	9	0.6
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	17	0.59
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	20	0.59
(1,1807)	2:158:B:ASN:H	2:159:B:ALA:H	5	0.59
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	17	0.59
(1,1867)	2:165:B:LYS:H	2:165:B:LYS:HB2	16	0.57
(1,1867)	2:165:B:LYS:H	2:165:B:LYS:HB3	16	0.57
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	6	0.56
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	6	0.56
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	6	0.56
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG21	9	0.54
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG22	9	0.54
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG23	9	0.54
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG21	9	0.54
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG22	9	0.54
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG23	9	0.54
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG21	9	0.54
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG22	9	0.54
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG23	9	0.54
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG21	9	0.54
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG22	9	0.54
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG23	9	0.54
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG21	9	0.54
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG22	9	0.54
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG23	9	0.54
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG21	9	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG22	9	0.54
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG23	9	0.54
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	8	0.54
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	8	0.54
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	8	0.54
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	8	0.54
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	8	0.54
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	8	0.54
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	18	0.53
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	18	0.53
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	18	0.53
(1,427)	2:33:B:ASN:H	2:33:B:ASN:HD22	13	0.53
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	16	0.52
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	11	0.52
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	11	0.52
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	11	0.52
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	7	0.51
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	8	0.5
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	7	0.5
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	14	0.5
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	20	0.49
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG21	14	0.48
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG22	14	0.48
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG23	14	0.48
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	15	0.48
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	3	0.47
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	3	0.47
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	3	0.47
(1,427)	2:33:B:ASN:H	2:33:B:ASN:HD22	9	0.47
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	4	0.46
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	4	0.46
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	4	0.46
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	1	0.46
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	8	0.46
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	19	0.46
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	2	0.46
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	2	0.46
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	2	0.46
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	8	0.45
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	8	0.45
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	8	0.45
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	4	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	2:97:B:TRP:H	2:97:B:TRP:HE1	14	0.45
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	12	0.45
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	9	0.45
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	9	0.45
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	9	0.45
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	9	0.45
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	9	0.45
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	9	0.45
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	7	0.44
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	7	0.44
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	7	0.44
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	15	0.44
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	15	0.44
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	15	0.44
(1,1787)	2:157:B:ASN:HB3	2:159:B:ALA:HA	16	0.44
(1,1198)	2:104:B:PHE:H	2:104:B:PHE:HE1	9	0.44
(1,1198)	2:104:B:PHE:H	2:104:B:PHE:HE2	9	0.44
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	6	0.44
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	3	0.44
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	10	0.44
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	3	0.44
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	5	0.44
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	5	0.44
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	5	0.44
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	9	0.43
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	9	0.43
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	9	0.43
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	11	0.43
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG21	12	0.43
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG22	12	0.43
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG23	12	0.43
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	8	0.43
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	6	0.43
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	16	0.43
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	13	0.43
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	14	0.42
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	3	0.42
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	6	0.42
(1,1867)	2:165:B:LYS:H	2:165:B:LYS:HB2	11	0.42
(1,1867)	2:165:B:LYS:H	2:165:B:LYS:HB3	11	0.42
(1,1606)	2:142:B:ILE:HG21	2:144:B:GLU:HG2	5	0.42
(1,1606)	2:142:B:ILE:HG22	2:144:B:GLU:HG2	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1606)	2:142:B:ILE:HG23	2:144:B:GLU:HG2	5	0.42
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	1	0.42
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	14	0.42
(1,1809)	2:158:B:ASN:H	2:161:B:ALA:H	20	0.41
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	18	0.41
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE1	1	0.41
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE2	1	0.41
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE1	1	0.41
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE2	1	0.41
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	5	0.41
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	15	0.41
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	18	0.41
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	3	0.41
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	16	0.41
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	7	0.41
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	7	0.41
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	7	0.41
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	7	0.41
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	7	0.41
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	7	0.41
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	7	0.41
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	7	0.41
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	7	0.41
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	18	0.41
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	18	0.41
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	18	0.41
(1,1634)	2:144:B:GLU:HG2	2:146:B:GLY:H	17	0.4
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	4	0.4
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	18	0.4
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	18	0.4
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	18	0.4
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	18	0.4
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	18	0.4
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	18	0.4
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD11	16	0.4
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD12	16	0.4
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD13	16	0.4
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	18	0.4
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	18	0.4
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	18	0.4
(1,333)	2:25:B:SER:HB2	2:26:B:GLN:H	4	0.4
(1,333)	2:25:B:SER:HB3	2:26:B:GLN:H	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	1	0.39
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	1	0.39
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	1	0.39
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD21	19	0.39
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD22	19	0.39
(1,2079)	1:322:A:LEU:HA	1:322:A:LEU:HD23	19	0.39
(1,1914)	2:169:B:ARG:H	2:169:B:ARG:HB2	7	0.39
(1,1914)	2:169:B:ARG:H	2:169:B:ARG:HB3	7	0.39
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	13	0.39
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	13	0.39
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	13	0.39
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	10	0.39
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	10	0.39
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	10	0.39
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	10	0.39
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	10	0.39
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	10	0.39
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	8	0.39
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	8	0.39
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	8	0.39
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD11	11	0.39
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD12	11	0.39
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD13	11	0.39
(1,774)	2:63:B:ARG:HD3	2:64:B:ALA:H	2	0.39
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	2	0.39
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	2	0.39
(1,453)	2:35:B:THR:HG21	2:36:B:GLU:HB3	5	0.39
(1,453)	2:35:B:THR:HG22	2:36:B:GLU:HB3	5	0.39
(1,453)	2:35:B:THR:HG23	2:36:B:GLU:HB3	5	0.39
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	12	0.39
(1,1911)	2:169:B:ARG:HD2	2:170:B:LEU:H	9	0.38
(1,1911)	2:169:B:ARG:HD3	2:170:B:LEU:H	9	0.38
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG21	4	0.38
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG22	4	0.38
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG23	4	0.38
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	12	0.38
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	20	0.38
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	10	0.38
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	10	0.38
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	10	0.38
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	10	0.38
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG21	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG22	1	0.38
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG23	1	0.38
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG21	1	0.38
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG22	1	0.38
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG23	1	0.38
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG21	1	0.38
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG22	1	0.38
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG23	1	0.38
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG21	1	0.38
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG22	1	0.38
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG23	1	0.38
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG21	1	0.38
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG22	1	0.38
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG23	1	0.38
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG21	1	0.38
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG22	1	0.38
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG23	1	0.38
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	10	0.38
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	1	0.38
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	1	0.38
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	1	0.38
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	2	0.38
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	2	0.38
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	2	0.38
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	19	0.37
(1,1808)	2:158:B:ASN:H	2:160:B:ALA:H	5	0.37
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	1	0.37
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	15	0.37
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	15	0.37
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	15	0.37
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	15	0.37
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	15	0.37
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	15	0.37
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	12	0.37
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	3	0.37
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	3	0.37
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	3	0.37
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	16	0.37
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	1	0.37
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD11	7	0.37
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD12	7	0.37
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD13	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD11	18	0.37
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD12	18	0.37
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD13	18	0.37
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	15	0.37
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	15	0.37
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	19	0.37
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	19	0.37
(1,395)	2:30:B:VAL:H	2:30:B:VAL:HG21	4	0.37
(1,395)	2:30:B:VAL:H	2:30:B:VAL:HG22	4	0.37
(1,395)	2:30:B:VAL:H	2:30:B:VAL:HG23	4	0.37
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	3	0.37
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	3	0.37
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	3	0.37
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	13	0.36
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	15	0.36
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	19	0.36
(1,1605)	2:142:B:ILE:HG21	2:144:B:GLU:HG3	3	0.36
(1,1605)	2:142:B:ILE:HG22	2:144:B:GLU:HG3	3	0.36
(1,1605)	2:142:B:ILE:HG23	2:144:B:GLU:HG3	3	0.36
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	3	0.36
(1,1113)	2:96:B:ASN:H	2:99:B:ARG:H	6	0.36
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD11	18	0.36
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD12	18	0.36
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD13	18	0.36
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	2	0.36
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	2	0.36
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	2	0.36
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	2	0.35
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG2	13	0.35
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG3	13	0.35
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	7	0.35
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	7	0.35
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	7	0.35
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	7	0.35
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	7	0.35
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	7	0.35
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	14	0.35
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	14	0.35
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	14	0.35
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	14	0.35
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	14	0.35
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	14	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	11	0.35
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	11	0.35
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	11	0.35
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	11	0.35
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	11	0.35
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	11	0.35
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	9	0.35
(1,1109)	2:96:B:ASN:H	2:97:B:TRP:HE1	4	0.35
(1,867)	2:74:B:ILE:HG21	2:117:B:LYS:HB3	2	0.35
(1,867)	2:74:B:ILE:HG22	2:117:B:LYS:HB3	2	0.35
(1,867)	2:74:B:ILE:HG23	2:117:B:LYS:HB3	2	0.35
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD11	4	0.35
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD12	4	0.35
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD13	4	0.35
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	15	0.35
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	15	0.35
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	15	0.35
(1,775)	2:63:B:ARG:HD2	2:64:B:ALA:H	19	0.35
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	10	0.35
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	10	0.35
(1,486)	2:37:B:ALA:H	2:39:B:GLU:H	16	0.35
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	3	0.35
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	3	0.35
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	20	0.35
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	8	0.35
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	8	0.35
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	8	0.35
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	10	0.35
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	10	0.35
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	10	0.35
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	17	0.34
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	18	0.34
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	18	0.34
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	16	0.34
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	16	0.34
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	16	0.34
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	16	0.34
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	16	0.34
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	16	0.34
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	6	0.34
(1,1113)	2:96:B:ASN:H	2:99:B:ARG:H	16	0.34
(1,1076)	2:95:B:VAL:HG11	2:96:B:ASN:HD22	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1076)	2:95:B:VAL:HG12	2:96:B:ASN:HD22	11	0.34
(1,1076)	2:95:B:VAL:HG13	2:96:B:ASN:HD22	11	0.34
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	1	0.34
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	1	0.34
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	1	0.34
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	14	0.34
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	4	0.34
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	4	0.34
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	4	0.34
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	11	0.34
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	11	0.34
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	11	0.34
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	4	0.34
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	4	0.34
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	4	0.34
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	4	0.34
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	4	0.34
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	4	0.34
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	4	0.34
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	4	0.34
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	4	0.34
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	20	0.34
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	9	0.34
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	9	0.34
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	6	0.34
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	6	0.34
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	5	0.34
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	5	0.34
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	5	0.34
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	5	0.34
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	5	0.34
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	5	0.34
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	11	0.34
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	8	0.34
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	16	0.34
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	16	0.34
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	16	0.34
(1,1)	2:1:B:MET:HA	2:3:B:GLN:H	4	0.34
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	4	0.33
(1,1507)	2:134:B:LEU:HD11	2:136:B:ASP:H	11	0.33
(1,1507)	2:134:B:LEU:HD12	2:136:B:ASP:H	11	0.33
(1,1507)	2:134:B:LEU:HD13	2:136:B:ASP:H	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	2:134:B:LEU:HD21	2:136:B:ASP:H	11	0.33
(1,1507)	2:134:B:LEU:HD22	2:136:B:ASP:H	11	0.33
(1,1507)	2:134:B:LEU:HD23	2:136:B:ASP:H	11	0.33
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	4	0.33
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	4	0.33
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	4	0.33
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	5	0.33
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	7	0.33
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	6	0.33
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	12	0.33
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	16	0.33
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	20	0.33
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	20	0.33
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	20	0.33
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD11	2	0.33
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD12	2	0.33
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD13	2	0.33
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	12	0.33
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	12	0.33
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	6	0.33
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	6	0.33
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	14	0.33
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	17	0.33
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	17	0.33
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	13	0.33
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	13	0.33
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	13	0.33
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	3	0.33
(1,1836)	2:162:B:GLU:H	2:162:B:GLU:HB2	5	0.32
(1,1793)	2:157:B:ASN:H	2:159:B:ALA:H	3	0.32
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	8	0.32
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	8	0.32
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	17	0.32
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	17	0.32
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	17	0.32
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	17	0.32
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	17	0.32
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	17	0.32
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	8	0.32
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	8	0.32
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	8	0.32
(1,1109)	2:96:B:ASN:H	2:97:B:TRP:HE1	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	7	0.32
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	9	0.32
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	9	0.32
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	9	0.32
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	4	0.32
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	10	0.32
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	10	0.32
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	10	0.32
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	17	0.32
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	17	0.32
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	17	0.32
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	16	0.32
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	16	0.32
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	16	0.32
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	16	0.32
(1,542)	2:41:B:THR:H	2:42:B:GLU:H	15	0.32
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	17	0.32
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	17	0.32
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	14	0.32
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	4	0.32
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	4	0.32
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	4	0.32
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	7	0.32
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	7	0.32
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	7	0.32
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	2	0.31
(1,1911)	2:169:B:ARG:HD2	2:170:B:LEU:H	18	0.31
(1,1911)	2:169:B:ARG:HD3	2:170:B:LEU:H	18	0.31
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	13	0.31
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	14	0.31
(1,1847)	2:164:B:ARG:H	2:164:B:ARG:HB3	10	0.31
(1,1847)	2:164:B:ARG:H	2:164:B:ARG:HB3	16	0.31
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	19	0.31
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	19	0.31
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	19	0.31
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	19	0.31
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	19	0.31
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	19	0.31
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	2	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	3	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	3	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	3	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	3	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	3	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	12	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	12	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	12	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	12	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	12	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	12	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	18	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	18	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	18	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	18	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	18	0.31
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	18	0.31
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	7	0.31
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	20	0.31
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	20	0.31
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	20	0.31
(1,1096)	2:96:B:ASN:HD21	2:99:B:ARG:H	1	0.31
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG21	10	0.31
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG22	10	0.31
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG23	10	0.31
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG21	10	0.31
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG22	10	0.31
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG23	10	0.31
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG21	10	0.31
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG22	10	0.31
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG23	10	0.31
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG21	10	0.31
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG22	10	0.31
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG23	10	0.31
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG21	10	0.31
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG22	10	0.31
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG23	10	0.31
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG21	10	0.31
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG22	10	0.31
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG23	10	0.31
(1,1044)	2:92:B:ARG:H	2:92:B:ARG:HB2	9	0.31
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	2	0.31
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	12	0.31
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	19	0.31
(1,1030)	2:92:B:ARG:HB3	2:94:B:GLY:H	17	0.31
(1,902)	2:81:B:GLN:HA	2:85:B:GLN:HB2	18	0.31
(1,902)	2:81:B:GLN:HA	2:85:B:GLN:HB3	18	0.31
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	10	0.31
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	10	0.31
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	10	0.31
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	10	0.31
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	10	0.31
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	10	0.31
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD11	1	0.31
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD12	1	0.31
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD13	1	0.31
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD11	6	0.31
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD12	6	0.31
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD13	6	0.31
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	4	0.31
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	9	0.31
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	9	0.31
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	5	0.31
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	5	0.31
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	5	0.31
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	5	0.31
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	19	0.31
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	19	0.31
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	10	0.31
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	10	0.31
(1,425)	2:33:B:ASN:H	2:33:B:ASN:HB2	8	0.31
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	20	0.31
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	11	0.31
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	11	0.31
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	19	0.31
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	19	0.31
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	11	0.31
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	19	0.31
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	19	0.31
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	19	0.31
(1,2052)	1:320:A:SER:HA	1:320:A:SER:HB2	10	0.3
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG21	17	0.3
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG22	17	0.3
(1,1949)	1:313:A:THR:H	1:313:A:THR:HG23	17	0.3
(1,1911)	2:169:B:ARG:HD2	2:170:B:LEU:H	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1911)	2:169:B:ARG:HD3	2:170:B:LEU:H	20	0.3
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	11	0.3
(1,1601)	2:142:B:ILE:HD11	2:147:B:GLY:H	17	0.3
(1,1601)	2:142:B:ILE:HD12	2:147:B:GLY:H	17	0.3
(1,1601)	2:142:B:ILE:HD13	2:147:B:GLY:H	17	0.3
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	15	0.3
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	15	0.3
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	15	0.3
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	15	0.3
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	15	0.3
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	15	0.3
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	14	0.3
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	14	0.3
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	14	0.3
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	14	0.3
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	14	0.3
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	14	0.3
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	11	0.3
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	19	0.3
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	9	0.3
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	9	0.3
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	9	0.3
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	12	0.3
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	12	0.3
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	12	0.3
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	2	0.3
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	2	0.3
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	2	0.3
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD11	6	0.3
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD12	6	0.3
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD13	6	0.3
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG21	19	0.3
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG22	19	0.3
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG23	19	0.3
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG21	19	0.3
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG22	19	0.3
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG23	19	0.3
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG21	19	0.3
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG22	19	0.3
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG23	19	0.3
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG21	19	0.3
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG22	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG23	19	0.3
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG21	19	0.3
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG22	19	0.3
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG23	19	0.3
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG21	19	0.3
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG22	19	0.3
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG23	19	0.3
(1,1076)	2:95:B:VAL:HG11	2:96:B:ASN:HD22	17	0.3
(1,1076)	2:95:B:VAL:HG12	2:96:B:ASN:HD22	17	0.3
(1,1076)	2:95:B:VAL:HG13	2:96:B:ASN:HD22	17	0.3
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA2	1	0.3
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA3	1	0.3
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA2	1	0.3
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA3	1	0.3
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA2	1	0.3
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA3	1	0.3
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	16	0.3
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	16	0.3
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	16	0.3
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	16	0.3
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	16	0.3
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	16	0.3
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	16	0.3
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	16	0.3
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	16	0.3
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	5	0.3
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	5	0.3
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	5	0.3
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	5	0.3
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	5	0.3
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	5	0.3
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	20	0.3
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	20	0.3
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	20	0.3
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	20	0.3
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	20	0.3
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	20	0.3
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	10	0.3
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	9	0.3
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	9	0.3
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	9	0.3
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD11	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD12	13	0.3
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD13	13	0.3
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	2	0.3
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	2	0.3
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	17	0.3
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	17	0.3
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	2	0.3
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	2	0.3
(1,530)	2:40:B:GLY:H	2:42:B:GLU:H	15	0.3
(1,507)	2:39:B:GLU:HG2	2:41:B:THR:HA	19	0.3
(1,507)	2:39:B:GLU:HG3	2:41:B:THR:HA	19	0.3
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB2	17	0.3
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB3	17	0.3
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	7	0.3
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	7	0.3
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	4	0.3
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	4	0.3
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	19	0.3
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	19	0.3
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	4	0.3
(1,211)	2:17:B:LEU:HD11	2:22:B:TYR:H	7	0.3
(1,211)	2:17:B:LEU:HD12	2:22:B:TYR:H	7	0.3
(1,211)	2:17:B:LEU:HD13	2:22:B:TYR:H	7	0.3
(1,211)	2:17:B:LEU:HD21	2:22:B:TYR:H	7	0.3
(1,211)	2:17:B:LEU:HD22	2:22:B:TYR:H	7	0.3
(1,211)	2:17:B:LEU:HD23	2:22:B:TYR:H	7	0.3
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	6	0.3
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	6	0.3
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	6	0.3
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	13	0.29
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	13	0.29
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	13	0.29
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	6	0.29
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	6	0.29
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	10	0.29
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	9	0.29
(1,1836)	2:162:B:GLU:H	2:162:B:GLU:HB2	4	0.29
(1,1606)	2:142:B:ILE:HG21	2:144:B:GLU:HG2	18	0.29
(1,1606)	2:142:B:ILE:HG22	2:144:B:GLU:HG2	18	0.29
(1,1606)	2:142:B:ILE:HG23	2:144:B:GLU:HG2	18	0.29
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	15	0.29
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD21	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD22	10	0.29
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD23	10	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	9	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	9	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	9	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	9	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	9	0.29
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	9	0.29
(1,1402)	2:121:B:VAL:H	2:121:B:VAL:HB	1	0.29
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	4	0.29
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	13	0.29
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	12	0.29
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	12	0.29
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	12	0.29
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	13	0.29
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	13	0.29
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	13	0.29
(1,1119)	2:97:B:TRP:H	2:97:B:TRP:HZ3	11	0.29
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	19	0.29
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	7	0.29
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	7	0.29
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	7	0.29
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG2	18	0.29
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG3	18	0.29
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	8	0.29
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	18	0.29
(1,1030)	2:92:B:ARG:HB3	2:94:B:GLY:H	18	0.29
(1,867)	2:74:B:ILE:HG21	2:117:B:LYS:HB3	9	0.29
(1,867)	2:74:B:ILE:HG22	2:117:B:LYS:HB3	9	0.29
(1,867)	2:74:B:ILE:HG23	2:117:B:LYS:HB3	9	0.29
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	1	0.29
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	1	0.29
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	1	0.29
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	1	0.29
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	1	0.29
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	1	0.29
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	20	0.29
(1,440)	2:34:B:ARG:H	2:34:B:ARG:HD2	19	0.29
(1,440)	2:34:B:ARG:H	2:34:B:ARG:HD3	19	0.29
(1,394)	2:30:B:VAL:H	2:30:B:VAL:HG11	13	0.29
(1,394)	2:30:B:VAL:H	2:30:B:VAL:HG12	13	0.29
(1,394)	2:30:B:VAL:H	2:30:B:VAL:HG13	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	2:17:B:LEU:HG	2:18:B:SER:H	7	0.29
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	20	0.29
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	20	0.29
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	20	0.29
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	9	0.28
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	17	0.28
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	7	0.28
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	3	0.28
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	2	0.28
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	2	0.28
(1,1847)	2:164:B:ARG:H	2:164:B:ARG:HB3	7	0.28
(1,1836)	2:162:B:GLU:H	2:162:B:GLU:HB2	11	0.28
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	19	0.28
(1,1793)	2:157:B:ASN:H	2:159:B:ALA:H	14	0.28
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	5	0.28
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	5	0.28
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	5	0.28
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	12	0.28
(1,1605)	2:142:B:ILE:HG21	2:144:B:GLU:HG3	8	0.28
(1,1605)	2:142:B:ILE:HG22	2:144:B:GLU:HG3	8	0.28
(1,1605)	2:142:B:ILE:HG23	2:144:B:GLU:HG3	8	0.28
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	5	0.28
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	5	0.28
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	5	0.28
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	5	0.28
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	5	0.28
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	5	0.28
(1,1402)	2:121:B:VAL:H	2:121:B:VAL:HB	17	0.28
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	3	0.28
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	3	0.28
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	3	0.28
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	20	0.28
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	20	0.28
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	20	0.28
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	1	0.28
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	6	0.28
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	6	0.28
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	6	0.28
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	16	0.28
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	16	0.28
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	16	0.28
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	20	0.28
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	20	0.28
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	20	0.28
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	20	0.28
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	20	0.28
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	18	0.28
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	18	0.28
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	18	0.28
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	18	0.28
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	18	0.28
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	18	0.28
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	18	0.28
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	18	0.28
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	18	0.28
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	18	0.28
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	14	0.28
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	14	0.28
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	14	0.28
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	14	0.28
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	9	0.28
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	9	0.28
(1,507)	2:39:B:GLU:HG2	2:41:B:THR:HA	8	0.28
(1,507)	2:39:B:GLU:HG3	2:41:B:THR:HA	8	0.28
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	17	0.28
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	17	0.28
(1,425)	2:33:B:ASN:H	2:33:B:ASN:HB2	10	0.28
(1,425)	2:33:B:ASN:H	2:33:B:ASN:HB2	15	0.28
(1,272)	2:20:B:LYS:HD2	2:22:B:TYR:H	12	0.28
(1,272)	2:20:B:LYS:HD3	2:22:B:TYR:H	12	0.28
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	15	0.28
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	15	0.28
(1,215)	2:17:B:LEU:HG	2:18:B:SER:H	4	0.28
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	1	0.28
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	1	0.28
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	1	0.28
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	14	0.28
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	14	0.28
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	14	0.28
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	18	0.27
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	18	0.27
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	18	0.27
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	13	0.27
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	20	0.27
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	20	0.27
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	20	0.27
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	20	0.27
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	20	0.27
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	20	0.27
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	13	0.27
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	15	0.27
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	18	0.27
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	6	0.27
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	6	0.27
(1,1847)	2:164:B:ARG:H	2:164:B:ARG:HB3	14	0.27
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	1	0.27
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	3	0.27
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	10	0.27
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	12	0.27
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	20	0.27
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	9	0.27
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	9	0.27
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	7	0.27
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	7	0.27
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	7	0.27
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	2	0.27
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	3	0.27
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	6	0.27
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	18	0.27
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	10	0.27
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	10	0.27
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	10	0.27
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	10	0.27
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	10	0.27
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	10	0.27
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	8	0.27
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	2	0.27
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	2	0.27
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	2	0.27
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	2	0.27
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	2	0.27
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	2	0.27
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	5	0.27
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	18	0.27
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	15	0.27
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	15	0.27
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	15	0.27
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	2	0.27
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	5	0.27
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	5	0.27
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	5	0.27
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	10	0.27
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	10	0.27
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	10	0.27
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	11	0.27
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	11	0.27
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	11	0.27
(1,1116)	2:97:B:TRP:H	2:97:B:TRP:HE1	6	0.27
(1,1108)	2:96:B:ASN:H	2:97:B:TRP:HB2	16	0.27
(1,1108)	2:96:B:ASN:H	2:97:B:TRP:HB3	16	0.27
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	8	0.27
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	8	0.27
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	8	0.27
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	8	0.27
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	8	0.27
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	8	0.27
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	4	0.27
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	5	0.27
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	15	0.27
(1,1030)	2:92:B:ARG:HB3	2:94:B:GLY:H	9	0.27
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD11	4	0.27
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD12	4	0.27
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD13	4	0.27
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	13	0.27
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	13	0.27
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	13	0.27
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	13	0.27
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	13	0.27
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	13	0.27
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	15	0.27
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	15	0.27
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	15	0.27
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	15	0.27
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	15	0.27
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD11	2	0.27
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD12	2	0.27
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD13	2	0.27
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	7	0.27
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	13	0.27
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	13	0.27
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	13	0.27
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	16	0.27
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	16	0.27
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	16	0.27
(1,774)	2:63:B:ARG:HD3	2:64:B:ALA:H	9	0.27
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	10	0.27
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	17	0.27
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	17	0.27
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	8	0.27
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	8	0.27
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	8	0.27
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	8	0.27
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	8	0.27
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	8	0.27
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	1	0.27
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	1	0.27
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	12	0.27
(1,458)	2:35:B:THR:H	2:35:B:THR:HB	13	0.27
(1,425)	2:33:B:ASN:H	2:33:B:ASN:HB2	2	0.27
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	3	0.27
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	6	0.27
(1,333)	2:25:B:SER:HB2	2:26:B:GLN:H	6	0.27
(1,333)	2:25:B:SER:HB3	2:26:B:GLN:H	6	0.27
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	10	0.27
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	10	0.27
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	18	0.27
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	18	0.27
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	18	0.27
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	18	0.27
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	19	0.27
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	19	0.27
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	20	0.27
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	20	0.27
(1,74)	2:8:B:LEU:HG	2:10:B:VAL:H	11	0.27
(1,2138)	2:101:B:VAL:HB	1:319:A:TRP:HH2	13	0.26
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	10	0.26
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	10	0.26
(1,2102)	1:323:A:GLU:H	1:321:A:SER:HB2	17	0.26
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	2	0.26
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	5	0.26
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	7	0.26
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	10	0.26
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	12	0.26
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	18	0.26
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	19	0.26
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	15	0.26
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	17	0.26
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	19	0.26
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	3	0.26
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	4	0.26
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	9	0.26
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	10	0.26
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB2	6	0.26
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB3	6	0.26
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	11	0.26
(1,1847)	2:164:B:ARG:H	2:164:B:ARG:HB3	8	0.26
(1,1847)	2:164:B:ARG:H	2:164:B:ARG:HB3	19	0.26
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	13	0.26
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	9	0.26
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	14	0.26
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	16	0.26
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	7	0.26
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	7	0.26
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	17	0.26
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	17	0.26
(1,1735)	2:152:B:VAL:HG21	2:156:B:GLY:H	1	0.26
(1,1735)	2:152:B:VAL:HG22	2:156:B:GLY:H	1	0.26
(1,1735)	2:152:B:VAL:HG23	2:156:B:GLY:H	1	0.26
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	3	0.26
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	3	0.26
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	3	0.26
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	16	0.26
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	16	0.26
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	16	0.26
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	8	0.26
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	11	0.26
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	11	0.26
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	15	0.26
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	15	0.26
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	15	0.26
(1,1655)	2:145:B:ASN:H	2:146:B:GLY:H	18	0.26
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	6	0.26
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	9	0.26
(1,1542)	2:137:B:HIS:H	2:138:B:LEU:HD11	2	0.26
(1,1542)	2:137:B:HIS:H	2:138:B:LEU:HD12	2	0.26
(1,1542)	2:137:B:HIS:H	2:138:B:LEU:HD13	2	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	4	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	4	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	4	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	4	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	4	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	4	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	17	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	17	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	17	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	17	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	17	0.26
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	17	0.26
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	12	0.26
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	12	0.26
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	12	0.26
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	12	0.26
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	12	0.26
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	12	0.26
(1,1382)	2:119:B:MET:HA	2:120:B:GLN:H	14	0.26
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	17	0.26
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	4	0.26
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	4	0.26
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	4	0.26
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG12	15	0.26
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG13	15	0.26
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG12	15	0.26
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG13	15	0.26
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE1	18	0.26
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE2	18	0.26
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE1	18	0.26
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE2	18	0.26
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	5	0.26
(1,1109)	2:96:B:ASN:H	2:97:B:TRP:HE1	8	0.26
(1,1044)	2:92:B:ARG:H	2:92:B:ARG:HB2	11	0.26
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	20	0.26
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	13	0.26
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	8	0.26
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	8	0.26
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	8	0.26
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	8	0.26
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	8	0.26
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	8	0.26
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	8	0.26
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	8	0.26
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	8	0.26
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	11	0.26
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	11	0.26
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	11	0.26
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	11	0.26
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	11	0.26
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	11	0.26
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD11	9	0.26
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD12	9	0.26
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD13	9	0.26
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	1	0.26
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	3	0.26
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	4	0.26
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	6	0.26
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	6	0.26
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	6	0.26
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	6	0.26
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	6	0.26
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	6	0.26
(1,542)	2:41:B:THR:H	2:42:B:GLU:H	10	0.26
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	12	0.26
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	18	0.26
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	18	0.26
(1,425)	2:33:B:ASN:H	2:33:B:ASN:HB2	7	0.26
(1,425)	2:33:B:ASN:H	2:33:B:ASN:HB2	14	0.26
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	12	0.26
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	16	0.26
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB2	4	0.26
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB3	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	10	0.26
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	10	0.26
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	10	0.26
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	3	0.26
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	3	0.26
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	9	0.26
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	9	0.26
(1,275)	2:20:B:LYS:HG2	2:22:B:TYR:H	10	0.26
(1,275)	2:20:B:LYS:HG3	2:22:B:TYR:H	10	0.26
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	12	0.26
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	12	0.26
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	13	0.26
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	13	0.26
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	15	0.26
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	15	0.26
(1,127)	2:11:B:ASP:HB2	2:47:B:LYS:HD2	6	0.26
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	18	0.25
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	18	0.25
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	18	0.25
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	1	0.25
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	4	0.25
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	16	0.25
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	17	0.25
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	14	0.25
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	16	0.25
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	18	0.25
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	3	0.25
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	11	0.25
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	11	0.25
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	11	0.25
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	11	0.25
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	2	0.25
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	18	0.25
(1,1866)	2:165:B:LYS:H	2:165:B:LYS:HB2	13	0.25
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	1	0.25
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	8	0.25
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	13	0.25
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	17	0.25
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	7	0.25
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	4	0.25
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	19	0.25
(1,1809)	2:158:B:ASN:H	2:161:B:ALA:H	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1808)	2:158:B:ASN:H	2:160:B:ALA:H	3	0.25
(1,1807)	2:158:B:ASN:H	2:159:B:ALA:H	3	0.25
(1,1786)	2:156:B:GLY:H	2:158:B:ASN:H	14	0.25
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	16	0.25
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	16	0.25
(1,1738)	2:152:B:VAL:HG11	2:155:B:TYR:HE1	8	0.25
(1,1738)	2:152:B:VAL:HG11	2:155:B:TYR:HE2	8	0.25
(1,1738)	2:152:B:VAL:HG12	2:155:B:TYR:HE1	8	0.25
(1,1738)	2:152:B:VAL:HG12	2:155:B:TYR:HE2	8	0.25
(1,1738)	2:152:B:VAL:HG13	2:155:B:TYR:HE1	8	0.25
(1,1738)	2:152:B:VAL:HG13	2:155:B:TYR:HE2	8	0.25
(1,1738)	2:152:B:VAL:HG21	2:155:B:TYR:HE1	8	0.25
(1,1738)	2:152:B:VAL:HG21	2:155:B:TYR:HE2	8	0.25
(1,1738)	2:152:B:VAL:HG22	2:155:B:TYR:HE1	8	0.25
(1,1738)	2:152:B:VAL:HG22	2:155:B:TYR:HE2	8	0.25
(1,1738)	2:152:B:VAL:HG23	2:155:B:TYR:HE1	8	0.25
(1,1738)	2:152:B:VAL:HG23	2:155:B:TYR:HE2	8	0.25
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	15	0.25
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	15	0.25
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	15	0.25
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	15	0.25
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	15	0.25
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	15	0.25
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	9	0.25
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	9	0.25
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	9	0.25
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	1	0.25
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	13	0.25
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	15	0.25
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	16	0.25
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	2	0.25
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	2	0.25
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	2	0.25
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	3	0.25
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	3	0.25
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	3	0.25
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	16	0.25
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	16	0.25
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	16	0.25
(1,1670)	2:148:B:TRP:HB2	2:150:B:THR:H	5	0.25
(1,1670)	2:148:B:TRP:HB3	2:150:B:THR:H	5	0.25
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	17	0.25
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	18	0.25
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	18	0.25
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	18	0.25
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	18	0.25
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	18	0.25
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	18	0.25
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	12	0.25
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	5	0.25
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	5	0.25
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	5	0.25
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	13	0.25
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	13	0.25
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	13	0.25
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	9	0.25
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	17	0.25
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE1	8	0.25
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE2	8	0.25
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE1	8	0.25
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE2	8	0.25
(1,1113)	2:96:B:ASN:H	2:99:B:ARG:H	14	0.25
(1,1095)	2:96:B:ASN:HD21	2:100:B:ILE:H	11	0.25
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	12	0.25
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	12	0.25
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	12	0.25
(1,1043)	2:92:B:ARG:H	2:92:B:ARG:HB3	1	0.25
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	14	0.25
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	20	0.25
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	8	0.25
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	8	0.25
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	8	0.25
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	8	0.25
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	8	0.25
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	8	0.25
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	19	0.25
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	19	0.25
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	19	0.25
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	9	0.25
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	9	0.25
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	9	0.25
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	9	0.25
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	9	0.25
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	9	0.25
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	9	0.25
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	9	0.25
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	2	0.25
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	2	0.25
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	9	0.25
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	9	0.25
(1,774)	2:63:B:ARG:HD3	2:64:B:ALA:H	4	0.25
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	2	0.25
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	12	0.25
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	15	0.25
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	20	0.25
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	1	0.25
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	6	0.25
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	1	0.25
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	1	0.25
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	1	0.25
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	11	0.25
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	11	0.25
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	11	0.25
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	11	0.25
(1,627)	2:47:B:LYS:H	2:47:B:LYS:HE3	3	0.25
(1,536)	2:41:B:THR:HG1	2:45:B:ALA:H	2	0.25
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	7	0.25
(1,451)	2:35:B:THR:HG1	2:36:B:GLU:H	9	0.25
(1,445)	2:35:B:THR:HA	2:36:B:GLU:HB3	19	0.25
(1,404)	2:31:B:GLU:H	2:31:B:GLU:HB2	13	0.25
(1,380)	2:29:B:ASP:H	2:30:B:VAL:HG21	4	0.25
(1,380)	2:29:B:ASP:H	2:30:B:VAL:HG22	4	0.25
(1,380)	2:29:B:ASP:H	2:30:B:VAL:HG23	4	0.25
(1,376)	2:29:B:ASP:HA	2:30:B:VAL:H	6	0.25
(1,266)	2:20:B:LYS:HB3	2:22:B:TYR:H	16	0.25
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	16	0.25
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	20	0.25
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	4	0.25
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	4	0.25
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	10	0.25
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	10	0.25
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	14	0.25
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	14	0.25
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	5	0.25
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	5	0.25
(1,74)	2:8:B:LEU:HG	2:10:B:VAL:H	15	0.25
(1,2152)	2:155:B:TYR:HD1	1:314:A:THR:HB	14	0.24
(1,2152)	2:155:B:TYR:HD2	1:314:A:THR:HB	14	0.24
(1,2135)	2:57:B:PHE:HB3	1:319:A:TRP:HA	20	0.24
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	1	0.24
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	1	0.24
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	1	0.24
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	15	0.24
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	15	0.24
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	15	0.24
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	8	0.24
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	14	0.24
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	15	0.24
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	20	0.24
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	2	0.24
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	4	0.24
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	5	0.24
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	9	0.24
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	10	0.24
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	9	0.24
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	9	0.24
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	9	0.24
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	9	0.24
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	9	0.24
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	9	0.24
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	2	0.24
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	16	0.24
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	1	0.24
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	8	0.24
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	18	0.24
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	6	0.24
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	9	0.24
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	2	0.24
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	7	0.24
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	18	0.24
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	20	0.24
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	5	0.24
(1,1808)	2:158:B:ASN:H	2:160:B:ALA:H	14	0.24
(1,1807)	2:158:B:ASN:H	2:159:B:ALA:H	14	0.24
(1,1788)	2:157:B:ASN:HB2	2:159:B:ALA:HA	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	19	0.24
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	19	0.24
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	20	0.24
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	20	0.24
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	12	0.24
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	12	0.24
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	12	0.24
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	10	0.24
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	11	0.24
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	14	0.24
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	13	0.24
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	13	0.24
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	13	0.24
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	19	0.24
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	19	0.24
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	19	0.24
(1,1634)	2:144:B:GLU:HG2	2:146:B:GLY:H	18	0.24
(1,1601)	2:142:B:ILE:HD11	2:147:B:GLY:H	1	0.24
(1,1601)	2:142:B:ILE:HD12	2:147:B:GLY:H	1	0.24
(1,1601)	2:142:B:ILE:HD13	2:147:B:GLY:H	1	0.24
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	8	0.24
(1,1551)	2:138:B:LEU:HD11	2:139:B:GLU:H	11	0.24
(1,1551)	2:138:B:LEU:HD12	2:139:B:GLU:H	11	0.24
(1,1551)	2:138:B:LEU:HD13	2:139:B:GLU:H	11	0.24
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	16	0.24
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	13	0.24
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	13	0.24
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	13	0.24
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	13	0.24
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	13	0.24
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	13	0.24
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	10	0.24
(1,1402)	2:121:B:VAL:H	2:121:B:VAL:HB	14	0.24
(1,1382)	2:119:B:MET:HA	2:120:B:GLN:H	2	0.24
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	8	0.24
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	19	0.24
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	19	0.24
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	19	0.24
(1,1183)	2:103:B:PHE:HB2	2:105:B:SER:HB2	20	0.24
(1,1183)	2:103:B:PHE:HB2	2:105:B:SER:HB3	20	0.24
(1,1183)	2:103:B:PHE:HB3	2:105:B:SER:HB2	20	0.24
(1,1183)	2:103:B:PHE:HB3	2:105:B:SER:HB3	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD1	6	0.24
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD2	6	0.24
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	2	0.24
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	2	0.24
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	18	0.24
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	18	0.24
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD11	18	0.24
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD12	18	0.24
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD13	18	0.24
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	15	0.24
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	15	0.24
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	15	0.24
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	14	0.24
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	14	0.24
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	14	0.24
(1,1044)	2:92:B:ARG:H	2:92:B:ARG:HB2	17	0.24
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG2	5	0.24
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG3	5	0.24
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	9	0.24
(1,1005)	2:90:B:LEU:HG	2:91:B:PHE:H	11	0.24
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	3	0.24
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	6	0.24
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	6	0.24
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	6	0.24
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	6	0.24
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	6	0.24
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	6	0.24
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	3	0.24
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	3	0.24
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	3	0.24
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	3	0.24
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	3	0.24
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	3	0.24
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	13	0.24
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	13	0.24
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	13	0.24
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	13	0.24
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	13	0.24
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	13	0.24
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	8	0.24
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	11	0.24
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	6	0.24
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	6	0.24
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	14	0.24
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	14	0.24
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	14	0.24
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	7	0.24
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	7	0.24
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	7	0.24
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	2	0.24
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	2	0.24
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	16	0.24
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	8	0.24
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	7	0.24
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	7	0.24
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	7	0.24
(1,551)	2:42:B:GLU:H	2:42:B:GLU:HG2	12	0.24
(1,507)	2:39:B:GLU:HG2	2:41:B:THR:HA	10	0.24
(1,507)	2:39:B:GLU:HG3	2:41:B:THR:HA	10	0.24
(1,503)	2:39:B:GLU:HB2	2:41:B:THR:HB	14	0.24
(1,503)	2:39:B:GLU:HB3	2:41:B:THR:HB	14	0.24
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	4	0.24
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	4	0.24
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	8	0.24
(1,486)	2:37:B:ALA:H	2:39:B:GLU:H	14	0.24
(1,444)	2:34:B:ARG:H	2:35:B:THR:H	19	0.24
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	4	0.24
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	5	0.24
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	17	0.24
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	19	0.24
(1,404)	2:31:B:GLU:H	2:31:B:GLU:HB2	17	0.24
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	16	0.24
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	16	0.24
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	16	0.24
(1,250)	2:19:B:GLN:HB2	2:21:B:GLY:H	6	0.24
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	17	0.24
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	2	0.24
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	2	0.24
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD11	8	0.24
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD12	8	0.24
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD13	8	0.24
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD21	8	0.24
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD22	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD23	8	0.24
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD11	8	0.24
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD12	8	0.24
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD13	8	0.24
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD21	8	0.24
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD22	8	0.24
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD23	8	0.24
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	13	0.24
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	13	0.24
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	13	0.24
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	9	0.23
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	9	0.23
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	9	0.23
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	13	0.23
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	7	0.23
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	14	0.23
(1,2046)	1:319:A:TRP:H	1:319:A:TRP:HB3	11	0.23
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	7	0.23
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	13	0.23
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	14	0.23
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	20	0.23
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	4	0.23
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	8	0.23
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	1	0.23
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	12	0.23
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	1	0.23
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	5	0.23
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	19	0.23
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	5	0.23
(1,1913)	2:169:B:ARG:H	2:169:B:ARG:HB2	11	0.23
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	17	0.23
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	19	0.23
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	20	0.23
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB2	10	0.23
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB3	10	0.23
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	2	0.23
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	15	0.23
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	4	0.23
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	7	0.23
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	10	0.23
(1,1835)	2:162:B:GLU:H	2:162:B:GLU:HB3	6	0.23
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	11	0.23
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB2	12	0.23
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB3	12	0.23
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	3	0.23
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	2	0.23
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	2	0.23
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	2	0.23
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	2	0.23
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	2	0.23
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	2	0.23
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	19	0.23
(1,1703)	2:150:B:THR:H	2:150:B:THR:HB	20	0.23
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	19	0.23
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD21	20	0.23
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD22	20	0.23
(1,1543)	2:137:B:HIS:H	2:138:B:LEU:HD23	20	0.23
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	1	0.23
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	5	0.23
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	9	0.23
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	17	0.23
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG11	11	0.23
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG12	11	0.23
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG13	11	0.23
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD1	18	0.23
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD2	18	0.23
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	15	0.23
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	15	0.23
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	20	0.23
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	20	0.23
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	8	0.23
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	8	0.23
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	8	0.23
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG2	6	0.23
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG3	6	0.23
(1,1030)	2:92:B:ARG:HB3	2:94:B:GLY:H	11	0.23
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	18	0.23
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	18	0.23
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	18	0.23
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	14	0.23
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	14	0.23
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	14	0.23
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	14	0.23
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	14	0.23
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	17	0.23
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	17	0.23
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	17	0.23
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	17	0.23
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	17	0.23
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	17	0.23
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG21	4	0.23
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG22	4	0.23
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG23	4	0.23
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG21	4	0.23
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG22	4	0.23
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG23	4	0.23
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG21	4	0.23
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG22	4	0.23
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG23	4	0.23
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	7	0.23
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	12	0.23
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	15	0.23
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	18	0.23
(1,775)	2:63:B:ARG:HD2	2:64:B:ALA:H	20	0.23
(1,774)	2:63:B:ARG:HD3	2:64:B:ALA:H	18	0.23
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	10	0.23
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	10	0.23
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	14	0.23
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	20	0.23
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	20	0.23
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	20	0.23
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	6	0.23
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	6	0.23
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	6	0.23
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	6	0.23
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	6	0.23
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	6	0.23
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	6	0.23
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	6	0.23
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	6	0.23
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	10	0.23
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	10	0.23
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	10	0.23
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	2	0.23
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	2	0.23
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	12	0.23
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	12	0.23
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	12	0.23
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	8	0.23
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	16	0.23
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	17	0.23
(1,530)	2:40:B:GLY:H	2:42:B:GLU:H	4	0.23
(1,530)	2:40:B:GLY:H	2:42:B:GLU:H	11	0.23
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	4	0.23
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	9	0.23
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	9	0.23
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	13	0.23
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	16	0.23
(1,449)	2:35:B:THR:HA	2:36:B:GLU:H	1	0.23
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	1	0.23
(1,404)	2:31:B:GLU:H	2:31:B:GLU:HB2	16	0.23
(1,376)	2:29:B:ASP:HA	2:30:B:VAL:H	18	0.23
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	18	0.23
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	18	0.23
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	8	0.23
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	8	0.23
(1,266)	2:20:B:LYS:HB3	2:22:B:TYR:H	6	0.23
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	1	0.23
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	7	0.23
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	18	0.23
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	19	0.23
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	13	0.23
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	3	0.23
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	3	0.23
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	13	0.23
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	13	0.23
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	3	0.23
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	3	0.23
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	16	0.23
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	16	0.23
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	11	0.23
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	11	0.23
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	11	0.23
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	15	0.23
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	15	0.23
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	2	0.23
(1,29)	2:4:B:SER:H	2:8:B:LEU:H	3	0.23
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD11	16	0.22
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD12	16	0.22
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD13	16	0.22
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD11	16	0.22
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD12	16	0.22
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD13	16	0.22
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	4	0.22
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	4	0.22
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	4	0.22
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	15	0.22
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	16	0.22
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	17	0.22
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	2	0.22
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	6	0.22
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	8	0.22
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	13	0.22
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	13	0.22
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	13	0.22
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	1	0.22
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	3	0.22
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	8	0.22
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	15	0.22
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	16	0.22
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	18	0.22
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	1	0.22
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	2	0.22
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	10	0.22
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	11	0.22
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	5	0.22
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	6	0.22
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	19	0.22
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	11	0.22
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	1	0.22
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	1	0.22
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	1	0.22
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	1	0.22
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	3	0.22
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	3	0.22
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	3	0.22
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	3	0.22
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	3	0.22
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	13	0.22
(1,1916)	2:169:B:ARG:H	2:169:B:ARG:HG3	4	0.22
(1,1916)	2:169:B:ARG:H	2:169:B:ARG:HG3	13	0.22
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	12	0.22
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	13	0.22
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	14	0.22
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	16	0.22
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB2	16	0.22
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB3	16	0.22
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	20	0.22
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG2	5	0.22
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG3	5	0.22
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG2	15	0.22
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG3	15	0.22
(1,1861)	2:165:B:LYS:HD2	2:166:B:GLY:H	17	0.22
(1,1861)	2:165:B:LYS:HD3	2:166:B:GLY:H	17	0.22
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	8	0.22
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	11	0.22
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	16	0.22
(1,1838)	2:162:B:GLU:H	2:162:B:GLU:HG2	15	0.22
(1,1838)	2:162:B:GLU:H	2:162:B:GLU:HG3	15	0.22
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	1	0.22
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	3	0.22
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	9	0.22
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	12	0.22
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	17	0.22
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	8	0.22
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	19	0.22
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	7	0.22
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	14	0.22
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	15	0.22
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	18	0.22
(1,1809)	2:158:B:ASN:H	2:161:B:ALA:H	3	0.22
(1,1809)	2:158:B:ASN:H	2:161:B:ALA:H	6	0.22
(1,1788)	2:157:B:ASN:HB2	2:159:B:ALA:HA	15	0.22
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	13	0.22
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	13	0.22
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	4	0.22
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	4	0.22
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	10	0.22
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	10	0.22
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	10	0.22
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	20	0.22
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	20	0.22
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	20	0.22
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	12	0.22
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	12	0.22
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	12	0.22
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	14	0.22
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	14	0.22
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	14	0.22
(1,1598)	2:142:B:ILE:HD11	2:146:B:GLY:H	4	0.22
(1,1598)	2:142:B:ILE:HD12	2:146:B:GLY:H	4	0.22
(1,1598)	2:142:B:ILE:HD13	2:146:B:GLY:H	4	0.22
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	9	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	3	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	3	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	3	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	3	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	3	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	3	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	5	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	5	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	5	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	5	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	5	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	5	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	14	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	14	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	14	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	14	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	14	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	14	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	15	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	15	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	15	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	15	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	15	0.22
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	15	0.22
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	13	0.22
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	18	0.22
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	1	0.22
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	6	0.22
(1,1391)	2:119:B:MET:H	2:121:B:VAL:H	16	0.22
(1,1382)	2:119:B:MET:HA	2:120:B:GLN:H	16	0.22
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	15	0.22
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	16	0.22
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG12	11	0.22
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG13	11	0.22
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG12	11	0.22
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG13	11	0.22
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG12	14	0.22
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG13	14	0.22
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG12	14	0.22
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG13	14	0.22
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD1	12	0.22
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD2	12	0.22
(1,1044)	2:92:B:ARG:H	2:92:B:ARG:HB2	18	0.22
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	12	0.22
(1,931)	2:85:B:GLN:HB2	2:86:B:VAL:HB	18	0.22
(1,931)	2:85:B:GLN:HB3	2:86:B:VAL:HB	18	0.22
(1,867)	2:74:B:ILE:HG21	2:117:B:LYS:HB3	6	0.22
(1,867)	2:74:B:ILE:HG22	2:117:B:LYS:HB3	6	0.22
(1,867)	2:74:B:ILE:HG23	2:117:B:LYS:HB3	6	0.22
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	6	0.22
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	6	0.22
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	6	0.22
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	6	0.22
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	6	0.22
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	6	0.22
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	6	0.22
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	6	0.22
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	6	0.22
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	19	0.22
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	19	0.22
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	19	0.22
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	19	0.22
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	19	0.22
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	19	0.22
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD11	16	0.22
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD12	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD13	16	0.22
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG21	16	0.22
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG22	16	0.22
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG23	16	0.22
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG21	16	0.22
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG22	16	0.22
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG23	16	0.22
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG21	16	0.22
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG22	16	0.22
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG23	16	0.22
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	16	0.22
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	16	0.22
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	10	0.22
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	10	0.22
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	8	0.22
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	11	0.22
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	6	0.22
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	17	0.22
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	15	0.22
(1,703)	2:51:B:ARG:H	2:51:B:ARG:HD2	15	0.22
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	6	0.22
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	6	0.22
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	6	0.22
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	1	0.22
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	1	0.22
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	15	0.22
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG21	3	0.22
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG22	3	0.22
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG23	3	0.22
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG11	9	0.22
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG12	9	0.22
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG13	9	0.22
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG21	9	0.22
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG22	9	0.22
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG23	9	0.22
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG11	9	0.22
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG12	9	0.22
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG13	9	0.22
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG21	9	0.22
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG22	9	0.22
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG23	9	0.22
(1,550)	2:42:B:GLU:H	2:42:B:GLU:HG3	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	4	0.22
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	1	0.22
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	8	0.22
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	20	0.22
(1,530)	2:40:B:GLY:H	2:42:B:GLU:H	17	0.22
(1,507)	2:39:B:GLU:HG2	2:41:B:THR:HA	16	0.22
(1,507)	2:39:B:GLU:HG3	2:41:B:THR:HA	16	0.22
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	4	0.22
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	12	0.22
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	13	0.22
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	13	0.22
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	11	0.22
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	15	0.22
(1,484)	2:37:B:ALA:H	2:38:B:PRO:HD2	4	0.22
(1,453)	2:35:B:THR:HG21	2:36:B:GLU:HB3	8	0.22
(1,453)	2:35:B:THR:HG22	2:36:B:GLU:HB3	8	0.22
(1,453)	2:35:B:THR:HG23	2:36:B:GLU:HB3	8	0.22
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	14	0.22
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	19	0.22
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	8	0.22
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	12	0.22
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	16	0.22
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD1	9	0.22
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD2	9	0.22
(1,155)	2:13:B:LEU:HG	2:14:B:SER:H	8	0.22
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	5	0.22
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	5	0.22
(1,106)	2:10:B:VAL:HG11	2:14:B:SER:H	11	0.22
(1,106)	2:10:B:VAL:HG12	2:14:B:SER:H	11	0.22
(1,106)	2:10:B:VAL:HG13	2:14:B:SER:H	11	0.22
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	10	0.22
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	18	0.22
(1,11)	2:3:B:GLN:HB2	2:4:B:SER:H	1	0.22
(1,11)	2:3:B:GLN:HB3	2:4:B:SER:H	1	0.22
(1,2133)	1:325:A:ASP:H	1:325:A:ASP:HB3	14	0.21
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	12	0.21
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	4	0.21
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	5	0.21
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	6	0.21
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	10	0.21
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	18	0.21
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	18	0.21
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	1	0.21
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	9	0.21
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	12	0.21
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	18	0.21
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	19	0.21
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	12	0.21
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD11	6	0.21
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD12	6	0.21
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD13	6	0.21
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	4	0.21
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	7	0.21
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	8	0.21
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	9	0.21
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	14	0.21
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	20	0.21
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	1	0.21
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	11	0.21
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	13	0.21
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	20	0.21
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	13	0.21
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	17	0.21
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	20	0.21
(1,1979)	1:315:A:PHE:H	1:314:A:THR:HA	10	0.21
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	3	0.21
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	3	0.21
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	3	0.21
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	3	0.21
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	5	0.21
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	4	0.21
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	13	0.21
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	13	0.21
(1,1861)	2:165:B:LYS:HD2	2:166:B:GLY:H	12	0.21
(1,1861)	2:165:B:LYS:HD3	2:166:B:GLY:H	12	0.21
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	20	0.21
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	8	0.21
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	18	0.21
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	19	0.21
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	1	0.21
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	20	0.21
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	16	0.21
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	2	0.21
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	2	0.21
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	4	0.21
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	4	0.21
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	11	0.21
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	11	0.21
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	11	0.21
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	15	0.21
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	15	0.21
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	15	0.21
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	20	0.21
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	20	0.21
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	20	0.21
(1,1660)	2:146:B:GLY:H	2:148:B:TRP:H	1	0.21
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG21	18	0.21
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG22	18	0.21
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG23	18	0.21
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	20	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	2	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	2	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	2	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	2	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	2	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	2	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	4	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	4	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	4	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	4	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	4	0.21
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	4	0.21
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	4	0.21
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	6	0.21
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	8	0.21
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	15	0.21
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	17	0.21
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	2	0.21
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	4	0.21
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	5	0.21
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	7	0.21
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	14	0.21
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	11	0.21
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	11	0.21
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	17	0.21
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	17	0.21
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	17	0.21
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	8	0.21
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	13	0.21
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	7	0.21
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	7	0.21
(1,1106)	2:96:B:ASN:H	2:97:B:TRP:HB3	6	0.21
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	9	0.21
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	9	0.21
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	9	0.21
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	4	0.21
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	4	0.21
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	4	0.21
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	4	0.21
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	4	0.21
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	4	0.21
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	1	0.21
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG21	15	0.21
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG22	15	0.21
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG23	15	0.21
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG21	15	0.21
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG22	15	0.21
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG23	15	0.21
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG21	15	0.21
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG22	15	0.21
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG23	15	0.21
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	13	0.21
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	6	0.21
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	6	0.21
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	10	0.21
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	19	0.21
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	7	0.21
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	8	0.21
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD21	14	0.21
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD22	14	0.21
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD23	14	0.21
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	5	0.21
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	5	0.21
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	5	0.21
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	5	0.21
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	5	0.21
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	5	0.21
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	5	0.21
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	5	0.21
(1,627)	2:47:B:LYS:H	2:47:B:LYS:HE3	6	0.21
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	9	0.21
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	9	0.21
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	9	0.21
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	9	0.21
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	9	0.21
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	9	0.21
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	2	0.21
(1,542)	2:41:B:THR:H	2:42:B:GLU:H	4	0.21
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	15	0.21
(1,505)	2:39:B:GLU:HG2	2:40:B:GLY:HA2	8	0.21
(1,505)	2:39:B:GLU:HG2	2:40:B:GLY:HA3	8	0.21
(1,505)	2:39:B:GLU:HG3	2:40:B:GLY:HA2	8	0.21
(1,505)	2:39:B:GLU:HG3	2:40:B:GLY:HA3	8	0.21
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	6	0.21
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	19	0.21
(1,465)	2:36:B:GLU:HB2	2:37:B:ALA:H	16	0.21
(1,465)	2:36:B:GLU:HB3	2:37:B:ALA:H	16	0.21
(1,458)	2:35:B:THR:H	2:35:B:THR:HB	14	0.21
(1,458)	2:35:B:THR:H	2:35:B:THR:HB	19	0.21
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	12	0.21
(1,445)	2:35:B:THR:HA	2:36:B:GLU:HB3	14	0.21
(1,424)	2:33:B:ASN:H	2:33:B:ASN:HB3	18	0.21
(1,404)	2:31:B:GLU:H	2:31:B:GLU:HB2	19	0.21
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	4	0.21
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	5	0.21
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	5	0.21
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	5	0.21
(1,275)	2:20:B:LYS:HG2	2:22:B:TYR:H	5	0.21
(1,275)	2:20:B:LYS:HG3	2:22:B:TYR:H	5	0.21
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	19	0.21
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	19	0.21
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	2	0.21
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	12	0.21
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	15	0.21
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	10	0.21
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG11	11	0.21
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG12	11	0.21
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG13	11	0.21
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG21	11	0.21
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG22	11	0.21
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG23	11	0.21
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG11	11	0.21
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG12	11	0.21
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG13	11	0.21
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG21	11	0.21
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG22	11	0.21
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG23	11	0.21
(1,155)	2:13:B:LEU:HG	2:14:B:SER:H	18	0.21
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	6	0.21
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	6	0.21
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	7	0.21
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	7	0.21
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	11	0.21
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	11	0.21
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	9	0.21
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	9	0.21
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	9	0.21
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	12	0.21
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	12	0.21
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	12	0.21
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	14	0.21
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	19	0.21
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	3	0.2
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	11	0.2
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	19	0.2
(1,2101)	1:323:A:GLU:H	1:321:A:SER:HB3	10	0.2
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	6	0.2
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	13	0.2
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	15	0.2
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	19	0.2
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	5	0.2
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	5	0.2
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	5	0.2
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	11	0.2
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	11	0.2
(1,2043)	1:319:A:TRP:H	1:318:A:LEU:HA	19	0.2
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	12	0.2
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	2	0.2
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	3	0.2
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	7	0.2
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	9	0.2
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	6	0.2
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	8	0.2
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	16	0.2
(1,1979)	1:315:A:PHE:H	1:314:A:THR:HA	8	0.2
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	15	0.2
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	15	0.2
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	15	0.2
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	15	0.2
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	19	0.2
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	19	0.2
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	19	0.2
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	19	0.2
(1,1912)	2:169:B:ARG:H	2:169:B:ARG:HB3	4	0.2
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	15	0.2
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	15	0.2
(1,1877)	2:166:B:GLY:H	2:167:B:GLN:HB2	7	0.2
(1,1877)	2:166:B:GLY:H	2:167:B:GLN:HB3	7	0.2
(1,1861)	2:165:B:LYS:HD2	2:166:B:GLY:H	3	0.2
(1,1861)	2:165:B:LYS:HD3	2:166:B:GLY:H	3	0.2
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	16	0.2
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	6	0.2
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	13	0.2
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	16	0.2
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	7	0.2
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	9	0.2
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	13	0.2
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	18	0.2
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	2	0.2
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	8	0.2
(1,1809)	2:158:B:ASN:H	2:161:B:ALA:H	2	0.2
(1,1786)	2:156:B:GLY:H	2:158:B:ASN:H	3	0.2
(1,1786)	2:156:B:GLY:H	2:158:B:ASN:H	17	0.2
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	5	0.2
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	5	0.2
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	5	0.2
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	5	0.2
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	5	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	2	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	2	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	2	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	6	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	6	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	6	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	8	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	8	0.2
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	8	0.2
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	18	0.2
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	18	0.2
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	18	0.2
(1,1695)	2:150:B:THR:HB	2:153:B:GLU:HG2	12	0.2
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	6	0.2
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	7	0.2
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	7	0.2
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	7	0.2
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	7	0.2
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	7	0.2
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	7	0.2
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	3	0.2
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	7	0.2
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	10	0.2
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	16	0.2
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	19	0.2
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	20	0.2
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	3	0.2
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	8	0.2
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	11	0.2
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	19	0.2
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	20	0.2
(1,1389)	2:119:B:MET:H	2:120:B:GLN:HE22	3	0.2
(1,1389)	2:119:B:MET:H	2:120:B:GLN:HE22	4	0.2
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE1	7	0.2
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE2	7	0.2
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE1	7	0.2
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE2	7	0.2
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE1	15	0.2
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE2	15	0.2
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE1	15	0.2
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE2	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	9	0.2
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	9	0.2
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	12	0.2
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	12	0.2
(1,1113)	2:96:B:ASN:H	2:99:B:ARG:H	7	0.2
(1,1106)	2:96:B:ASN:H	2:97:B:TRP:HB3	7	0.2
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	3	0.2
(1,1101)	2:96:B:ASN:H	2:100:B:ILE:H	9	0.2
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD11	9	0.2
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD12	9	0.2
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD13	9	0.2
(1,1095)	2:96:B:ASN:HD21	2:100:B:ILE:H	13	0.2
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	1	0.2
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	1	0.2
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	1	0.2
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	18	0.2
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	18	0.2
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	18	0.2
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	19	0.2
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	19	0.2
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	19	0.2
(1,1071)	2:94:B:GLY:H	2:96:B:ASN:HD22	3	0.2
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	8	0.2
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	20	0.2
(1,1036)	2:92:B:ARG:HG3	2:94:B:GLY:H	19	0.2
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	11	0.2
(1,893)	2:80:B:TYR:HE1	2:81:B:GLN:H	10	0.2
(1,893)	2:80:B:TYR:HE2	2:81:B:GLN:H	10	0.2
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD11	15	0.2
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD12	15	0.2
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD13	15	0.2
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	13	0.2
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	13	0.2
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	13	0.2
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	13	0.2
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	13	0.2
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	13	0.2
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	13	0.2
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	13	0.2
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	13	0.2
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	15	0.2
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	15	0.2
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	15	0.2
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	15	0.2
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	15	0.2
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	17	0.2
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	17	0.2
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	17	0.2
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	17	0.2
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	17	0.2
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	17	0.2
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	17	0.2
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	17	0.2
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	17	0.2
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD21	18	0.2
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD22	18	0.2
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD23	18	0.2
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	9	0.2
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	1	0.2
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	3	0.2
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	9	0.2
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	16	0.2
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	18	0.2
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	9	0.2
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	19	0.2
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	19	0.2
(1,703)	2:51:B:ARG:H	2:51:B:ARG:HD2	10	0.2
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	4	0.2
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	4	0.2
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	4	0.2
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	16	0.2
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	16	0.2
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	16	0.2
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	16	0.2
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	16	0.2
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	16	0.2
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	16	0.2
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	16	0.2
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	16	0.2
(1,627)	2:47:B:LYS:H	2:47:B:LYS:HE3	13	0.2
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	10	0.2
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	10	0.2
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	17	0.2
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	18	0.2
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	8	0.2
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	3	0.2
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	18	0.2
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	14	0.2
(1,453)	2:35:B:THR:HG21	2:36:B:GLU:HB3	1	0.2
(1,453)	2:35:B:THR:HG22	2:36:B:GLU:HB3	1	0.2
(1,453)	2:35:B:THR:HG23	2:36:B:GLU:HB3	1	0.2
(1,430)	2:33:B:ASN:H	2:35:B:THR:HG1	20	0.2
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	18	0.2
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB2	8	0.2
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB3	8	0.2
(1,373)	2:28:B:SER:H	2:30:B:VAL:HG21	13	0.2
(1,373)	2:28:B:SER:H	2:30:B:VAL:HG22	13	0.2
(1,373)	2:28:B:SER:H	2:30:B:VAL:HG23	13	0.2
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	8	0.2
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	8	0.2
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	14	0.2
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	14	0.2
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	12	0.2
(1,333)	2:25:B:SER:HB2	2:26:B:GLN:H	10	0.2
(1,333)	2:25:B:SER:HB3	2:26:B:GLN:H	10	0.2
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	3	0.2
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	3	0.2
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG11	3	0.2
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG12	3	0.2
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG13	3	0.2
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG21	3	0.2
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG22	3	0.2
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG23	3	0.2
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	13	0.2
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	13	0.2
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	14	0.2
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	14	0.2
(1,275)	2:20:B:LYS:HG2	2:22:B:TYR:H	13	0.2
(1,275)	2:20:B:LYS:HG3	2:22:B:TYR:H	13	0.2
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	1	0.2
(1,250)	2:19:B:GLN:HB2	2:21:B:GLY:H	9	0.2
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	6	0.2
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	12	0.2
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	5	0.2
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	5	0.2
(1,127)	2:11:B:ASP:HB2	2:47:B:LYS:HD2	10	0.2
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	9	0.2
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	15	0.2
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	17	0.2
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	7	0.19
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	7	0.19
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	7	0.19
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	19	0.19
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	19	0.19
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	19	0.19
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	9	0.19
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	4	0.19
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	9	0.19
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	12	0.19
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	16	0.19
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	4	0.19
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	5	0.19
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	10	0.19
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	17	0.19
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	17	0.19
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	17	0.19
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	17	0.19
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	16	0.19
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	18	0.19
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	19	0.19
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	12	0.19
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	5	0.19
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	9	0.19
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	10	0.19
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	20	0.19
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	11	0.19
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	11	0.19
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	16	0.19
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	16	0.19
(1,1877)	2:166:B:GLY:H	2:167:B:GLN:HB2	8	0.19
(1,1877)	2:166:B:GLY:H	2:167:B:GLN:HB3	8	0.19
(1,1861)	2:165:B:LYS:HD2	2:166:B:GLY:H	9	0.19
(1,1861)	2:165:B:LYS:HD3	2:166:B:GLY:H	9	0.19
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	2	0.19
(1,1847)	2:164:B:ARG:H	2:164:B:ARG:HB3	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	5	0.19
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	14	0.19
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	15	0.19
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	6	0.19
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	12	0.19
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	14	0.19
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB2	1	0.19
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB3	1	0.19
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	6	0.19
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	9	0.19
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	11	0.19
(1,1787)	2:157:B:ASN:HB3	2:159:B:ALA:HA	12	0.19
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	7	0.19
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	7	0.19
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	11	0.19
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	11	0.19
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	12	0.19
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	12	0.19
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	14	0.19
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	14	0.19
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	11	0.19
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	11	0.19
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	11	0.19
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	11	0.19
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	11	0.19
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	11	0.19
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	18	0.19
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	18	0.19
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	18	0.19
(1,1670)	2:148:B:TRP:HB2	2:150:B:THR:H	15	0.19
(1,1670)	2:148:B:TRP:HB3	2:150:B:THR:H	15	0.19
(1,1655)	2:145:B:ASN:H	2:146:B:GLY:H	14	0.19
(1,1639)	2:144:B:GLU:H	2:145:B:ASN:HD21	19	0.19
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD11	17	0.19
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD12	17	0.19
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD13	17	0.19
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	19	0.19
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	14	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	11	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	11	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	11	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	11	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	11	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	17	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	17	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	17	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	17	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	17	0.19
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	17	0.19
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	12	0.19
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	14	0.19
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	15	0.19
(1,1367)	2:117:B:LYS:H	2:117:B:LYS:HD3	9	0.19
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	2	0.19
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	6	0.19
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	9	0.19
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	12	0.19
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	15	0.19
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	17	0.19
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	11	0.19
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	18	0.19
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	10	0.19
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	1	0.19
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	1	0.19
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	8	0.19
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	8	0.19
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	19	0.19
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	19	0.19
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	15	0.19
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	15	0.19
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	15	0.19
(1,1034)	2:92:B:ARG:HD2	2:93:B:ASP:H	5	0.19
(1,1034)	2:92:B:ARG:HD3	2:93:B:ASP:H	5	0.19
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	5	0.19
(1,931)	2:85:B:GLN:HB2	2:86:B:VAL:HB	20	0.19
(1,931)	2:85:B:GLN:HB3	2:86:B:VAL:HB	20	0.19
(1,894)	2:80:B:TYR:H	2:129:B:TRP:HD1	2	0.19
(1,894)	2:80:B:TYR:H	2:129:B:TRP:HD1	20	0.19
(1,861)	2:74:B:ILE:HD11	2:119:B:MET:HB2	2	0.19
(1,861)	2:74:B:ILE:HD11	2:119:B:MET:HB3	2	0.19
(1,861)	2:74:B:ILE:HD12	2:119:B:MET:HB2	2	0.19
(1,861)	2:74:B:ILE:HD12	2:119:B:MET:HB3	2	0.19
(1,861)	2:74:B:ILE:HD13	2:119:B:MET:HB2	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,861)	2:74:B:ILE:HD13	2:119:B:MET:HB3	2	0.19
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	2	0.19
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	2	0.19
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	2	0.19
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	2	0.19
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	2	0.19
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	2	0.19
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	15	0.19
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD11	16	0.19
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD12	16	0.19
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD13	16	0.19
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	5	0.19
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	5	0.19
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	5	0.19
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	5	0.19
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	5	0.19
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	5	0.19
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	5	0.19
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	5	0.19
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	5	0.19
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	15	0.19
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	15	0.19
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	15	0.19
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	15	0.19
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	15	0.19
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	15	0.19
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	15	0.19
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	15	0.19
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	15	0.19
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	13	0.19
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	13	0.19
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	5	0.19
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	5	0.19
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	6	0.19
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	6	0.19
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	10	0.19
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	5	0.19
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	7	0.19
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	11	0.19
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	2	0.19
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD1	12	0.19
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD2	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	2	0.19
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	2	0.19
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	2	0.19
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	19	0.19
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	19	0.19
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	19	0.19
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	11	0.19
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	11	0.19
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	11	0.19
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	11	0.19
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	11	0.19
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	11	0.19
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	11	0.19
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	11	0.19
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	11	0.19
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	18	0.19
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	18	0.19
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	18	0.19
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	18	0.19
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	20	0.19
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	20	0.19
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	20	0.19
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	20	0.19
(1,628)	2:47:B:LYS:H	2:47:B:LYS:HE2	20	0.19
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	2	0.19
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	10	0.19
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	10	0.19
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	10	0.19
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	10	0.19
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	10	0.19
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	10	0.19
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	5	0.19
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	14	0.19
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	15	0.19
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	9	0.19
(1,527)	2:40:B:GLY:H	2:41:B:THR:HG1	13	0.19
(1,527)	2:40:B:GLY:H	2:41:B:THR:HG1	14	0.19
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG21	19	0.19
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG22	19	0.19
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG23	19	0.19
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	3	0.19
(1,502)	2:39:B:GLU:HB2	2:41:B:THR:HA	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	2:39:B:GLU:HB3	2:41:B:THR:HA	20	0.19
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	7	0.19
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	7	0.19
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	4	0.19
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	5	0.19
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB1	3	0.19
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB2	3	0.19
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB3	3	0.19
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB1	7	0.19
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB2	7	0.19
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB3	7	0.19
(1,479)	2:37:B:ALA:HB1	2:40:B:GLY:H	1	0.19
(1,479)	2:37:B:ALA:HB2	2:40:B:GLY:H	1	0.19
(1,479)	2:37:B:ALA:HB3	2:40:B:GLY:H	1	0.19
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	9	0.19
(1,442)	2:34:B:ARG:H	2:35:B:THR:HB	6	0.19
(1,404)	2:31:B:GLU:H	2:31:B:GLU:HB2	2	0.19
(1,385)	2:30:B:VAL:HA	2:31:B:GLU:H	6	0.19
(1,375)	2:28:B:SER:H	2:30:B:VAL:H	3	0.19
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	10	0.19
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	10	0.19
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	12	0.19
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	12	0.19
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG11	1	0.19
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG12	1	0.19
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG13	1	0.19
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG21	1	0.19
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG22	1	0.19
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG23	1	0.19
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	16	0.19
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	16	0.19
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	15	0.19
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	15	0.19
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	5	0.19
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	10	0.19
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	15	0.19
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	1	0.19
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	2	0.19
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG11	20	0.19
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG12	20	0.19
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG13	20	0.19
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG21	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG22	20	0.19
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG23	20	0.19
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG11	20	0.19
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG12	20	0.19
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG13	20	0.19
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG21	20	0.19
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG22	20	0.19
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG23	20	0.19
(1,155)	2:13:B:LEU:HG	2:14:B:SER:H	17	0.19
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	9	0.19
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	9	0.19
(1,127)	2:11:B:ASP:HB2	2:47:B:LYS:HD2	9	0.19
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG2	3	0.19
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG3	3	0.19
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	3	0.19
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	4	0.19
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	13	0.19
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	2	0.18
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	7	0.18
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	14	0.18
(1,2101)	1:323:A:GLU:H	1:321:A:SER:HB3	19	0.18
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	1	0.18
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	3	0.18
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	5	0.18
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	11	0.18
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	17	0.18
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	20	0.18
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	3	0.18
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	13	0.18
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	20	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	11	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	11	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	11	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	15	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	15	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	15	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	19	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	19	0.18
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	19	0.18
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	20	0.18
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	9	0.18
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	15	0.18
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	2	0.18
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	4	0.18
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	7	0.18
(1,1979)	1:315:A:PHE:H	1:314:A:THR:HA	1	0.18
(1,1979)	1:315:A:PHE:H	1:314:A:THR:HA	4	0.18
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	3	0.18
(1,1916)	2:169:B:ARG:H	2:169:B:ARG:HG3	19	0.18
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	6	0.18
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	6	0.18
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	9	0.18
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	9	0.18
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	5	0.18
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	10	0.18
(1,1843)	2:163:B:SER:HB2	2:165:B:LYS:H	13	0.18
(1,1843)	2:163:B:SER:HB3	2:165:B:LYS:H	13	0.18
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	7	0.18
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	16	0.18
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	11	0.18
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	5	0.18
(1,1794)	2:158:B:ASN:HA	2:159:B:ALA:H	19	0.18
(1,1735)	2:152:B:VAL:HG21	2:156:B:GLY:H	13	0.18
(1,1735)	2:152:B:VAL:HG22	2:156:B:GLY:H	13	0.18
(1,1735)	2:152:B:VAL:HG23	2:156:B:GLY:H	13	0.18
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	5	0.18
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	9	0.18
(1,1660)	2:146:B:GLY:H	2:148:B:TRP:H	10	0.18
(1,1657)	2:145:B:ASN:H	2:148:B:TRP:H	10	0.18
(1,1657)	2:145:B:ASN:H	2:148:B:TRP:H	17	0.18
(1,1601)	2:142:B:ILE:HD11	2:147:B:GLY:H	4	0.18
(1,1601)	2:142:B:ILE:HD12	2:147:B:GLY:H	4	0.18
(1,1601)	2:142:B:ILE:HD13	2:147:B:GLY:H	4	0.18
(1,1590)	2:141:B:TRP:H	2:142:B:ILE:HB	4	0.18
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	1	0.18
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	1	0.18
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	1	0.18
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	1	0.18
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	1	0.18
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	1	0.18
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	16	0.18
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	16	0.18
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	16	0.18
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	16	0.18
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	16	0.18
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	13	0.18
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	2	0.18
(1,1487)	2:131:B:ALA:H	2:130:B:MET:HA	9	0.18
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	12	0.18
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	13	0.18
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	16	0.18
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	16	0.18
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	2	0.18
(1,1374)	2:117:B:LYS:H	2:120:B:GLN:H	10	0.18
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD11	12	0.18
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD12	12	0.18
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD13	12	0.18
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD21	12	0.18
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD22	12	0.18
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD23	12	0.18
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	10	0.18
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	11	0.18
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	20	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	1	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	3	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	5	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	7	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	10	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	13	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	14	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	18	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	19	0.18
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	20	0.18
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	4	0.18
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	4	0.18
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	4	0.18
(1,1113)	2:96:B:ASN:H	2:99:B:ARG:H	15	0.18
(1,1108)	2:96:B:ASN:H	2:97:B:TRP:HB2	19	0.18
(1,1108)	2:96:B:ASN:H	2:97:B:TRP:HB3	19	0.18
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	9	0.18
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	9	0.18
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	9	0.18
(1,931)	2:85:B:GLN:HB2	2:86:B:VAL:HB	6	0.18
(1,931)	2:85:B:GLN:HB3	2:86:B:VAL:HB	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,928)	2:85:B:GLN:HB3	2:87:B:VAL:H	18	0.18
(1,910)	2:81:B:GLN:H	2:85:B:GLN:H	8	0.18
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	10	0.18
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	10	0.18
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	10	0.18
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	10	0.18
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	10	0.18
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	10	0.18
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	10	0.18
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	10	0.18
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	10	0.18
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	19	0.18
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	19	0.18
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	19	0.18
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	19	0.18
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	19	0.18
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	19	0.18
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	19	0.18
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	19	0.18
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	19	0.18
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	16	0.18
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	16	0.18
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	16	0.18
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	16	0.18
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	16	0.18
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	16	0.18
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD11	12	0.18
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD12	12	0.18
(1,837)	2:72:B:LEU:HA	2:74:B:ILE:HD13	12	0.18
(1,836)	2:72:B:LEU:HA	2:74:B:ILE:HA	9	0.18
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	14	0.18
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	17	0.18
(1,809)	2:69:B:THR:HG1	2:110:B:LEU:H	8	0.18
(1,809)	2:69:B:THR:HG1	2:110:B:LEU:H	13	0.18
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD11	7	0.18
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD12	7	0.18
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD13	7	0.18
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD21	12	0.18
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD22	12	0.18
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD23	12	0.18
(1,775)	2:63:B:ARG:HD2	2:64:B:ALA:H	16	0.18
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	15	0.18
(1,703)	2:51:B:ARG:H	2:51:B:ARG:HD2	3	0.18
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	4	0.18
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	4	0.18
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	12	0.18
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	19	0.18
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	10	0.18
(1,526)	2:40:B:GLY:H	2:40:B:GLY:HA2	16	0.18
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	20	0.18
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	9	0.18
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	9	0.18
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	20	0.18
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	20	0.18
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	11	0.18
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	9	0.18
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	9	0.18
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB1	2	0.18
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB2	2	0.18
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB3	2	0.18
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB1	15	0.18
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB2	15	0.18
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB3	15	0.18
(1,480)	2:37:B:ALA:H	2:37:B:ALA:HA	18	0.18
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	11	0.18
(1,465)	2:36:B:GLU:HB2	2:37:B:ALA:H	1	0.18
(1,465)	2:36:B:GLU:HB3	2:37:B:ALA:H	1	0.18
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	15	0.18
(1,449)	2:35:B:THR:HA	2:36:B:GLU:H	14	0.18
(1,449)	2:35:B:THR:HA	2:36:B:GLU:H	19	0.18
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	18	0.18
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	18	0.18
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	18	0.18
(1,398)	2:30:B:VAL:H	2:31:B:GLU:HG2	10	0.18
(1,398)	2:30:B:VAL:H	2:31:B:GLU:HG3	10	0.18
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	13	0.18
(1,333)	2:25:B:SER:HB2	2:26:B:GLN:H	8	0.18
(1,333)	2:25:B:SER:HB3	2:26:B:GLN:H	8	0.18
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	20	0.18
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	20	0.18
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	1	0.18
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	1	0.18
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	6	0.18
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	18	0.18
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	18	0.18
(1,272)	2:20:B:LYS:HD2	2:22:B:TYR:H	19	0.18
(1,272)	2:20:B:LYS:HD3	2:22:B:TYR:H	19	0.18
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	8	0.18
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	8	0.18
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	9	0.18
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	9	0.18
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	15	0.18
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	19	0.18
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	3	0.18
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	2	0.18
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	11	0.18
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	4	0.18
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	4	0.18
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG11	2	0.18
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG12	2	0.18
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG13	2	0.18
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG21	2	0.18
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG22	2	0.18
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG23	2	0.18
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG11	2	0.18
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG12	2	0.18
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG13	2	0.18
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG21	2	0.18
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG22	2	0.18
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG23	2	0.18
(1,155)	2:13:B:LEU:HG	2:14:B:SER:H	3	0.18
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	11	0.18
(1,3)	2:1:B:MET:HG2	2:2:B:SER:HA	10	0.18
(1,3)	2:1:B:MET:HG3	2:2:B:SER:HA	10	0.18
(1,2102)	1:323:A:GLU:H	1:321:A:SER:HB2	5	0.17
(1,2101)	1:323:A:GLU:H	1:321:A:SER:HB3	6	0.17
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	7	0.17
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	15	0.17
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	16	0.17
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	13	0.17
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	15	0.17
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	8	0.17
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD11	13	0.17
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD12	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2034)	1:319:A:TRP:HE1	1:318:A:LEU:HD13	13	0.17
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	6	0.17
(1,2005)	1:317:A:HIS:H	1:316:A:GLU:HA	10	0.17
(1,2003)	1:317:A:HIS:H	1:314:A:THR:HA	17	0.17
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	14	0.17
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	15	0.17
(1,1989)	1:316:A:GLU:H	1:315:A:PHE:HA	18	0.17
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	19	0.17
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	19	0.17
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	19	0.17
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	19	0.17
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	19	0.17
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	19	0.17
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	9	0.17
(1,1916)	2:169:B:ARG:H	2:169:B:ARG:HG3	14	0.17
(1,1908)	2:169:B:ARG:HA	2:170:B:LEU:H	12	0.17
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	9	0.17
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	9	0.17
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	7	0.17
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	20	0.17
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	12	0.17
(1,1864)	2:165:B:LYS:HG2	2:166:B:GLY:H	16	0.17
(1,1860)	2:165:B:LYS:HB2	2:168:B:GLU:H	18	0.17
(1,1846)	2:164:B:ARG:HD2	2:165:B:LYS:H	18	0.17
(1,1846)	2:164:B:ARG:HD3	2:165:B:LYS:H	18	0.17
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	4	0.17
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	10	0.17
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	17	0.17
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	2	0.17
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	10	0.17
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	15	0.17
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	17	0.17
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	1	0.17
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	4	0.17
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	12	0.17
(1,1786)	2:156:B:GLY:H	2:158:B:ASN:H	18	0.17
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	14	0.17
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	14	0.17
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	3	0.17
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	3	0.17
(1,1738)	2:152:B:VAL:HG11	2:155:B:TYR:HE1	9	0.17
(1,1738)	2:152:B:VAL:HG11	2:155:B:TYR:HE2	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1738)	2:152:B:VAL:HG12	2:155:B:TYR:HE1	9	0.17
(1,1738)	2:152:B:VAL:HG12	2:155:B:TYR:HE2	9	0.17
(1,1738)	2:152:B:VAL:HG13	2:155:B:TYR:HE1	9	0.17
(1,1738)	2:152:B:VAL:HG13	2:155:B:TYR:HE2	9	0.17
(1,1738)	2:152:B:VAL:HG21	2:155:B:TYR:HE1	9	0.17
(1,1738)	2:152:B:VAL:HG21	2:155:B:TYR:HE2	9	0.17
(1,1738)	2:152:B:VAL:HG22	2:155:B:TYR:HE1	9	0.17
(1,1738)	2:152:B:VAL:HG22	2:155:B:TYR:HE2	9	0.17
(1,1738)	2:152:B:VAL:HG23	2:155:B:TYR:HE1	9	0.17
(1,1738)	2:152:B:VAL:HG23	2:155:B:TYR:HE2	9	0.17
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	4	0.17
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	4	0.17
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	4	0.17
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	4	0.17
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	4	0.17
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	4	0.17
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	14	0.17
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	14	0.17
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	14	0.17
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	14	0.17
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	14	0.17
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	14	0.17
(1,1735)	2:152:B:VAL:HG21	2:156:B:GLY:H	15	0.17
(1,1735)	2:152:B:VAL:HG22	2:156:B:GLY:H	15	0.17
(1,1735)	2:152:B:VAL:HG23	2:156:B:GLY:H	15	0.17
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	2	0.17
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	2	0.17
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	10	0.17
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	10	0.17
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	15	0.17
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	15	0.17
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	13	0.17
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	13	0.17
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	13	0.17
(1,1655)	2:145:B:ASN:H	2:146:B:GLY:H	4	0.17
(1,1655)	2:145:B:ASN:H	2:146:B:GLY:H	12	0.17
(1,1590)	2:141:B:TRP:H	2:142:B:ILE:HB	9	0.17
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	14	0.17
(1,1507)	2:134:B:LEU:HD11	2:136:B:ASP:H	3	0.17
(1,1507)	2:134:B:LEU:HD12	2:136:B:ASP:H	3	0.17
(1,1507)	2:134:B:LEU:HD13	2:136:B:ASP:H	3	0.17
(1,1507)	2:134:B:LEU:HD21	2:136:B:ASP:H	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	2:134:B:LEU:HD22	2:136:B:ASP:H	3	0.17
(1,1507)	2:134:B:LEU:HD23	2:136:B:ASP:H	3	0.17
(1,1483)	2:131:B:ALA:HA	2:132:B:THR:H	18	0.17
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	10	0.17
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	1	0.17
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	1	0.17
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	1	0.17
(1,1292)	2:112:B:VAL:HG11	2:113:B:GLU:H	14	0.17
(1,1292)	2:112:B:VAL:HG12	2:113:B:GLU:H	14	0.17
(1,1292)	2:112:B:VAL:HG13	2:113:B:GLU:H	14	0.17
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	11	0.17
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	16	0.17
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	15	0.17
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	14	0.17
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	19	0.17
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE1	16	0.17
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE2	16	0.17
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE1	16	0.17
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE2	16	0.17
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE1	20	0.17
(1,1202)	2:105:B:SER:HB2	2:106:B:PHE:HE2	20	0.17
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE1	20	0.17
(1,1202)	2:105:B:SER:HB3	2:106:B:PHE:HE2	20	0.17
(1,1183)	2:103:B:PHE:HB2	2:105:B:SER:HB2	12	0.17
(1,1183)	2:103:B:PHE:HB2	2:105:B:SER:HB3	12	0.17
(1,1183)	2:103:B:PHE:HB3	2:105:B:SER:HB2	12	0.17
(1,1183)	2:103:B:PHE:HB3	2:105:B:SER:HB3	12	0.17
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD11	1	0.17
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD12	1	0.17
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD13	1	0.17
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD11	19	0.17
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD12	19	0.17
(1,1100)	2:96:B:ASN:H	2:100:B:ILE:HD13	19	0.17
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD11	15	0.17
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD12	15	0.17
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD13	15	0.17
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	16	0.17
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	16	0.17
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	16	0.17
(1,1070)	2:94:B:GLY:H	2:96:B:ASN:HD21	4	0.17
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	5	0.17
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	5	0.17
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	11	0.17
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	14	0.17
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	19	0.17
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	3	0.17
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	3	0.17
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	3	0.17
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	3	0.17
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	3	0.17
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	3	0.17
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	3	0.17
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	3	0.17
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	3	0.17
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD11	3	0.17
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD12	3	0.17
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD13	3	0.17
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	5	0.17
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	5	0.17
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	5	0.17
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	5	0.17
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	5	0.17
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	5	0.17
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD21	3	0.17
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD22	3	0.17
(1,824)	2:71:B:GLN:HA	2:72:B:LEU:HD23	3	0.17
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	3	0.17
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	8	0.17
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	9	0.17
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	10	0.17
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	20	0.17
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	12	0.17
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	12	0.17
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	12	0.17
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG21	20	0.17
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG22	20	0.17
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG23	20	0.17
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG21	20	0.17
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG22	20	0.17
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG23	20	0.17
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG21	20	0.17
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG22	20	0.17
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG23	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	14	0.17
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	14	0.17
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	13	0.17
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	19	0.17
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD1	1	0.17
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD2	1	0.17
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD1	3	0.17
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD2	3	0.17
(1,702)	2:51:B:ARG:H	2:51:B:ARG:HD3	13	0.17
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	11	0.17
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	11	0.17
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	11	0.17
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	15	0.17
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	15	0.17
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	15	0.17
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	17	0.17
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	17	0.17
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	17	0.17
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	18	0.17
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	18	0.17
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	18	0.17
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	12	0.17
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	12	0.17
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	12	0.17
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	12	0.17
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	12	0.17
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	12	0.17
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	12	0.17
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	12	0.17
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	12	0.17
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	1	0.17
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	1	0.17
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	1	0.17
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	1	0.17
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	12	0.17
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	12	0.17
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	9	0.17
(1,612)	2:47:B:LYS:HB2	2:51:B:ARG:HA	14	0.17
(1,612)	2:47:B:LYS:HB3	2:51:B:ARG:HA	14	0.17
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	3	0.17
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	16	0.17
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	16	0.17
(1,526)	2:40:B:GLY:H	2:40:B:GLY:HA2	3	0.17
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	18	0.17
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	18	0.17
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	9	0.17
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	17	0.17
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	16	0.17
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	16	0.17
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	11	0.17
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	11	0.17
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	19	0.17
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	19	0.17
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG2	8	0.17
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG3	8	0.17
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG2	8	0.17
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG3	8	0.17
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG2	8	0.17
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG3	8	0.17
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	2	0.17
(1,436)	2:34:B:ARG:HD2	2:35:B:THR:H	2	0.17
(1,436)	2:34:B:ARG:HD3	2:35:B:THR:H	2	0.17
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	13	0.17
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	7	0.17
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	7	0.17
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	7	0.17
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	1	0.17
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	2	0.17
(1,410)	2:32:B:GLU:HG2	2:34:B:ARG:H	1	0.17
(1,410)	2:32:B:GLU:HG3	2:34:B:ARG:H	1	0.17
(1,410)	2:32:B:GLU:HG2	2:34:B:ARG:H	16	0.17
(1,410)	2:32:B:GLU:HG3	2:34:B:ARG:H	16	0.17
(1,401)	2:30:B:VAL:H	2:33:B:ASN:H	10	0.17
(1,387)	2:30:B:VAL:HG11	2:32:B:GLU:H	12	0.17
(1,387)	2:30:B:VAL:HG12	2:32:B:GLU:H	12	0.17
(1,387)	2:30:B:VAL:HG13	2:32:B:GLU:H	12	0.17
(1,387)	2:30:B:VAL:HG11	2:32:B:GLU:H	17	0.17
(1,387)	2:30:B:VAL:HG12	2:32:B:GLU:H	17	0.17
(1,387)	2:30:B:VAL:HG13	2:32:B:GLU:H	17	0.17
(1,385)	2:30:B:VAL:HA	2:31:B:GLU:H	10	0.17
(1,376)	2:29:B:ASP:HA	2:30:B:VAL:H	8	0.17
(1,375)	2:28:B:SER:H	2:30:B:VAL:H	17	0.17
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG11	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG12	6	0.17
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG13	6	0.17
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	15	0.17
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	15	0.17
(1,333)	2:25:B:SER:HB2	2:26:B:GLN:H	16	0.17
(1,333)	2:25:B:SER:HB3	2:26:B:GLN:H	16	0.17
(1,316)	2:23:B:SER:H	2:25:B:SER:H	6	0.17
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG11	17	0.17
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG12	17	0.17
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG13	17	0.17
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG21	17	0.17
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG22	17	0.17
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG23	17	0.17
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	12	0.17
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	12	0.17
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	8	0.17
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	8	0.17
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	4	0.17
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	4	0.17
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	16	0.17
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	5	0.17
(1,187)	2:16:B:LYS:H	2:16:B:LYS:HE2	15	0.17
(1,187)	2:16:B:LYS:H	2:16:B:LYS:HE3	15	0.17
(1,155)	2:13:B:LEU:HG	2:14:B:SER:H	12	0.17
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	5	0.17
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	3	0.16
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	3	0.16
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	3	0.16
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	6	0.16
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	6	0.16
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	6	0.16
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	1	0.16
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	2	0.16
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	8	0.16
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	7	0.16
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	10	0.16
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	4	0.16
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	5	0.16
(1,2003)	1:317:A:HIS:H	1:314:A:THR:HA	19	0.16
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	5	0.16
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	5	0.16
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	5	0.16
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	12	0.16
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	12	0.16
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	12	0.16
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	12	0.16
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	12	0.16
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	12	0.16
(1,1923)	2:170:B:LEU:HG	2:171:B:GLU:H	15	0.16
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	10	0.16
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	18	0.16
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	3	0.16
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	5	0.16
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	12	0.16
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	4	0.16
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB2	20	0.16
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB3	20	0.16
(1,1809)	2:158:B:ASN:H	2:161:B:ALA:H	14	0.16
(1,1794)	2:158:B:ASN:HA	2:159:B:ALA:H	18	0.16
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	5	0.16
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	5	0.16
(1,1735)	2:152:B:VAL:HG21	2:156:B:GLY:H	11	0.16
(1,1735)	2:152:B:VAL:HG22	2:156:B:GLY:H	11	0.16
(1,1735)	2:152:B:VAL:HG23	2:156:B:GLY:H	11	0.16
(1,1661)	2:146:B:GLY:H	2:149:B:ASP:H	2	0.16
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	1	0.16
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	10	0.16
(1,1614)	2:143:B:GLN:HA	2:147:B:GLY:H	6	0.16
(1,1598)	2:142:B:ILE:HD11	2:146:B:GLY:H	14	0.16
(1,1598)	2:142:B:ILE:HD12	2:146:B:GLY:H	14	0.16
(1,1598)	2:142:B:ILE:HD13	2:146:B:GLY:H	14	0.16
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	5	0.16
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	6	0.16
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	12	0.16
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	2	0.16
(1,1394)	2:120:B:GLN:H	2:120:B:GLN:HB2	16	0.16
(1,1394)	2:120:B:GLN:H	2:120:B:GLN:HB3	16	0.16
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD11	6	0.16
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD12	6	0.16
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD13	6	0.16
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD21	6	0.16
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD22	6	0.16
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD23	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	2	0.16
(1,1239)	2:109:B:ALA:HA	2:110:B:LEU:H	4	0.16
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	7	0.16
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	8	0.16
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	14	0.16
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	5	0.16
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	11	0.16
(1,1198)	2:104:B:PHE:H	2:104:B:PHE:HE1	8	0.16
(1,1198)	2:104:B:PHE:H	2:104:B:PHE:HE2	8	0.16
(1,1192)	2:104:B:PHE:HD1	2:106:B:PHE:H	11	0.16
(1,1192)	2:104:B:PHE:HD2	2:106:B:PHE:H	11	0.16
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	16	0.16
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	16	0.16
(1,1119)	2:97:B:TRP:H	2:97:B:TRP:HZ3	2	0.16
(1,1119)	2:97:B:TRP:H	2:97:B:TRP:HZ3	10	0.16
(1,1112)	2:96:B:ASN:H	2:99:B:ARG:HB2	7	0.16
(1,1112)	2:96:B:ASN:H	2:99:B:ARG:HB3	7	0.16
(1,1108)	2:96:B:ASN:H	2:97:B:TRP:HB2	13	0.16
(1,1108)	2:96:B:ASN:H	2:97:B:TRP:HB3	13	0.16
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG21	12	0.16
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG22	12	0.16
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG23	12	0.16
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG21	12	0.16
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG22	12	0.16
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG23	12	0.16
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG21	12	0.16
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG22	12	0.16
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG23	12	0.16
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG21	12	0.16
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG22	12	0.16
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG23	12	0.16
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG21	12	0.16
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG22	12	0.16
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG23	12	0.16
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG21	12	0.16
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG22	12	0.16
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG23	12	0.16
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	6	0.16
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	6	0.16
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	6	0.16
(1,1071)	2:94:B:GLY:H	2:96:B:ASN:HD22	20	0.16
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	19	0.16
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	19	0.16
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	3	0.16
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG2	9	0.16
(1,1041)	2:92:B:ARG:H	2:89:B:GLU:HG3	9	0.16
(1,1030)	2:92:B:ARG:HB3	2:94:B:GLY:H	1	0.16
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG21	18	0.16
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG22	18	0.16
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG23	18	0.16
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	16	0.16
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	16	0.16
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	16	0.16
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	1	0.16
(1,910)	2:81:B:GLN:H	2:85:B:GLN:H	19	0.16
(1,867)	2:74:B:ILE:HG21	2:117:B:LYS:HB3	5	0.16
(1,867)	2:74:B:ILE:HG22	2:117:B:LYS:HB3	5	0.16
(1,867)	2:74:B:ILE:HG23	2:117:B:LYS:HB3	5	0.16
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	7	0.16
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	7	0.16
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	7	0.16
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	7	0.16
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	7	0.16
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	7	0.16
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	7	0.16
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	7	0.16
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	7	0.16
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	11	0.16
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	11	0.16
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	11	0.16
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	11	0.16
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	11	0.16
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	11	0.16
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	1	0.16
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	2	0.16
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	5	0.16
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	11	0.16
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	12	0.16
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	15	0.16
(1,814)	2:69:B:THR:HG21	2:110:B:LEU:HD11	15	0.16
(1,814)	2:69:B:THR:HG21	2:110:B:LEU:HD12	15	0.16
(1,814)	2:69:B:THR:HG21	2:110:B:LEU:HD13	15	0.16
(1,814)	2:69:B:THR:HG22	2:110:B:LEU:HD11	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	2:69:B:THR:HG22	2:110:B:LEU:HD12	15	0.16
(1,814)	2:69:B:THR:HG22	2:110:B:LEU:HD13	15	0.16
(1,814)	2:69:B:THR:HG23	2:110:B:LEU:HD11	15	0.16
(1,814)	2:69:B:THR:HG23	2:110:B:LEU:HD12	15	0.16
(1,814)	2:69:B:THR:HG23	2:110:B:LEU:HD13	15	0.16
(1,812)	2:69:B:THR:HG21	2:106:B:PHE:HE1	14	0.16
(1,812)	2:69:B:THR:HG21	2:106:B:PHE:HE2	14	0.16
(1,812)	2:69:B:THR:HG22	2:106:B:PHE:HE1	14	0.16
(1,812)	2:69:B:THR:HG22	2:106:B:PHE:HE2	14	0.16
(1,812)	2:69:B:THR:HG23	2:106:B:PHE:HE1	14	0.16
(1,812)	2:69:B:THR:HG23	2:106:B:PHE:HE2	14	0.16
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	19	0.16
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	19	0.16
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	17	0.16
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	13	0.16
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	13	0.16
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	16	0.16
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	16	0.16
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	2	0.16
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	5	0.16
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	10	0.16
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	20	0.16
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	19	0.16
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	15	0.16
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	15	0.16
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	15	0.16
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	15	0.16
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	15	0.16
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	15	0.16
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	15	0.16
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	15	0.16
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	15	0.16
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	17	0.16
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	17	0.16
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	17	0.16
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	17	0.16
(1,627)	2:47:B:LYS:H	2:47:B:LYS:HE3	11	0.16
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	20	0.16
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	20	0.16
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	6	0.16
(1,538)	2:41:B:THR:HG21	2:43:B:SER:H	5	0.16
(1,538)	2:41:B:THR:HG22	2:43:B:SER:H	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	2:41:B:THR:HG23	2:43:B:SER:H	5	0.16
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	13	0.16
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	6	0.16
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	13	0.16
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	14	0.16
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	14	0.16
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	16	0.16
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	16	0.16
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG21	1	0.16
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG22	1	0.16
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG23	1	0.16
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG21	20	0.16
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG22	20	0.16
(1,518)	2:39:B:GLU:H	2:41:B:THR:HG23	20	0.16
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	7	0.16
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	8	0.16
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	15	0.16
(1,502)	2:39:B:GLU:HB2	2:41:B:THR:HA	13	0.16
(1,502)	2:39:B:GLU:HB3	2:41:B:THR:HA	13	0.16
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	2	0.16
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	6	0.16
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	11	0.16
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	4	0.16
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	13	0.16
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	17	0.16
(1,451)	2:35:B:THR:HG1	2:36:B:GLU:H	10	0.16
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	1	0.16
(1,410)	2:32:B:GLU:HG2	2:34:B:ARG:H	19	0.16
(1,410)	2:32:B:GLU:HG3	2:34:B:ARG:H	19	0.16
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB2	1	0.16
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB3	1	0.16
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	1	0.16
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	10	0.16
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	16	0.16
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	16	0.16
(1,345)	2:26:B:GLN:HG2	2:27:B:PHE:H	13	0.16
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	5	0.16
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	20	0.16
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	20	0.16
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	6	0.16
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	6	0.16
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	1	0.16
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	6	0.16
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	6	0.16
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	18	0.16
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	18	0.16
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	16	0.16
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	18	0.16
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	8	0.16
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	19	0.16
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	7	0.16
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	15	0.16
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	2	0.16
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	2	0.16
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	9	0.16
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	9	0.16
(1,187)	2:16:B:LYS:H	2:16:B:LYS:HE2	10	0.16
(1,187)	2:16:B:LYS:H	2:16:B:LYS:HE3	10	0.16
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG11	6	0.16
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG12	6	0.16
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG13	6	0.16
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG21	6	0.16
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG22	6	0.16
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG23	6	0.16
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG11	6	0.16
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG12	6	0.16
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG13	6	0.16
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG21	6	0.16
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG22	6	0.16
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG23	6	0.16
(1,155)	2:13:B:LEU:HG	2:14:B:SER:H	11	0.16
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE1	1	0.16
(1,139)	2:12:B:PHE:H	2:12:B:PHE:HE2	1	0.16
(1,104)	2:10:B:VAL:HG11	2:12:B:PHE:H	12	0.16
(1,104)	2:10:B:VAL:HG12	2:12:B:PHE:H	12	0.16
(1,104)	2:10:B:VAL:HG13	2:12:B:PHE:H	12	0.16
(1,74)	2:8:B:LEU:HG	2:10:B:VAL:H	18	0.16
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	6	0.16
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	8	0.16
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	12	0.16
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	16	0.16
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	20	0.16
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	18	0.15
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	6	0.15
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	12	0.15
(1,2048)	1:319:A:TRP:H	1:319:A:TRP:HD1	6	0.15
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	14	0.15
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	17	0.15
(1,2025)	1:318:A:LEU:H	1:317:A:HIS:HA	17	0.15
(1,1979)	1:315:A:PHE:H	1:314:A:THR:HA	9	0.15
(1,1946)	1:313:A:THR:H	1:312:A:GLY:HA3	8	0.15
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	2	0.15
(1,1919)	2:169:B:ARG:H	2:170:B:LEU:HA	5	0.15
(1,1916)	2:169:B:ARG:H	2:169:B:ARG:HG3	2	0.15
(1,1908)	2:169:B:ARG:HA	2:170:B:LEU:H	16	0.15
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB2	7	0.15
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB3	7	0.15
(1,1896)	2:168:B:GLU:HG3	2:170:B:LEU:H	4	0.15
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	5	0.15
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	5	0.15
(1,1874)	2:166:B:GLY:HA2	2:167:B:GLN:H	13	0.15
(1,1861)	2:165:B:LYS:HD2	2:166:B:GLY:H	14	0.15
(1,1861)	2:165:B:LYS:HD3	2:166:B:GLY:H	14	0.15
(1,1854)	2:165:B:LYS:HA	2:166:B:GLY:H	6	0.15
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	6	0.15
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	14	0.15
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	16	0.15
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB2	18	0.15
(1,1814)	2:160:B:ALA:HA	2:163:B:SER:HB3	18	0.15
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	10	0.15
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	17	0.15
(1,1788)	2:157:B:ASN:HB2	2:159:B:ALA:HA	5	0.15
(1,1787)	2:157:B:ASN:HB3	2:159:B:ALA:HA	5	0.15
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	6	0.15
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	6	0.15
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	9	0.15
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	9	0.15
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	17	0.15
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	17	0.15
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	17	0.15
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	19	0.15
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	19	0.15
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	19	0.15
(1,1707)	2:150:B:THR:H	2:151:B:PHE:HE1	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1707)	2:150:B:THR:H	2:151:B:PHE:HE2	19	0.15
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	1	0.15
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	1	0.15
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	1	0.15
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	17	0.15
(1,1640)	2:144:B:GLU:H	2:145:B:ASN:HD22	18	0.15
(1,1631)	2:144:B:GLU:HG3	2:145:B:ASN:H	8	0.15
(1,1600)	2:142:B:ILE:HD11	2:147:B:GLY:HA2	4	0.15
(1,1600)	2:142:B:ILE:HD12	2:147:B:GLY:HA2	4	0.15
(1,1600)	2:142:B:ILE:HD13	2:147:B:GLY:HA2	4	0.15
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD11	5	0.15
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD12	5	0.15
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD13	5	0.15
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	8	0.15
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	17	0.15
(1,1562)	2:138:B:LEU:H	2:139:B:GLU:HG2	2	0.15
(1,1562)	2:138:B:LEU:H	2:139:B:GLU:HG3	2	0.15
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	15	0.15
(1,1551)	2:138:B:LEU:HD11	2:139:B:GLU:H	4	0.15
(1,1551)	2:138:B:LEU:HD12	2:139:B:GLU:H	4	0.15
(1,1551)	2:138:B:LEU:HD13	2:139:B:GLU:H	4	0.15
(1,1531)	2:135:B:ASN:H	2:137:B:HIS:H	18	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	10	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	10	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	10	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	10	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	10	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	10	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD11	19	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD12	19	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD13	19	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD21	19	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD22	19	0.15
(1,1516)	2:134:B:LEU:H	2:134:B:LEU:HD23	19	0.15
(1,1507)	2:134:B:LEU:HD11	2:136:B:ASP:H	1	0.15
(1,1507)	2:134:B:LEU:HD12	2:136:B:ASP:H	1	0.15
(1,1507)	2:134:B:LEU:HD13	2:136:B:ASP:H	1	0.15
(1,1507)	2:134:B:LEU:HD21	2:136:B:ASP:H	1	0.15
(1,1507)	2:134:B:LEU:HD22	2:136:B:ASP:H	1	0.15
(1,1507)	2:134:B:LEU:HD23	2:136:B:ASP:H	1	0.15
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	16	0.15
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	16	0.15
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	16	0.15
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	16	0.15
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	16	0.15
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	11	0.15
(1,1367)	2:117:B:LYS:H	2:117:B:LYS:HD3	8	0.15
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	6	0.15
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	6	0.15
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	6	0.15
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	7	0.15
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	7	0.15
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	7	0.15
(1,1338)	2:115:B:VAL:HG11	2:119:B:MET:H	7	0.15
(1,1338)	2:115:B:VAL:HG12	2:119:B:MET:H	7	0.15
(1,1338)	2:115:B:VAL:HG13	2:119:B:MET:H	7	0.15
(1,1292)	2:112:B:VAL:HG11	2:113:B:GLU:H	20	0.15
(1,1292)	2:112:B:VAL:HG12	2:113:B:GLU:H	20	0.15
(1,1292)	2:112:B:VAL:HG13	2:113:B:GLU:H	20	0.15
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	3	0.15
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	10	0.15
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	13	0.15
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	16	0.15
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD1	13	0.15
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD2	13	0.15
(1,1144)	2:100:B:ILE:HG21	2:138:B:LEU:HG	6	0.15
(1,1144)	2:100:B:ILE:HG22	2:138:B:LEU:HG	6	0.15
(1,1144)	2:100:B:ILE:HG23	2:138:B:LEU:HG	6	0.15
(1,1113)	2:96:B:ASN:H	2:99:B:ARG:H	12	0.15
(1,1106)	2:96:B:ASN:H	2:97:B:TRP:HB3	5	0.15
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD11	14	0.15
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD12	14	0.15
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD13	14	0.15
(1,1071)	2:94:B:GLY:H	2:96:B:ASN:HD22	2	0.15
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG11	18	0.15
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG12	18	0.15
(1,1066)	2:94:B:GLY:H	2:95:B:VAL:HG13	18	0.15
(1,1060)	2:93:B:ASP:H	2:94:B:GLY:HA2	10	0.15
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	11	0.15
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD1	11	0.15
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD2	11	0.15
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD1	11	0.15
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD2	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD1	11	0.15
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD2	11	0.15
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD1	13	0.15
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD2	13	0.15
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD1	13	0.15
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD2	13	0.15
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD1	13	0.15
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD2	13	0.15
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	13	0.15
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	17	0.15
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA2	7	0.15
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA3	7	0.15
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA2	7	0.15
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA3	7	0.15
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA2	7	0.15
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA3	7	0.15
(1,867)	2:74:B:ILE:HG21	2:117:B:LYS:HB3	4	0.15
(1,867)	2:74:B:ILE:HG22	2:117:B:LYS:HB3	4	0.15
(1,867)	2:74:B:ILE:HG23	2:117:B:LYS:HB3	4	0.15
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	20	0.15
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	20	0.15
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	20	0.15
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	20	0.15
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	20	0.15
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	20	0.15
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	20	0.15
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	20	0.15
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	20	0.15
(1,861)	2:74:B:ILE:HD11	2:119:B:MET:HB2	14	0.15
(1,861)	2:74:B:ILE:HD11	2:119:B:MET:HB3	14	0.15
(1,861)	2:74:B:ILE:HD12	2:119:B:MET:HB2	14	0.15
(1,861)	2:74:B:ILE:HD12	2:119:B:MET:HB3	14	0.15
(1,861)	2:74:B:ILE:HD13	2:119:B:MET:HB2	14	0.15
(1,861)	2:74:B:ILE:HD13	2:119:B:MET:HB3	14	0.15
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	7	0.15
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	7	0.15
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	7	0.15
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	7	0.15
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	7	0.15
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	7	0.15
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	8	0.15
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	8	0.15
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	8	0.15
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	8	0.15
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	8	0.15
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	8	0.15
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	8	0.15
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	8	0.15
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD21	20	0.15
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD22	20	0.15
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD23	20	0.15
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	9	0.15
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	9	0.15
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	17	0.15
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	17	0.15
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	2	0.15
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	14	0.15
(1,775)	2:63:B:ARG:HD2	2:64:B:ALA:H	13	0.15
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	11	0.15
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	11	0.15
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	12	0.15
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	12	0.15
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	6	0.15
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	14	0.15
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	7	0.15
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	9	0.15
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	13	0.15
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	13	0.15
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	4	0.15
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	4	0.15
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	17	0.15
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	17	0.15
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD1	11	0.15
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD2	11	0.15
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	3	0.15
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	3	0.15
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	3	0.15
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	3	0.15
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	3	0.15
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	3	0.15
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	3	0.15
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	3	0.15
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	15	0.15
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	15	0.15
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	15	0.15
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	15	0.15
(1,627)	2:47:B:LYS:H	2:47:B:LYS:HE3	4	0.15
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	12	0.15
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	17	0.15
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	19	0.15
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	3	0.15
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	3	0.15
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	3	0.15
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	3	0.15
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	3	0.15
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	3	0.15
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	19	0.15
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	19	0.15
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	19	0.15
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	19	0.15
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	19	0.15
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	19	0.15
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	9	0.15
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	9	0.15
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	9	0.15
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG11	3	0.15
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG12	3	0.15
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG13	3	0.15
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG11	13	0.15
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG12	13	0.15
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG13	13	0.15
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG21	13	0.15
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG22	13	0.15
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG23	13	0.15
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	1	0.15
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	9	0.15
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	18	0.15
(1,551)	2:42:B:GLU:H	2:42:B:GLU:HG2	16	0.15
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	2	0.15
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	11	0.15
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	8	0.15
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	8	0.15
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	13	0.15
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	19	0.15
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	19	0.15
(1,492)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	17	0.15
(1,492)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	17	0.15
(1,492)	2:38:B:PRO:HD3	2:39:B:GLU:HG2	17	0.15
(1,492)	2:38:B:PRO:HD3	2:39:B:GLU:HG3	17	0.15
(1,484)	2:37:B:ALA:H	2:38:B:PRO:HD2	19	0.15
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB1	9	0.15
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB2	9	0.15
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB3	9	0.15
(1,480)	2:37:B:ALA:H	2:37:B:ALA:HA	4	0.15
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG2	12	0.15
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG3	12	0.15
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG2	12	0.15
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG3	12	0.15
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG2	12	0.15
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG3	12	0.15
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG2	13	0.15
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG3	13	0.15
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG2	13	0.15
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG3	13	0.15
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG2	13	0.15
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG3	13	0.15
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	5	0.15
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	2	0.15
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	14	0.15
(1,449)	2:35:B:THR:HA	2:36:B:GLU:H	8	0.15
(1,446)	2:35:B:THR:HA	2:36:B:GLU:HB2	19	0.15
(1,444)	2:34:B:ARG:H	2:35:B:THR:H	18	0.15
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	8	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	2	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	2	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	2	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	8	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	8	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	8	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	15	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	15	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	15	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	20	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	20	0.15
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	15	0.15
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	18	0.15
(1,410)	2:32:B:GLU:HG2	2:34:B:ARG:H	15	0.15
(1,410)	2:32:B:GLU:HG3	2:34:B:ARG:H	15	0.15
(1,404)	2:31:B:GLU:H	2:31:B:GLU:HB2	9	0.15
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG11	8	0.15
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG12	8	0.15
(1,372)	2:28:B:SER:H	2:30:B:VAL:HG13	8	0.15
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	9	0.15
(1,321)	2:24:B:TRP:HB2	2:26:B:GLN:H	6	0.15
(1,321)	2:24:B:TRP:HB3	2:26:B:GLN:H	6	0.15
(1,275)	2:20:B:LYS:HG2	2:22:B:TYR:H	17	0.15
(1,275)	2:20:B:LYS:HG3	2:22:B:TYR:H	17	0.15
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	11	0.15
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	11	0.15
(1,270)	2:20:B:LYS:HD2	2:112:B:VAL:HG11	12	0.15
(1,270)	2:20:B:LYS:HD2	2:112:B:VAL:HG12	12	0.15
(1,270)	2:20:B:LYS:HD2	2:112:B:VAL:HG13	12	0.15
(1,270)	2:20:B:LYS:HD2	2:112:B:VAL:HG21	12	0.15
(1,270)	2:20:B:LYS:HD2	2:112:B:VAL:HG22	12	0.15
(1,270)	2:20:B:LYS:HD2	2:112:B:VAL:HG23	12	0.15
(1,270)	2:20:B:LYS:HD3	2:112:B:VAL:HG11	12	0.15
(1,270)	2:20:B:LYS:HD3	2:112:B:VAL:HG12	12	0.15
(1,270)	2:20:B:LYS:HD3	2:112:B:VAL:HG13	12	0.15
(1,270)	2:20:B:LYS:HD3	2:112:B:VAL:HG21	12	0.15
(1,270)	2:20:B:LYS:HD3	2:112:B:VAL:HG22	12	0.15
(1,270)	2:20:B:LYS:HD3	2:112:B:VAL:HG23	12	0.15
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	20	0.15
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	20	0.15
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	2	0.15
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	13	0.15
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	18	0.15
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	12	0.15
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	12	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG11	7	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG12	7	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG13	7	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG21	7	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG22	7	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG23	7	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG11	7	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG12	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG13	7	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG21	7	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG22	7	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG23	7	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG11	8	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG12	8	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG13	8	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG21	8	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG22	8	0.15
(1,183)	2:16:B:LYS:HG2	2:112:B:VAL:HG23	8	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG11	8	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG12	8	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG13	8	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG21	8	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG22	8	0.15
(1,183)	2:16:B:LYS:HG3	2:112:B:VAL:HG23	8	0.15
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD1	8	0.15
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD2	8	0.15
(1,74)	2:8:B:LEU:HG	2:10:B:VAL:H	3	0.15
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG2	17	0.15
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG3	17	0.15
(1,30)	2:5:B:ASN:HA	2:6:B:ARG:H	7	0.15
(1,3)	2:1:B:MET:HG2	2:2:B:SER:HA	6	0.15
(1,3)	2:1:B:MET:HG3	2:2:B:SER:HA	6	0.15
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	4	0.14
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	6	0.14
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	10	0.14
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	17	0.14
(1,2103)	1:323:A:GLU:H	1:322:A:LEU:HA	8	0.14
(1,2102)	1:323:A:GLU:H	1:321:A:SER:HB2	4	0.14
(1,2102)	1:323:A:GLU:H	1:321:A:SER:HB2	15	0.14
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	14	0.14
(1,2069)	1:321:A:SER:H	1:320:A:SER:HA	11	0.14
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	16	0.14
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	16	0.14
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	16	0.14
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	1	0.14
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	2	0.14
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	3	0.14
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	4	0.14
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	19	0.14
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	7	0.14
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	10	0.14
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	18	0.14
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	5	0.14
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	5	0.14
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	5	0.14
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	5	0.14
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	5	0.14
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	5	0.14
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	14	0.14
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	15	0.14
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	1	0.14
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	10	0.14
(1,1923)	2:170:B:LEU:HG	2:171:B:GLU:H	2	0.14
(1,1917)	2:169:B:ARG:H	2:169:B:ARG:HG2	12	0.14
(1,1898)	2:168:B:GLU:HG2	2:170:B:LEU:H	1	0.14
(1,1898)	2:168:B:GLU:HG2	2:170:B:LEU:H	8	0.14
(1,1898)	2:168:B:GLU:HG2	2:170:B:LEU:H	20	0.14
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG2	2	0.14
(1,1889)	2:167:B:GLN:H	2:167:B:GLN:HG3	2	0.14
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	14	0.14
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	14	0.14
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	16	0.14
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	16	0.14
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	14	0.14
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	17	0.14
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	19	0.14
(1,1866)	2:165:B:LYS:H	2:165:B:LYS:HB2	16	0.14
(1,1862)	2:165:B:LYS:HD2	2:167:B:GLN:H	14	0.14
(1,1862)	2:165:B:LYS:HD3	2:167:B:GLN:H	14	0.14
(1,1860)	2:165:B:LYS:HB2	2:168:B:GLU:H	15	0.14
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	15	0.14
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	18	0.14
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	11	0.14
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	18	0.14
(1,1829)	2:162:B:GLU:HA	2:163:B:SER:H	10	0.14
(1,1819)	2:161:B:ALA:HA	2:162:B:GLU:H	3	0.14
(1,1812)	2:160:B:ALA:HA	2:161:B:ALA:H	13	0.14
(1,1787)	2:157:B:ASN:HB3	2:159:B:ALA:HA	14	0.14
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	10	0.14
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	10	0.14
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	13	0.14
(1,1735)	2:152:B:VAL:HG21	2:156:B:GLY:H	19	0.14
(1,1735)	2:152:B:VAL:HG22	2:156:B:GLY:H	19	0.14
(1,1735)	2:152:B:VAL:HG23	2:156:B:GLY:H	19	0.14
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	4	0.14
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	4	0.14
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	19	0.14
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	19	0.14
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	10	0.14
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	10	0.14
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	10	0.14
(1,1694)	2:150:B:THR:HB	2:153:B:GLU:HG3	2	0.14
(1,1661)	2:146:B:GLY:H	2:149:B:ASP:H	6	0.14
(1,1661)	2:146:B:GLY:H	2:149:B:ASP:H	11	0.14
(1,1661)	2:146:B:GLY:H	2:149:B:ASP:H	19	0.14
(1,1657)	2:145:B:ASN:H	2:148:B:TRP:H	1	0.14
(1,1628)	2:143:B:GLN:H	2:145:B:ASN:H	14	0.14
(1,1614)	2:143:B:GLN:HA	2:147:B:GLY:H	3	0.14
(1,1614)	2:143:B:GLN:HA	2:147:B:GLY:H	16	0.14
(1,1601)	2:142:B:ILE:HD11	2:147:B:GLY:H	9	0.14
(1,1601)	2:142:B:ILE:HD12	2:147:B:GLY:H	9	0.14
(1,1601)	2:142:B:ILE:HD13	2:147:B:GLY:H	9	0.14
(1,1598)	2:142:B:ILE:HD11	2:146:B:GLY:H	15	0.14
(1,1598)	2:142:B:ILE:HD12	2:146:B:GLY:H	15	0.14
(1,1598)	2:142:B:ILE:HD13	2:146:B:GLY:H	15	0.14
(1,1590)	2:141:B:TRP:H	2:142:B:ILE:HB	17	0.14
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	2	0.14
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	9	0.14
(1,1552)	2:138:B:LEU:HD21	2:139:B:GLU:H	17	0.14
(1,1552)	2:138:B:LEU:HD22	2:139:B:GLU:H	17	0.14
(1,1552)	2:138:B:LEU:HD23	2:139:B:GLU:H	17	0.14
(1,1551)	2:138:B:LEU:HD11	2:139:B:GLU:H	3	0.14
(1,1551)	2:138:B:LEU:HD12	2:139:B:GLU:H	3	0.14
(1,1551)	2:138:B:LEU:HD13	2:139:B:GLU:H	3	0.14
(1,1541)	2:137:B:HIS:H	2:137:B:HIS:HD2	15	0.14
(1,1531)	2:135:B:ASN:H	2:137:B:HIS:H	17	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	9	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	9	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	9	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	9	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	9	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	18	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	18	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	18	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	18	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	18	0.14
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	18	0.14
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	8	0.14
(1,1389)	2:119:B:MET:H	2:120:B:GLN:HE22	1	0.14
(1,1361)	2:116:B:ASP:H	2:119:B:MET:H	11	0.14
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG11	4	0.14
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG12	4	0.14
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG13	4	0.14
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG21	4	0.14
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG22	4	0.14
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG23	4	0.14
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG11	4	0.14
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG12	4	0.14
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG13	4	0.14
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG21	4	0.14
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG22	4	0.14
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG23	4	0.14
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG11	4	0.14
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG12	4	0.14
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG13	4	0.14
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG21	4	0.14
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG22	4	0.14
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG23	4	0.14
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG11	4	0.14
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG12	4	0.14
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG13	4	0.14
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG21	4	0.14
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG22	4	0.14
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG23	4	0.14
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG11	4	0.14
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG12	4	0.14
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG13	4	0.14
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG21	4	0.14
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG22	4	0.14
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG23	4	0.14
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG11	4	0.14
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG12	4	0.14
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG13	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG21	4	0.14
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG22	4	0.14
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG23	4	0.14
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD11	1	0.14
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD12	1	0.14
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD13	1	0.14
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD21	1	0.14
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD22	1	0.14
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD23	1	0.14
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	4	0.14
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	13	0.14
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	16	0.14
(1,1292)	2:112:B:VAL:HG11	2:113:B:GLU:H	7	0.14
(1,1292)	2:112:B:VAL:HG12	2:113:B:GLU:H	7	0.14
(1,1292)	2:112:B:VAL:HG13	2:113:B:GLU:H	7	0.14
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG11	4	0.14
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG12	4	0.14
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG13	4	0.14
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	12	0.14
(1,1144)	2:100:B:ILE:HG21	2:138:B:LEU:HG	9	0.14
(1,1144)	2:100:B:ILE:HG22	2:138:B:LEU:HG	9	0.14
(1,1144)	2:100:B:ILE:HG23	2:138:B:LEU:HG	9	0.14
(1,1137)	2:100:B:ILE:HD11	2:142:B:ILE:HG21	11	0.14
(1,1137)	2:100:B:ILE:HD11	2:142:B:ILE:HG22	11	0.14
(1,1137)	2:100:B:ILE:HD11	2:142:B:ILE:HG23	11	0.14
(1,1137)	2:100:B:ILE:HD12	2:142:B:ILE:HG21	11	0.14
(1,1137)	2:100:B:ILE:HD12	2:142:B:ILE:HG22	11	0.14
(1,1137)	2:100:B:ILE:HD12	2:142:B:ILE:HG23	11	0.14
(1,1137)	2:100:B:ILE:HD13	2:142:B:ILE:HG21	11	0.14
(1,1137)	2:100:B:ILE:HD13	2:142:B:ILE:HG22	11	0.14
(1,1137)	2:100:B:ILE:HD13	2:142:B:ILE:HG23	11	0.14
(1,1116)	2:97:B:TRP:H	2:97:B:TRP:HE1	1	0.14
(1,1116)	2:97:B:TRP:H	2:97:B:TRP:HE1	7	0.14
(1,1111)	2:96:B:ASN:H	2:97:B:TRP:HZ3	17	0.14
(1,1110)	2:96:B:ASN:H	2:97:B:TRP:H	2	0.14
(1,1107)	2:96:B:ASN:H	2:97:B:TRP:HB2	18	0.14
(1,1096)	2:96:B:ASN:HD21	2:99:B:ARG:H	9	0.14
(1,1076)	2:95:B:VAL:HG11	2:96:B:ASN:HD22	14	0.14
(1,1076)	2:95:B:VAL:HG12	2:96:B:ASN:HD22	14	0.14
(1,1076)	2:95:B:VAL:HG13	2:96:B:ASN:HD22	14	0.14
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	2	0.14
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	17	0.14
(1,1032)	2:92:B:ARG:HB2	2:94:B:GLY:H	17	0.14
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	1	0.14
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	1	0.14
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	1	0.14
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	8	0.14
(1,881)	2:77:B:GLY:HA3	2:122:B:LEU:HD21	4	0.14
(1,881)	2:77:B:GLY:HA3	2:122:B:LEU:HD22	4	0.14
(1,881)	2:77:B:GLY:HA3	2:122:B:LEU:HD23	4	0.14
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA2	11	0.14
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA3	11	0.14
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA2	11	0.14
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA3	11	0.14
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA2	11	0.14
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA3	11	0.14
(1,867)	2:74:B:ILE:HG21	2:117:B:LYS:HB3	1	0.14
(1,867)	2:74:B:ILE:HG22	2:117:B:LYS:HB3	1	0.14
(1,867)	2:74:B:ILE:HG23	2:117:B:LYS:HB3	1	0.14
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	12	0.14
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	12	0.14
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	12	0.14
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	12	0.14
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	12	0.14
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	12	0.14
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	12	0.14
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	12	0.14
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	12	0.14
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	7	0.14
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	7	0.14
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	7	0.14
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	7	0.14
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	7	0.14
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	7	0.14
(1,847)	2:72:B:LEU:HD11	2:85:B:GLN:HG2	19	0.14
(1,847)	2:72:B:LEU:HD11	2:85:B:GLN:HG3	19	0.14
(1,847)	2:72:B:LEU:HD12	2:85:B:GLN:HG2	19	0.14
(1,847)	2:72:B:LEU:HD12	2:85:B:GLN:HG3	19	0.14
(1,847)	2:72:B:LEU:HD13	2:85:B:GLN:HG2	19	0.14
(1,847)	2:72:B:LEU:HD13	2:85:B:GLN:HG3	19	0.14
(1,847)	2:72:B:LEU:HD21	2:85:B:GLN:HG2	19	0.14
(1,847)	2:72:B:LEU:HD21	2:85:B:GLN:HG3	19	0.14
(1,847)	2:72:B:LEU:HD22	2:85:B:GLN:HG2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	2:72:B:LEU:HD22	2:85:B:GLN:HG3	19	0.14
(1,847)	2:72:B:LEU:HD23	2:85:B:GLN:HG2	19	0.14
(1,847)	2:72:B:LEU:HD23	2:85:B:GLN:HG3	19	0.14
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD11	2	0.14
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD12	2	0.14
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD13	2	0.14
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD21	2	0.14
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD22	2	0.14
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD23	2	0.14
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD11	2	0.14
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD12	2	0.14
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD13	2	0.14
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD21	2	0.14
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD22	2	0.14
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD23	2	0.14
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD11	2	0.14
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD12	2	0.14
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD13	2	0.14
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD21	2	0.14
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD22	2	0.14
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD23	2	0.14
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD11	2	0.14
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD12	2	0.14
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD13	2	0.14
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD21	2	0.14
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD22	2	0.14
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD23	2	0.14
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD11	2	0.14
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD12	2	0.14
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD13	2	0.14
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD21	2	0.14
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD22	2	0.14
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD23	2	0.14
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD11	2	0.14
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD12	2	0.14
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD13	2	0.14
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD21	2	0.14
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD22	2	0.14
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD23	2	0.14
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	4	0.14
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	6	0.14
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	18	0.14
(1,809)	2:69:B:THR:HG1	2:110:B:LEU:H	2	0.14
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	14	0.14
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	14	0.14
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD1	16	0.14
(1,784)	2:64:B:ALA:H	2:65:B:PHE:HD2	16	0.14
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	19	0.14
(1,775)	2:63:B:ARG:HD2	2:64:B:ALA:H	5	0.14
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	9	0.14
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	12	0.14
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	16	0.14
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	14	0.14
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	11	0.14
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	2	0.14
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	2	0.14
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD1	7	0.14
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD2	7	0.14
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD1	15	0.14
(1,713)	2:52:B:GLU:H	2:155:B:TYR:HD2	15	0.14
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD21	16	0.14
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD22	16	0.14
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD23	16	0.14
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	1	0.14
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	1	0.14
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	1	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	1	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	1	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	1	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	1	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	1	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	1	0.14
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	2	0.14
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	2	0.14
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	2	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	2	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	2	0.14
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	2	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	2	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	2	0.14
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	2	0.14
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	9	0.14
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	9	0.14
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	9	0.14
(1,628)	2:47:B:LYS:H	2:47:B:LYS:HE2	6	0.14
(1,613)	2:47:B:LYS:HD3	2:48:B:GLN:H	5	0.14
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG11	11	0.14
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG12	11	0.14
(1,585)	2:45:B:ALA:H	2:152:B:VAL:HG13	11	0.14
(1,580)	2:45:B:ALA:HB1	2:152:B:VAL:HG21	7	0.14
(1,580)	2:45:B:ALA:HB1	2:152:B:VAL:HG22	7	0.14
(1,580)	2:45:B:ALA:HB1	2:152:B:VAL:HG23	7	0.14
(1,580)	2:45:B:ALA:HB2	2:152:B:VAL:HG21	7	0.14
(1,580)	2:45:B:ALA:HB2	2:152:B:VAL:HG22	7	0.14
(1,580)	2:45:B:ALA:HB2	2:152:B:VAL:HG23	7	0.14
(1,580)	2:45:B:ALA:HB3	2:152:B:VAL:HG21	7	0.14
(1,580)	2:45:B:ALA:HB3	2:152:B:VAL:HG22	7	0.14
(1,580)	2:45:B:ALA:HB3	2:152:B:VAL:HG23	7	0.14
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	7	0.14
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	15	0.14
(1,550)	2:42:B:GLU:H	2:42:B:GLU:HG3	1	0.14
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	11	0.14
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	17	0.14
(1,536)	2:41:B:THR:HG1	2:45:B:ALA:H	9	0.14
(1,536)	2:41:B:THR:HG1	2:45:B:ALA:H	13	0.14
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	3	0.14
(1,526)	2:40:B:GLY:H	2:40:B:GLY:HA2	14	0.14
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	9	0.14
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	2	0.14
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	2	0.14
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	10	0.14
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	5	0.14
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	5	0.14
(1,486)	2:37:B:ALA:H	2:39:B:GLU:H	9	0.14
(1,465)	2:36:B:GLU:HB2	2:37:B:ALA:H	2	0.14
(1,465)	2:36:B:GLU:HB3	2:37:B:ALA:H	2	0.14
(1,442)	2:34:B:ARG:H	2:35:B:THR:HB	14	0.14
(1,422)	2:33:B:ASN:HD22	2:34:B:ARG:H	6	0.14
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	5	0.14
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	11	0.14
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	12	0.14
(1,345)	2:26:B:GLN:HG2	2:27:B:PHE:H	5	0.14
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	13	0.14
(1,334)	2:25:B:SER:HB2	2:29:B:ASP:H	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	2:25:B:SER:HB3	2:29:B:ASP:H	16	0.14
(1,324)	2:24:B:TRP:HD1	2:25:B:SER:H	19	0.14
(1,321)	2:24:B:TRP:HB2	2:26:B:GLN:H	4	0.14
(1,321)	2:24:B:TRP:HB3	2:26:B:GLN:H	4	0.14
(1,309)	2:23:B:SER:HA	2:26:B:GLN:H	9	0.14
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	1	0.14
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	1	0.14
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	2	0.14
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	2	0.14
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	9	0.14
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	9	0.14
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	15	0.14
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	15	0.14
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	13	0.14
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	13	0.14
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG11	14	0.14
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG12	14	0.14
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG13	14	0.14
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG21	14	0.14
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG22	14	0.14
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG23	14	0.14
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	14	0.14
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	14	0.14
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	7	0.14
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	7	0.14
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	14	0.14
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	14	0.14
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	6	0.14
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	15	0.14
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	1	0.14
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	7	0.14
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	6	0.14
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	13	0.14
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	1	0.14
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	1	0.14
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	6	0.14
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	6	0.14
(1,211)	2:17:B:LEU:HD11	2:22:B:TYR:H	12	0.14
(1,211)	2:17:B:LEU:HD12	2:22:B:TYR:H	12	0.14
(1,211)	2:17:B:LEU:HD13	2:22:B:TYR:H	12	0.14
(1,211)	2:17:B:LEU:HD21	2:22:B:TYR:H	12	0.14
(1,211)	2:17:B:LEU:HD22	2:22:B:TYR:H	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	2:17:B:LEU:HD23	2:22:B:TYR:H	12	0.14
(1,173)	2:14:B:SER:H	2:24:B:TRP:HE1	13	0.14
(1,173)	2:14:B:SER:H	2:24:B:TRP:HE1	19	0.14
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD1	20	0.14
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD2	20	0.14
(1,104)	2:10:B:VAL:HG11	2:12:B:PHE:H	3	0.14
(1,104)	2:10:B:VAL:HG12	2:12:B:PHE:H	3	0.14
(1,104)	2:10:B:VAL:HG13	2:12:B:PHE:H	3	0.14
(1,104)	2:10:B:VAL:HG11	2:12:B:PHE:H	19	0.14
(1,104)	2:10:B:VAL:HG12	2:12:B:PHE:H	19	0.14
(1,104)	2:10:B:VAL:HG13	2:12:B:PHE:H	19	0.14
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG2	5	0.14
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG3	5	0.14
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG2	11	0.14
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG3	11	0.14
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD11	13	0.13
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD12	13	0.13
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD13	13	0.13
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD11	13	0.13
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD12	13	0.13
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD13	13	0.13
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	19	0.13
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	16	0.13
(1,2048)	1:319:A:TRP:H	1:319:A:TRP:HD1	20	0.13
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	1	0.13
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	12	0.13
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	15	0.13
(1,1979)	1:315:A:PHE:H	1:314:A:THR:HA	20	0.13
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	18	0.13
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	18	0.13
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	18	0.13
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	18	0.13
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	18	0.13
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	18	0.13
(1,1923)	2:170:B:LEU:HG	2:171:B:GLU:H	16	0.13
(1,1908)	2:169:B:ARG:HA	2:170:B:LEU:H	19	0.13
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	10	0.13
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	10	0.13
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB2	2	0.13
(1,1900)	2:168:B:GLU:H	2:168:B:GLU:HB3	2	0.13
(1,1895)	2:168:B:GLU:HG3	2:169:B:ARG:H	7	0.13
(1,1895)	2:168:B:GLU:HG3	2:169:B:ARG:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	9	0.13
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	11	0.13
(1,1862)	2:165:B:LYS:HD2	2:167:B:GLN:H	11	0.13
(1,1862)	2:165:B:LYS:HD3	2:167:B:GLN:H	11	0.13
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	2	0.13
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	5	0.13
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	9	0.13
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	19	0.13
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	4	0.13
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	20	0.13
(1,1809)	2:158:B:ASN:H	2:161:B:ALA:H	13	0.13
(1,1793)	2:157:B:ASN:H	2:159:B:ALA:H	5	0.13
(1,1787)	2:157:B:ASN:HB3	2:159:B:ALA:HA	9	0.13
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	1	0.13
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	1	0.13
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	10	0.13
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	10	0.13
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	6	0.13
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	6	0.13
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	6	0.13
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	6	0.13
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	6	0.13
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	6	0.13
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	16	0.13
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	16	0.13
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	16	0.13
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	16	0.13
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	16	0.13
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	16	0.13
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	17	0.13
(1,1670)	2:148:B:TRP:HB2	2:150:B:THR:H	12	0.13
(1,1670)	2:148:B:TRP:HB3	2:150:B:THR:H	12	0.13
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG21	17	0.13
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG22	17	0.13
(1,1662)	2:146:B:GLY:H	2:150:B:THR:HG23	17	0.13
(1,1658)	2:145:B:ASN:H	2:149:B:ASP:H	6	0.13
(1,1657)	2:145:B:ASN:H	2:148:B:TRP:H	12	0.13
(1,1655)	2:145:B:ASN:H	2:146:B:GLY:H	15	0.13
(1,1648)	2:145:B:ASN:HD22	2:146:B:GLY:H	20	0.13
(1,1643)	2:144:B:GLU:H	2:147:B:GLY:H	1	0.13
(1,1640)	2:144:B:GLU:H	2:145:B:ASN:HD22	17	0.13
(1,1615)	2:143:B:GLN:HB3	2:144:B:GLU:HA	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1598)	2:142:B:ILE:HD11	2:146:B:GLY:H	13	0.13
(1,1598)	2:142:B:ILE:HD12	2:146:B:GLY:H	13	0.13
(1,1598)	2:142:B:ILE:HD13	2:146:B:GLY:H	13	0.13
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	10	0.13
(1,1553)	2:138:B:LEU:HD11	2:141:B:TRP:H	20	0.13
(1,1553)	2:138:B:LEU:HD12	2:141:B:TRP:H	20	0.13
(1,1553)	2:138:B:LEU:HD13	2:141:B:TRP:H	20	0.13
(1,1553)	2:138:B:LEU:HD21	2:141:B:TRP:H	20	0.13
(1,1553)	2:138:B:LEU:HD22	2:141:B:TRP:H	20	0.13
(1,1553)	2:138:B:LEU:HD23	2:141:B:TRP:H	20	0.13
(1,1545)	2:137:B:HIS:H	2:138:B:LEU:HG	7	0.13
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	2	0.13
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	3	0.13
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	5	0.13
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	13	0.13
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	15	0.13
(1,1361)	2:116:B:ASP:H	2:119:B:MET:H	9	0.13
(1,1361)	2:116:B:ASP:H	2:119:B:MET:H	14	0.13
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	16	0.13
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	16	0.13
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	16	0.13
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD11	8	0.13
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD12	8	0.13
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD13	8	0.13
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD21	8	0.13
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD22	8	0.13
(1,1328)	2:114:B:SER:H	2:122:B:LEU:HD23	8	0.13
(1,1327)	2:114:B:SER:H	2:119:B:MET:H	19	0.13
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD11	17	0.13
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD12	17	0.13
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD13	17	0.13
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	6	0.13
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	1	0.13
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	6	0.13
(1,1211)	2:106:B:PHE:HE1	2:109:B:ALA:HB1	12	0.13
(1,1211)	2:106:B:PHE:HE1	2:109:B:ALA:HB2	12	0.13
(1,1211)	2:106:B:PHE:HE1	2:109:B:ALA:HB3	12	0.13
(1,1211)	2:106:B:PHE:HE2	2:109:B:ALA:HB1	12	0.13
(1,1211)	2:106:B:PHE:HE2	2:109:B:ALA:HB2	12	0.13
(1,1211)	2:106:B:PHE:HE2	2:109:B:ALA:HB3	12	0.13
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	14	0.13
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	14	0.13
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	16	0.13
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	16	0.13
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	16	0.13
(1,1116)	2:97:B:TRP:H	2:97:B:TRP:HE1	13	0.13
(1,1109)	2:96:B:ASN:H	2:97:B:TRP:HE1	15	0.13
(1,1106)	2:96:B:ASN:H	2:97:B:TRP:HB3	12	0.13
(1,1085)	2:95:B:VAL:HG11	2:141:B:TRP:H	19	0.13
(1,1085)	2:95:B:VAL:HG12	2:141:B:TRP:H	19	0.13
(1,1085)	2:95:B:VAL:HG13	2:141:B:TRP:H	19	0.13
(1,1085)	2:95:B:VAL:HG21	2:141:B:TRP:H	19	0.13
(1,1085)	2:95:B:VAL:HG22	2:141:B:TRP:H	19	0.13
(1,1085)	2:95:B:VAL:HG23	2:141:B:TRP:H	19	0.13
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	10	0.13
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	10	0.13
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	10	0.13
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	14	0.13
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	14	0.13
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	14	0.13
(1,1060)	2:93:B:ASP:H	2:94:B:GLY:HA2	9	0.13
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	13	0.13
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	4	0.13
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	6	0.13
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	20	0.13
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	13	0.13
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	13	0.13
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	13	0.13
(1,947)	2:86:B:VAL:HG11	2:87:B:VAL:HB	7	0.13
(1,947)	2:86:B:VAL:HG12	2:87:B:VAL:HB	7	0.13
(1,947)	2:86:B:VAL:HG13	2:87:B:VAL:HB	7	0.13
(1,947)	2:86:B:VAL:HG21	2:87:B:VAL:HB	7	0.13
(1,947)	2:86:B:VAL:HG22	2:87:B:VAL:HB	7	0.13
(1,947)	2:86:B:VAL:HG23	2:87:B:VAL:HB	7	0.13
(1,910)	2:81:B:GLN:H	2:85:B:GLN:H	7	0.13
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD11	20	0.13
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD12	20	0.13
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD13	20	0.13
(1,867)	2:74:B:ILE:HG21	2:117:B:LYS:HB3	12	0.13
(1,867)	2:74:B:ILE:HG22	2:117:B:LYS:HB3	12	0.13
(1,867)	2:74:B:ILE:HG23	2:117:B:LYS:HB3	12	0.13
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	5	0.13
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	5	0.13
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	5	0.13
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	5	0.13
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	5	0.13
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	5	0.13
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	5	0.13
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	5	0.13
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	17	0.13
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	17	0.13
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	17	0.13
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	17	0.13
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	17	0.13
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	17	0.13
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	7	0.13
(1,809)	2:69:B:THR:HG1	2:110:B:LEU:H	14	0.13
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD21	2	0.13
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD22	2	0.13
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD23	2	0.13
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	10	0.13
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	10	0.13
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	12	0.13
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	12	0.13
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	19	0.13
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	19	0.13
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	5	0.13
(1,783)	2:64:B:ALA:H	2:65:B:PHE:HA	6	0.13
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	5	0.13
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	5	0.13
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	18	0.13
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	18	0.13
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	19	0.13
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	19	0.13
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	7	0.13
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	8	0.13
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	10	0.13
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	11	0.13
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	18	0.13
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	6	0.13
(1,730)	2:54:B:GLY:H	2:55:B:ASP:HA	13	0.13
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	12	0.13
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	14	0.13
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	12	0.13
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	18	0.13
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	18	0.13
(1,711)	2:52:B:GLU:HG3	2:53:B:ALA:H	10	0.13
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	8	0.13
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	8	0.13
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	8	0.13
(1,666)	2:49:B:ALA:H	2:53:B:ALA:H	20	0.13
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	18	0.13
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	18	0.13
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	18	0.13
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	18	0.13
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	18	0.13
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	18	0.13
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	18	0.13
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	18	0.13
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	18	0.13
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	13	0.13
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	13	0.13
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	13	0.13
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	13	0.13
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	19	0.13
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	19	0.13
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	19	0.13
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	19	0.13
(1,627)	2:47:B:LYS:H	2:47:B:LYS:HE3	18	0.13
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	1	0.13
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	1	0.13
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	1	0.13
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	1	0.13
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	1	0.13
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	1	0.13
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	2	0.13
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	2	0.13
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	2	0.13
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	2	0.13
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	2	0.13
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	2	0.13
(1,599)	2:46:B:VAL:HG11	2:151:B:PHE:H	17	0.13
(1,599)	2:46:B:VAL:HG12	2:151:B:PHE:H	17	0.13
(1,599)	2:46:B:VAL:HG13	2:151:B:PHE:H	17	0.13
(1,599)	2:46:B:VAL:HG21	2:151:B:PHE:H	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	2:46:B:VAL:HG22	2:151:B:PHE:H	17	0.13
(1,599)	2:46:B:VAL:HG23	2:151:B:PHE:H	17	0.13
(1,597)	2:46:B:VAL:HG21	2:149:B:ASP:H	11	0.13
(1,597)	2:46:B:VAL:HG22	2:149:B:ASP:H	11	0.13
(1,597)	2:46:B:VAL:HG23	2:149:B:ASP:H	11	0.13
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	17	0.13
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	17	0.13
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	17	0.13
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	19	0.13
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	19	0.13
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	19	0.13
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG11	2	0.13
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG12	2	0.13
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG13	2	0.13
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG21	2	0.13
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG22	2	0.13
(1,570)	2:44:B:GLU:HG2	2:46:B:VAL:HG23	2	0.13
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG11	2	0.13
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG12	2	0.13
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG13	2	0.13
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG21	2	0.13
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG22	2	0.13
(1,570)	2:44:B:GLU:HG3	2:46:B:VAL:HG23	2	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG11	10	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG12	10	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG13	10	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG21	10	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG22	10	0.13
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG23	10	0.13
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	10	0.13
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	13	0.13
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	17	0.13
(1,550)	2:42:B:GLU:H	2:42:B:GLU:HG3	15	0.13
(1,535)	2:41:B:THR:HG1	2:44:B:GLU:H	5	0.13
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	19	0.13
(1,527)	2:40:B:GLY:H	2:41:B:THR:HG1	6	0.13
(1,527)	2:40:B:GLY:H	2:41:B:THR:HG1	20	0.13
(1,526)	2:40:B:GLY:H	2:40:B:GLY:HA2	19	0.13
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	18	0.13
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	3	0.13
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	3	0.13
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	2:38:B:PRO:HD3	2:39:B:GLU:HA	2	0.13
(1,486)	2:37:B:ALA:H	2:39:B:GLU:H	7	0.13
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB1	14	0.13
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB2	14	0.13
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB3	14	0.13
(1,457)	2:35:B:THR:HG21	2:37:B:ALA:H	6	0.13
(1,457)	2:35:B:THR:HG22	2:37:B:ALA:H	6	0.13
(1,457)	2:35:B:THR:HG23	2:37:B:ALA:H	6	0.13
(1,446)	2:35:B:THR:HA	2:36:B:GLU:HB2	14	0.13
(1,436)	2:34:B:ARG:HD2	2:35:B:THR:H	18	0.13
(1,436)	2:34:B:ARG:HD3	2:35:B:THR:H	18	0.13
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	7	0.13
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	17	0.13
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	18	0.13
(1,422)	2:33:B:ASN:HD22	2:34:B:ARG:H	17	0.13
(1,415)	2:32:B:GLU:H	2:33:B:ASN:H	9	0.13
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	6	0.13
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	13	0.13
(1,410)	2:32:B:GLU:HG2	2:34:B:ARG:H	12	0.13
(1,410)	2:32:B:GLU:HG3	2:34:B:ARG:H	12	0.13
(1,401)	2:30:B:VAL:H	2:33:B:ASN:H	6	0.13
(1,385)	2:30:B:VAL:HA	2:31:B:GLU:H	2	0.13
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	3	0.13
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	8	0.13
(1,333)	2:25:B:SER:HB2	2:26:B:GLN:H	17	0.13
(1,333)	2:25:B:SER:HB3	2:26:B:GLN:H	17	0.13
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	5	0.13
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	5	0.13
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	5	0.13
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	12	0.13
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	12	0.13
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	12	0.13
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG11	14	0.13
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG12	14	0.13
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG13	14	0.13
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG21	14	0.13
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG22	14	0.13
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG23	14	0.13
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	12	0.13
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	12	0.13
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	15	0.13
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	2:20:B:LYS:H	2:20:B:LYS:HE2	16	0.13
(1,281)	2:20:B:LYS:H	2:20:B:LYS:HE3	16	0.13
(1,272)	2:20:B:LYS:HD2	2:22:B:TYR:H	2	0.13
(1,272)	2:20:B:LYS:HD3	2:22:B:TYR:H	2	0.13
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	1	0.13
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	1	0.13
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	9	0.13
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	9	0.13
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	20	0.13
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	20	0.13
(1,257)	2:19:B:GLN:H	2:19:B:GLN:HE22	8	0.13
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	4	0.13
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	4	0.13
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	6	0.13
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	8	0.13
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	10	0.13
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	12	0.13
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	15	0.13
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	15	0.13
(1,211)	2:17:B:LEU:HD11	2:22:B:TYR:H	9	0.13
(1,211)	2:17:B:LEU:HD12	2:22:B:TYR:H	9	0.13
(1,211)	2:17:B:LEU:HD13	2:22:B:TYR:H	9	0.13
(1,211)	2:17:B:LEU:HD21	2:22:B:TYR:H	9	0.13
(1,211)	2:17:B:LEU:HD22	2:22:B:TYR:H	9	0.13
(1,211)	2:17:B:LEU:HD23	2:22:B:TYR:H	9	0.13
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD1	13	0.13
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD2	13	0.13
(1,148)	2:13:B:LEU:HD11	2:130:B:MET:HE1	7	0.13
(1,148)	2:13:B:LEU:HD11	2:130:B:MET:HE2	7	0.13
(1,148)	2:13:B:LEU:HD11	2:130:B:MET:HE3	7	0.13
(1,148)	2:13:B:LEU:HD12	2:130:B:MET:HE1	7	0.13
(1,148)	2:13:B:LEU:HD12	2:130:B:MET:HE2	7	0.13
(1,148)	2:13:B:LEU:HD12	2:130:B:MET:HE3	7	0.13
(1,148)	2:13:B:LEU:HD13	2:130:B:MET:HE1	7	0.13
(1,148)	2:13:B:LEU:HD13	2:130:B:MET:HE2	7	0.13
(1,148)	2:13:B:LEU:HD13	2:130:B:MET:HE3	7	0.13
(1,128)	2:11:B:ASP:HB2	2:13:B:LEU:H	1	0.13
(1,128)	2:11:B:ASP:HB3	2:13:B:LEU:H	1	0.13
(1,109)	2:10:B:VAL:HG21	2:12:B:PHE:H	17	0.13
(1,109)	2:10:B:VAL:HG22	2:12:B:PHE:H	17	0.13
(1,109)	2:10:B:VAL:HG23	2:12:B:PHE:H	17	0.13
(1,74)	2:8:B:LEU:HG	2:10:B:VAL:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:1:B:MET:HA	2:3:B:GLN:H	3	0.13
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD11	3	0.12
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD12	3	0.12
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD13	3	0.12
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD11	3	0.12
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD12	3	0.12
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD13	3	0.12
(1,2151)	2:155:B:TYR:HD1	1:315:A:PHE:HA	10	0.12
(1,2151)	2:155:B:TYR:HD2	1:315:A:PHE:HA	10	0.12
(1,2151)	2:155:B:TYR:HD1	1:315:A:PHE:HA	16	0.12
(1,2151)	2:155:B:TYR:HD2	1:315:A:PHE:HA	16	0.12
(1,2128)	1:325:A:ASP:H	1:322:A:LEU:HG	10	0.12
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	8	0.12
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	8	0.12
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	8	0.12
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	7	0.12
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	13	0.12
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	15	0.12
(1,2101)	1:323:A:GLU:H	1:321:A:SER:HB3	18	0.12
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	3	0.12
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	3	0.12
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	3	0.12
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	5	0.12
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	8	0.12
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	13	0.12
(1,2003)	1:317:A:HIS:H	1:314:A:THR:HA	18	0.12
(1,1997)	1:317:A:HIS:HD1	1:317:A:HIS:HA	8	0.12
(1,1997)	1:317:A:HIS:HD1	1:317:A:HIS:HA	14	0.12
(1,1988)	1:316:A:GLU:H	1:314:A:THR:HA	10	0.12
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	7	0.12
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	7	0.12
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	7	0.12
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	7	0.12
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	7	0.12
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	7	0.12
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	11	0.12
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	11	0.12
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	11	0.12
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	11	0.12
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	11	0.12
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	11	0.12
(1,1948)	1:313:A:THR:H	1:313:A:THR:HB	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1946)	1:313:A:THR:H	1:312:A:GLY:HA3	1	0.12
(1,1923)	2:170:B:LEU:HG	2:171:B:GLU:H	3	0.12
(1,1923)	2:170:B:LEU:HG	2:171:B:GLU:H	10	0.12
(1,1919)	2:169:B:ARG:H	2:170:B:LEU:HA	7	0.12
(1,1919)	2:169:B:ARG:H	2:170:B:LEU:HA	9	0.12
(1,1911)	2:169:B:ARG:HD2	2:170:B:LEU:H	17	0.12
(1,1911)	2:169:B:ARG:HD3	2:170:B:LEU:H	17	0.12
(1,1908)	2:169:B:ARG:HA	2:170:B:LEU:H	1	0.12
(1,1908)	2:169:B:ARG:HA	2:170:B:LEU:H	6	0.12
(1,1898)	2:168:B:GLU:HG2	2:170:B:LEU:H	9	0.12
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	1	0.12
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	1	0.12
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	8	0.12
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	8	0.12
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	18	0.12
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	18	0.12
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	4	0.12
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	9	0.12
(1,1877)	2:166:B:GLY:H	2:167:B:GLN:HB2	1	0.12
(1,1877)	2:166:B:GLY:H	2:167:B:GLN:HB3	1	0.12
(1,1841)	2:163:B:SER:HA	2:164:B:ARG:H	12	0.12
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	1	0.12
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	13	0.12
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	15	0.12
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	2	0.12
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	2	0.12
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE1	9	0.12
(1,1774)	2:154:B:LEU:H	2:155:B:TYR:HE2	9	0.12
(1,1748)	2:153:B:GLU:HG2	2:154:B:LEU:H	17	0.12
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	10	0.12
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	10	0.12
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	10	0.12
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	10	0.12
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	10	0.12
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	10	0.12
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	13	0.12
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	13	0.12
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	13	0.12
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	13	0.12
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	13	0.12
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	13	0.12
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	3	0.12
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	13	0.12
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	13	0.12
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	16	0.12
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	16	0.12
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG11	14	0.12
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG12	14	0.12
(1,1710)	2:150:B:THR:H	2:152:B:VAL:HG13	14	0.12
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	6	0.12
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	6	0.12
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	6	0.12
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG11	20	0.12
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG12	20	0.12
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG13	20	0.12
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG21	20	0.12
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG22	20	0.12
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG23	20	0.12
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	7	0.12
(1,1628)	2:143:B:GLN:H	2:145:B:ASN:H	12	0.12
(1,1594)	2:141:B:TRP:H	2:144:B:GLU:H	2	0.12
(1,1590)	2:141:B:TRP:H	2:142:B:ILE:HB	1	0.12
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD11	4	0.12
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD12	4	0.12
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD13	4	0.12
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	1	0.12
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	3	0.12
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	14	0.12
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	1	0.12
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	16	0.12
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	20	0.12
(1,1541)	2:137:B:HIS:H	2:137:B:HIS:HD2	8	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	13	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	13	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	13	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	13	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	13	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	13	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD11	19	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD12	19	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD13	19	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD21	19	0.12
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD22	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	2:133:B:TYR:H	2:134:B:LEU:HD23	19	0.12
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	14	0.12
(1,1367)	2:117:B:LYS:H	2:117:B:LYS:HD3	5	0.12
(1,1367)	2:117:B:LYS:H	2:117:B:LYS:HD3	12	0.12
(1,1361)	2:116:B:ASP:H	2:119:B:MET:H	2	0.12
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG11	8	0.12
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG12	8	0.12
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG13	8	0.12
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG21	8	0.12
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG22	8	0.12
(1,1346)	2:115:B:VAL:HG11	2:123:B:VAL:HG23	8	0.12
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG11	8	0.12
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG12	8	0.12
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG13	8	0.12
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG21	8	0.12
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG22	8	0.12
(1,1346)	2:115:B:VAL:HG12	2:123:B:VAL:HG23	8	0.12
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG11	8	0.12
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG12	8	0.12
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG13	8	0.12
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG21	8	0.12
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG22	8	0.12
(1,1346)	2:115:B:VAL:HG13	2:123:B:VAL:HG23	8	0.12
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG11	8	0.12
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG12	8	0.12
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG13	8	0.12
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG21	8	0.12
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG22	8	0.12
(1,1346)	2:115:B:VAL:HG21	2:123:B:VAL:HG23	8	0.12
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG11	8	0.12
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG12	8	0.12
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG13	8	0.12
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG21	8	0.12
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG22	8	0.12
(1,1346)	2:115:B:VAL:HG22	2:123:B:VAL:HG23	8	0.12
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG11	8	0.12
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG12	8	0.12
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG13	8	0.12
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG21	8	0.12
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG22	8	0.12
(1,1346)	2:115:B:VAL:HG23	2:123:B:VAL:HG23	8	0.12
(1,1292)	2:112:B:VAL:HG11	2:113:B:GLU:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	2:112:B:VAL:HG12	2:113:B:GLU:H	2	0.12
(1,1292)	2:112:B:VAL:HG13	2:113:B:GLU:H	2	0.12
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD11	11	0.12
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD12	11	0.12
(1,1255)	2:109:B:ALA:H	2:110:B:LEU:HD13	11	0.12
(1,1223)	2:106:B:PHE:H	2:110:B:LEU:HG	20	0.12
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD1	1	0.12
(1,1174)	2:102:B:ALA:H	2:104:B:PHE:HD2	1	0.12
(1,1165)	2:101:B:VAL:H	2:104:B:PHE:H	14	0.12
(1,1132)	2:100:B:ILE:HD11	2:103:B:PHE:H	17	0.12
(1,1132)	2:100:B:ILE:HD12	2:103:B:PHE:H	17	0.12
(1,1132)	2:100:B:ILE:HD13	2:103:B:PHE:H	17	0.12
(1,1119)	2:97:B:TRP:H	2:97:B:TRP:HZ3	19	0.12
(1,1119)	2:97:B:TRP:H	2:97:B:TRP:HZ3	20	0.12
(1,1113)	2:96:B:ASN:H	2:99:B:ARG:H	13	0.12
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG21	5	0.12
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG22	5	0.12
(1,1082)	2:95:B:VAL:HG11	2:100:B:ILE:HG23	5	0.12
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG21	5	0.12
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG22	5	0.12
(1,1082)	2:95:B:VAL:HG12	2:100:B:ILE:HG23	5	0.12
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG21	5	0.12
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG22	5	0.12
(1,1082)	2:95:B:VAL:HG13	2:100:B:ILE:HG23	5	0.12
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG21	5	0.12
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG22	5	0.12
(1,1082)	2:95:B:VAL:HG21	2:100:B:ILE:HG23	5	0.12
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG21	5	0.12
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG22	5	0.12
(1,1082)	2:95:B:VAL:HG22	2:100:B:ILE:HG23	5	0.12
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG21	5	0.12
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG22	5	0.12
(1,1082)	2:95:B:VAL:HG23	2:100:B:ILE:HG23	5	0.12
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	4	0.12
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	4	0.12
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	4	0.12
(1,1079)	2:95:B:VAL:HG21	2:96:B:ASN:HD22	12	0.12
(1,1079)	2:95:B:VAL:HG22	2:96:B:ASN:HD22	12	0.12
(1,1079)	2:95:B:VAL:HG23	2:96:B:ASN:HD22	12	0.12
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	5	0.12
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	16	0.12
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG21	8	0.12
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG22	8	0.12
(1,1012)	2:91:B:PHE:HA	2:95:B:VAL:HG23	8	0.12
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	6	0.12
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	6	0.12
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	6	0.12
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	8	0.12
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	8	0.12
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	8	0.12
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB1	2	0.12
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB2	2	0.12
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB3	2	0.12
(1,997)	2:90:B:LEU:HD11	2:102:B:ALA:H	13	0.12
(1,997)	2:90:B:LEU:HD12	2:102:B:ALA:H	13	0.12
(1,997)	2:90:B:LEU:HD13	2:102:B:ALA:H	13	0.12
(1,997)	2:90:B:LEU:HD21	2:102:B:ALA:H	13	0.12
(1,997)	2:90:B:LEU:HD22	2:102:B:ALA:H	13	0.12
(1,997)	2:90:B:LEU:HD23	2:102:B:ALA:H	13	0.12
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD1	7	0.12
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD2	7	0.12
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD1	7	0.12
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD2	7	0.12
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD1	7	0.12
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD2	7	0.12
(1,902)	2:81:B:GLN:HA	2:85:B:GLN:HB2	8	0.12
(1,902)	2:81:B:GLN:HA	2:85:B:GLN:HB3	8	0.12
(1,901)	2:81:B:GLN:HA	2:84:B:GLU:H	19	0.12
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD11	3	0.12
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD12	3	0.12
(1,880)	2:77:B:GLY:HA3	2:122:B:LEU:HD13	3	0.12
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA2	15	0.12
(1,879)	2:75:B:THR:HG21	2:77:B:GLY:HA3	15	0.12
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA2	15	0.12
(1,879)	2:75:B:THR:HG22	2:77:B:GLY:HA3	15	0.12
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA2	15	0.12
(1,879)	2:75:B:THR:HG23	2:77:B:GLY:HA3	15	0.12
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	2	0.12
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	2	0.12
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	2	0.12
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	2	0.12
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	2	0.12
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	2	0.12
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	2	0.12
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	2	0.12
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB1	14	0.12
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB2	14	0.12
(1,865)	2:74:B:ILE:HD11	2:79:B:ALA:HB3	14	0.12
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB1	14	0.12
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB2	14	0.12
(1,865)	2:74:B:ILE:HD12	2:79:B:ALA:HB3	14	0.12
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB1	14	0.12
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB2	14	0.12
(1,865)	2:74:B:ILE:HD13	2:79:B:ALA:HB3	14	0.12
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB2	3	0.12
(1,860)	2:74:B:ILE:HD11	2:117:B:LYS:HB3	3	0.12
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB2	3	0.12
(1,860)	2:74:B:ILE:HD12	2:117:B:LYS:HB3	3	0.12
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB2	3	0.12
(1,860)	2:74:B:ILE:HD13	2:117:B:LYS:HB3	3	0.12
(1,846)	2:72:B:LEU:HD11	2:74:B:ILE:HB	19	0.12
(1,846)	2:72:B:LEU:HD12	2:74:B:ILE:HB	19	0.12
(1,846)	2:72:B:LEU:HD13	2:74:B:ILE:HB	19	0.12
(1,846)	2:72:B:LEU:HD21	2:74:B:ILE:HB	19	0.12
(1,846)	2:72:B:LEU:HD22	2:74:B:ILE:HB	19	0.12
(1,846)	2:72:B:LEU:HD23	2:74:B:ILE:HB	19	0.12
(1,842)	2:72:B:LEU:HD21	2:86:B:VAL:HB	2	0.12
(1,842)	2:72:B:LEU:HD22	2:86:B:VAL:HB	2	0.12
(1,842)	2:72:B:LEU:HD23	2:86:B:VAL:HB	2	0.12
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD11	12	0.12
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD12	12	0.12
(1,823)	2:71:B:GLN:HA	2:72:B:LEU:HD13	12	0.12
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	19	0.12
(1,809)	2:69:B:THR:HG1	2:110:B:LEU:H	5	0.12
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD21	5	0.12
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD22	5	0.12
(1,807)	2:68:B:LEU:H	2:72:B:LEU:HD23	5	0.12
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	16	0.12
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	16	0.12
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	16	0.12
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	16	0.12
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	16	0.12
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	16	0.12
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	16	0.12
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	16	0.12
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	5	0.12
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	5	0.12
(1,775)	2:63:B:ARG:HD2	2:64:B:ALA:H	12	0.12
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	1	0.12
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	3	0.12
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	4	0.12
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	11	0.12
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	3	0.12
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	12	0.12
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	15	0.12
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	3	0.12
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	4	0.12
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD21	13	0.12
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD22	13	0.12
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD23	13	0.12
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	7	0.12
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	7	0.12
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	7	0.12
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	7	0.12
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	7	0.12
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	7	0.12
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	7	0.12
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	7	0.12
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	7	0.12
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	17	0.12
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	17	0.12
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	17	0.12
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	17	0.12
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	17	0.12
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	17	0.12
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	17	0.12
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	17	0.12
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	17	0.12
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG2	5	0.12
(1,637)	2:48:B:GLN:HB2	2:52:B:GLU:HG3	5	0.12
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG2	5	0.12
(1,637)	2:48:B:GLN:HB3	2:52:B:GLU:HG3	5	0.12
(1,628)	2:47:B:LYS:H	2:47:B:LYS:HE2	19	0.12
(1,620)	2:47:B:LYS:HG2	2:50:B:LEU:H	3	0.12
(1,620)	2:47:B:LYS:HG3	2:50:B:LEU:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	2:47:B:LYS:HD2	2:48:B:GLN:H	15	0.12
(1,596)	2:46:B:VAL:HG21	2:148:B:TRP:H	8	0.12
(1,596)	2:46:B:VAL:HG22	2:148:B:TRP:H	8	0.12
(1,596)	2:46:B:VAL:HG23	2:148:B:TRP:H	8	0.12
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG21	8	0.12
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG22	8	0.12
(1,587)	2:45:B:ALA:H	2:152:B:VAL:HG23	8	0.12
(1,550)	2:42:B:GLU:H	2:42:B:GLU:HG3	10	0.12
(1,542)	2:41:B:THR:H	2:42:B:GLU:H	11	0.12
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	2	0.12
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	6	0.12
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	7	0.12
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	14	0.12
(1,502)	2:39:B:GLU:HB2	2:41:B:THR:HA	3	0.12
(1,502)	2:39:B:GLU:HB3	2:41:B:THR:HA	3	0.12
(1,502)	2:39:B:GLU:HB2	2:41:B:THR:HA	7	0.12
(1,502)	2:39:B:GLU:HB3	2:41:B:THR:HA	7	0.12
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	7	0.12
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	15	0.12
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	3	0.12
(1,490)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	3	0.12
(1,486)	2:37:B:ALA:H	2:39:B:GLU:H	3	0.12
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB1	10	0.12
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB2	10	0.12
(1,481)	2:37:B:ALA:H	2:37:B:ALA:HB3	10	0.12
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG2	10	0.12
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG3	10	0.12
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG2	10	0.12
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG3	10	0.12
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG2	10	0.12
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG3	10	0.12
(1,468)	2:36:B:GLU:H	2:36:B:GLU:HB2	8	0.12
(1,468)	2:36:B:GLU:H	2:36:B:GLU:HB3	8	0.12
(1,468)	2:36:B:GLU:H	2:36:B:GLU:HB2	16	0.12
(1,468)	2:36:B:GLU:H	2:36:B:GLU:HB3	16	0.12
(1,467)	2:36:B:GLU:H	2:36:B:GLU:HA	3	0.12
(1,465)	2:36:B:GLU:HB2	2:37:B:ALA:H	11	0.12
(1,465)	2:36:B:GLU:HB3	2:37:B:ALA:H	11	0.12
(1,457)	2:35:B:THR:HG21	2:37:B:ALA:H	10	0.12
(1,457)	2:35:B:THR:HG22	2:37:B:ALA:H	10	0.12
(1,457)	2:35:B:THR:HG23	2:37:B:ALA:H	10	0.12
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	10	0.12
(1,451)	2:35:B:THR:HG1	2:36:B:GLU:H	18	0.12
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	17	0.12
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	17	0.12
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	17	0.12
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	7	0.12
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	14	0.12
(1,415)	2:32:B:GLU:H	2:33:B:ASN:H	19	0.12
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	20	0.12
(1,410)	2:32:B:GLU:HG2	2:34:B:ARG:H	14	0.12
(1,410)	2:32:B:GLU:HG3	2:34:B:ARG:H	14	0.12
(1,387)	2:30:B:VAL:HG11	2:32:B:GLU:H	8	0.12
(1,387)	2:30:B:VAL:HG12	2:32:B:GLU:H	8	0.12
(1,387)	2:30:B:VAL:HG13	2:32:B:GLU:H	8	0.12
(1,387)	2:30:B:VAL:HG11	2:32:B:GLU:H	11	0.12
(1,387)	2:30:B:VAL:HG12	2:32:B:GLU:H	11	0.12
(1,387)	2:30:B:VAL:HG13	2:32:B:GLU:H	11	0.12
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB2	11	0.12
(1,383)	2:30:B:VAL:HA	2:31:B:GLU:HB3	11	0.12
(1,379)	2:29:B:ASP:H	2:30:B:VAL:HG11	4	0.12
(1,379)	2:29:B:ASP:H	2:30:B:VAL:HG12	4	0.12
(1,379)	2:29:B:ASP:H	2:30:B:VAL:HG13	4	0.12
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	7	0.12
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	20	0.12
(1,334)	2:25:B:SER:HB2	2:29:B:ASP:H	19	0.12
(1,334)	2:25:B:SER:HB3	2:29:B:ASP:H	19	0.12
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	3	0.12
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	3	0.12
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	3	0.12
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	4	0.12
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	4	0.12
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	6	0.12
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	6	0.12
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	13	0.12
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	13	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG11	20	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG12	20	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG13	20	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG21	20	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG22	20	0.12
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG23	20	0.12
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	10	0.12
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	19	0.12
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	19	0.12
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG11	1	0.12
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG12	1	0.12
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG13	1	0.12
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG21	1	0.12
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG22	1	0.12
(1,287)	2:21:B:GLY:H	2:112:B:VAL:HG23	1	0.12
(1,272)	2:20:B:LYS:HD2	2:22:B:TYR:H	5	0.12
(1,272)	2:20:B:LYS:HD3	2:22:B:TYR:H	5	0.12
(1,248)	2:19:B:GLN:HB3	2:21:B:GLY:H	14	0.12
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	19	0.12
(1,234)	2:18:B:SER:HB2	2:21:B:GLY:H	13	0.12
(1,234)	2:18:B:SER:HB2	2:21:B:GLY:H	16	0.12
(1,233)	2:18:B:SER:HB2	2:20:B:LYS:H	9	0.12
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	16	0.12
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	16	0.12
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD11	9	0.12
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD12	9	0.12
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD13	9	0.12
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD21	9	0.12
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD22	9	0.12
(1,137)	2:12:B:PHE:HE1	2:13:B:LEU:HD23	9	0.12
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD11	9	0.12
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD12	9	0.12
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD13	9	0.12
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD21	9	0.12
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD22	9	0.12
(1,137)	2:12:B:PHE:HE2	2:13:B:LEU:HD23	9	0.12
(1,124)	2:11:B:ASP:HB3	2:47:B:LYS:HD2	1	0.12
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD11	17	0.11
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD12	17	0.11
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD13	17	0.11
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD11	17	0.11
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD12	17	0.11
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD13	17	0.11
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD21	11	0.11
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD22	11	0.11
(1,2127)	1:325:A:ASP:H	1:322:A:LEU:HD23	11	0.11
(1,2087)	1:322:A:LEU:H	1:321:A:SER:HA	10	0.11
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD21	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD22	6	0.11
(1,2062)	1:320:A:SER:H	1:322:A:LEU:HD23	6	0.11
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	9	0.11
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	14	0.11
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	18	0.11
(1,2048)	1:319:A:TRP:H	1:319:A:TRP:HD1	16	0.11
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	3	0.11
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	5	0.11
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	11	0.11
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	16	0.11
(1,2037)	1:319:A:TRP:HE1	1:319:A:TRP:HB3	19	0.11
(1,2027)	1:318:A:LEU:H	1:318:A:LEU:HA	5	0.11
(1,2027)	1:318:A:LEU:H	1:318:A:LEU:HA	12	0.11
(1,1997)	1:317:A:HIS:HD1	1:317:A:HIS:HA	2	0.11
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	12	0.11
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	12	0.11
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	12	0.11
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	12	0.11
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB2	16	0.11
(1,1972)	1:315:A:PHE:HE1	1:318:A:LEU:HB3	16	0.11
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB2	16	0.11
(1,1972)	1:315:A:PHE:HE2	1:318:A:LEU:HB3	16	0.11
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	2	0.11
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	2	0.11
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	2	0.11
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	2	0.11
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	2	0.11
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	2	0.11
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD11	10	0.11
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD12	10	0.11
(1,1967)	1:315:A:PHE:HD1	1:318:A:LEU:HD13	10	0.11
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD11	10	0.11
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD12	10	0.11
(1,1967)	1:315:A:PHE:HD2	1:318:A:LEU:HD13	10	0.11
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	4	0.11
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	16	0.11
(1,1923)	2:170:B:LEU:HG	2:171:B:GLU:H	4	0.11
(1,1923)	2:170:B:LEU:HG	2:171:B:GLU:H	20	0.11
(1,1917)	2:169:B:ARG:H	2:169:B:ARG:HG2	6	0.11
(1,1908)	2:169:B:ARG:HA	2:170:B:LEU:H	10	0.11
(1,1908)	2:169:B:ARG:HA	2:170:B:LEU:H	17	0.11
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	15	0.11
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	18	0.11
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	18	0.11
(1,1895)	2:168:B:GLU:HG3	2:169:B:ARG:H	2	0.11
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	17	0.11
(1,1883)	2:167:B:GLN:HG2	2:170:B:LEU:H	12	0.11
(1,1883)	2:167:B:GLN:HG3	2:170:B:LEU:H	12	0.11
(1,1880)	2:167:B:GLN:HA	2:168:B:GLU:H	16	0.11
(1,1863)	2:165:B:LYS:HG3	2:166:B:GLY:H	3	0.11
(1,1863)	2:165:B:LYS:HG3	2:166:B:GLY:H	12	0.11
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	2	0.11
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	6	0.11
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	8	0.11
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	14	0.11
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	19	0.11
(1,1807)	2:158:B:ASN:H	2:159:B:ALA:H	19	0.11
(1,1793)	2:157:B:ASN:H	2:159:B:ALA:H	18	0.11
(1,1786)	2:156:B:GLY:H	2:158:B:ASN:H	5	0.11
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	4	0.11
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	4	0.11
(1,1780)	2:155:B:TYR:HE1	2:156:B:GLY:H	5	0.11
(1,1780)	2:155:B:TYR:HE2	2:156:B:GLY:H	5	0.11
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	6	0.11
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	6	0.11
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	8	0.11
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	8	0.11
(1,1720)	2:151:B:PHE:HE1	2:152:B:VAL:H	11	0.11
(1,1720)	2:151:B:PHE:HE2	2:152:B:VAL:H	11	0.11
(1,1700)	2:150:B:THR:HG21	2:153:B:GLU:H	1	0.11
(1,1700)	2:150:B:THR:HG22	2:153:B:GLU:H	1	0.11
(1,1700)	2:150:B:THR:HG23	2:153:B:GLU:H	1	0.11
(1,1697)	2:150:B:THR:HG21	2:152:B:VAL:H	8	0.11
(1,1697)	2:150:B:THR:HG22	2:152:B:VAL:H	8	0.11
(1,1697)	2:150:B:THR:HG23	2:152:B:VAL:H	8	0.11
(1,1695)	2:150:B:THR:HB	2:153:B:GLU:HG2	17	0.11
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	3	0.11
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	10	0.11
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	16	0.11
(1,1682)	2:149:B:ASP:H	2:150:B:THR:HA	19	0.11
(1,1660)	2:146:B:GLY:H	2:148:B:TRP:H	19	0.11
(1,1622)	2:143:B:GLN:H	2:139:B:GLU:HG2	17	0.11
(1,1622)	2:143:B:GLN:H	2:139:B:GLU:HG3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1615)	2:143:B:GLN:HB3	2:144:B:GLU:HA	19	0.11
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD11	4	0.11
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD12	4	0.11
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD13	4	0.11
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD11	9	0.11
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD12	9	0.11
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD13	9	0.11
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD11	1	0.11
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD12	1	0.11
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD13	1	0.11
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD11	9	0.11
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD12	9	0.11
(1,1578)	2:141:B:TRP:HB3	2:142:B:ILE:HD13	9	0.11
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG21	2	0.11
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG22	2	0.11
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG23	2	0.11
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	10	0.11
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	16	0.11
(1,1552)	2:138:B:LEU:HD21	2:139:B:GLU:H	10	0.11
(1,1552)	2:138:B:LEU:HD22	2:139:B:GLU:H	10	0.11
(1,1552)	2:138:B:LEU:HD23	2:139:B:GLU:H	10	0.11
(1,1507)	2:134:B:LEU:HD11	2:136:B:ASP:H	8	0.11
(1,1507)	2:134:B:LEU:HD12	2:136:B:ASP:H	8	0.11
(1,1507)	2:134:B:LEU:HD13	2:136:B:ASP:H	8	0.11
(1,1507)	2:134:B:LEU:HD21	2:136:B:ASP:H	8	0.11
(1,1507)	2:134:B:LEU:HD22	2:136:B:ASP:H	8	0.11
(1,1507)	2:134:B:LEU:HD23	2:136:B:ASP:H	8	0.11
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	4	0.11
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	6	0.11
(1,1469)	2:129:B:TRP:H	2:129:B:TRP:HZ2	9	0.11
(1,1394)	2:120:B:GLN:H	2:120:B:GLN:HB2	2	0.11
(1,1394)	2:120:B:GLN:H	2:120:B:GLN:HB3	2	0.11
(1,1341)	2:115:B:VAL:HG21	2:118:B:GLU:H	18	0.11
(1,1341)	2:115:B:VAL:HG22	2:118:B:GLU:H	18	0.11
(1,1341)	2:115:B:VAL:HG23	2:118:B:GLU:H	18	0.11
(1,1338)	2:115:B:VAL:HG11	2:119:B:MET:H	16	0.11
(1,1338)	2:115:B:VAL:HG12	2:119:B:MET:H	16	0.11
(1,1338)	2:115:B:VAL:HG13	2:119:B:MET:H	16	0.11
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG11	20	0.11
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG12	20	0.11
(1,1276)	2:111:B:CYS:HB2	2:112:B:VAL:HG13	20	0.11
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	2	0.11
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	4	0.11
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	12	0.11
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	17	0.11
(1,1192)	2:104:B:PHE:HD1	2:106:B:PHE:H	3	0.11
(1,1192)	2:104:B:PHE:HD2	2:106:B:PHE:H	3	0.11
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD1	14	0.11
(1,1172)	2:102:B:ALA:H	2:103:B:PHE:HD2	14	0.11
(1,1131)	2:100:B:ILE:HD11	2:101:B:VAL:H	9	0.11
(1,1131)	2:100:B:ILE:HD12	2:101:B:VAL:H	9	0.11
(1,1131)	2:100:B:ILE:HD13	2:101:B:VAL:H	9	0.11
(1,1107)	2:96:B:ASN:H	2:97:B:TRP:HB2	4	0.11
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD11	5	0.11
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD12	5	0.11
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD13	5	0.11
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD11	16	0.11
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD12	16	0.11
(1,1097)	2:96:B:ASN:HD22	2:100:B:ILE:HD13	16	0.11
(1,1085)	2:95:B:VAL:HG11	2:141:B:TRP:H	11	0.11
(1,1085)	2:95:B:VAL:HG12	2:141:B:TRP:H	11	0.11
(1,1085)	2:95:B:VAL:HG13	2:141:B:TRP:H	11	0.11
(1,1085)	2:95:B:VAL:HG21	2:141:B:TRP:H	11	0.11
(1,1085)	2:95:B:VAL:HG22	2:141:B:TRP:H	11	0.11
(1,1085)	2:95:B:VAL:HG23	2:141:B:TRP:H	11	0.11
(1,1075)	2:95:B:VAL:HG11	2:96:B:ASN:HD21	17	0.11
(1,1075)	2:95:B:VAL:HG12	2:96:B:ASN:HD21	17	0.11
(1,1075)	2:95:B:VAL:HG13	2:96:B:ASN:HD21	17	0.11
(1,1060)	2:93:B:ASP:H	2:94:B:GLY:HA2	19	0.11
(1,1059)	2:93:B:ASP:H	2:94:B:GLY:HA3	15	0.11
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	3	0.11
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	5	0.11
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG11	19	0.11
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG12	19	0.11
(1,1011)	2:91:B:PHE:HA	2:95:B:VAL:HG13	19	0.11
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB1	13	0.11
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB2	13	0.11
(1,1004)	2:90:B:LEU:HG	2:102:B:ALA:HB3	13	0.11
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD1	5	0.11
(1,995)	2:90:B:LEU:HD21	2:91:B:PHE:HD2	5	0.11
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD1	5	0.11
(1,995)	2:90:B:LEU:HD22	2:91:B:PHE:HD2	5	0.11
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD1	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	2:90:B:LEU:HD23	2:91:B:PHE:HD2	5	0.11
(1,941)	2:86:B:VAL:HA	2:89:B:GLU:H	20	0.11
(1,910)	2:81:B:GLN:H	2:85:B:GLN:H	2	0.11
(1,838)	2:72:B:LEU:HD11	2:83:B:PHE:HA	6	0.11
(1,838)	2:72:B:LEU:HD12	2:83:B:PHE:HA	6	0.11
(1,838)	2:72:B:LEU:HD13	2:83:B:PHE:HA	6	0.11
(1,818)	2:69:B:THR:H	2:69:B:THR:HA	13	0.11
(1,812)	2:69:B:THR:HG21	2:106:B:PHE:HE1	16	0.11
(1,812)	2:69:B:THR:HG21	2:106:B:PHE:HE2	16	0.11
(1,812)	2:69:B:THR:HG22	2:106:B:PHE:HE1	16	0.11
(1,812)	2:69:B:THR:HG22	2:106:B:PHE:HE2	16	0.11
(1,812)	2:69:B:THR:HG23	2:106:B:PHE:HE1	16	0.11
(1,812)	2:69:B:THR:HG23	2:106:B:PHE:HE2	16	0.11
(1,809)	2:69:B:THR:HG1	2:110:B:LEU:H	7	0.11
(1,809)	2:69:B:THR:HG1	2:110:B:LEU:H	18	0.11
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD11	3	0.11
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD12	3	0.11
(1,806)	2:68:B:LEU:H	2:72:B:LEU:HD13	3	0.11
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG21	14	0.11
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG22	14	0.11
(1,799)	2:68:B:LEU:HD21	2:69:B:THR:HG23	14	0.11
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG21	14	0.11
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG22	14	0.11
(1,799)	2:68:B:LEU:HD22	2:69:B:THR:HG23	14	0.11
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG21	14	0.11
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG22	14	0.11
(1,799)	2:68:B:LEU:HD23	2:69:B:THR:HG23	14	0.11
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG21	3	0.11
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG22	3	0.11
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG23	3	0.11
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG21	3	0.11
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG22	3	0.11
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG23	3	0.11
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG21	3	0.11
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG22	3	0.11
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG23	3	0.11
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG21	10	0.11
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG22	10	0.11
(1,797)	2:68:B:LEU:HD11	2:69:B:THR:HG23	10	0.11
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG21	10	0.11
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG22	10	0.11
(1,797)	2:68:B:LEU:HD12	2:69:B:THR:HG23	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG21	10	0.11
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG22	10	0.11
(1,797)	2:68:B:LEU:HD13	2:69:B:THR:HG23	10	0.11
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD21	3	0.11
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD22	3	0.11
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD23	3	0.11
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD21	16	0.11
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD22	16	0.11
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD23	16	0.11
(1,791)	2:67:B:ASP:H	2:68:B:LEU:HD11	10	0.11
(1,791)	2:67:B:ASP:H	2:68:B:LEU:HD12	10	0.11
(1,791)	2:67:B:ASP:H	2:68:B:LEU:HD13	10	0.11
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE1	6	0.11
(1,785)	2:64:B:ALA:H	2:65:B:PHE:HE2	6	0.11
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	7	0.11
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	7	0.11
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	17	0.11
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	1	0.11
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	2	0.11
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	5	0.11
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	3	0.11
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	3	0.11
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	3	0.11
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	3	0.11
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	3	0.11
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	7	0.11
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	7	0.11
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	7	0.11
(1,668)	2:50:B:LEU:HD11	2:101:B:VAL:HG11	8	0.11
(1,668)	2:50:B:LEU:HD11	2:101:B:VAL:HG12	8	0.11
(1,668)	2:50:B:LEU:HD11	2:101:B:VAL:HG13	8	0.11
(1,668)	2:50:B:LEU:HD12	2:101:B:VAL:HG11	8	0.11
(1,668)	2:50:B:LEU:HD12	2:101:B:VAL:HG12	8	0.11
(1,668)	2:50:B:LEU:HD12	2:101:B:VAL:HG13	8	0.11
(1,668)	2:50:B:LEU:HD13	2:101:B:VAL:HG11	8	0.11
(1,668)	2:50:B:LEU:HD13	2:101:B:VAL:HG12	8	0.11
(1,668)	2:50:B:LEU:HD13	2:101:B:VAL:HG13	8	0.11
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD21	5	0.11
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD22	5	0.11
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD23	5	0.11
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD21	15	0.11
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD22	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	2:49:B:ALA:H	2:50:B:LEU:HD23	15	0.11
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	14	0.11
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	14	0.11
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	14	0.11
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	14	0.11
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	14	0.11
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	14	0.11
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	14	0.11
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	14	0.11
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	14	0.11
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	19	0.11
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	19	0.11
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	19	0.11
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	19	0.11
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	19	0.11
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	19	0.11
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	19	0.11
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	19	0.11
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	19	0.11
(1,619)	2:47:B:LYS:HG2	2:49:B:ALA:H	15	0.11
(1,619)	2:47:B:LYS:HG3	2:49:B:ALA:H	15	0.11
(1,614)	2:47:B:LYS:HD2	2:48:B:GLN:H	20	0.11
(1,612)	2:47:B:LYS:HB2	2:51:B:ARG:HA	2	0.11
(1,612)	2:47:B:LYS:HB3	2:51:B:ARG:HA	2	0.11
(1,612)	2:47:B:LYS:HB2	2:51:B:ARG:HA	5	0.11
(1,612)	2:47:B:LYS:HB3	2:51:B:ARG:HA	5	0.11
(1,612)	2:47:B:LYS:HB2	2:51:B:ARG:HA	15	0.11
(1,612)	2:47:B:LYS:HB3	2:51:B:ARG:HA	15	0.11
(1,612)	2:47:B:LYS:HB2	2:51:B:ARG:HA	16	0.11
(1,612)	2:47:B:LYS:HB3	2:51:B:ARG:HA	16	0.11
(1,604)	2:46:B:VAL:HG11	2:49:B:ALA:HA	11	0.11
(1,604)	2:46:B:VAL:HG12	2:49:B:ALA:HA	11	0.11
(1,604)	2:46:B:VAL:HG13	2:49:B:ALA:HA	11	0.11
(1,604)	2:46:B:VAL:HG21	2:49:B:ALA:HA	11	0.11
(1,604)	2:46:B:VAL:HG22	2:49:B:ALA:HA	11	0.11
(1,604)	2:46:B:VAL:HG23	2:49:B:ALA:HA	11	0.11
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG11	5	0.11
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG12	5	0.11
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG13	5	0.11
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG21	5	0.11
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG22	5	0.11
(1,562)	2:44:B:GLU:HA	2:46:B:VAL:HG23	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	2:42:B:GLU:H	2:42:B:GLU:HG2	20	0.11
(1,543)	2:42:B:GLU:HA	2:43:B:SER:H	14	0.11
(1,525)	2:40:B:GLY:H	2:40:B:GLY:HA3	5	0.11
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	1	0.11
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	1	0.11
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	5	0.11
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	5	0.11
(1,515)	2:39:B:GLU:H	2:40:B:GLY:HA2	16	0.11
(1,515)	2:39:B:GLU:H	2:40:B:GLY:HA3	16	0.11
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	13	0.11
(1,510)	2:39:B:GLU:H	2:39:B:GLU:HA	17	0.11
(1,508)	2:39:B:GLU:HG2	2:41:B:THR:HB	9	0.11
(1,508)	2:39:B:GLU:HG3	2:41:B:THR:HB	9	0.11
(1,508)	2:39:B:GLU:HG2	2:41:B:THR:HB	15	0.11
(1,508)	2:39:B:GLU:HG3	2:41:B:THR:HB	15	0.11
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	13	0.11
(1,497)	2:39:B:GLU:HA	2:40:B:GLY:H	18	0.11
(1,486)	2:37:B:ALA:H	2:39:B:GLU:H	5	0.11
(1,480)	2:37:B:ALA:H	2:37:B:ALA:HA	17	0.11
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG2	9	0.11
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG3	9	0.11
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG2	9	0.11
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG3	9	0.11
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG2	9	0.11
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG3	9	0.11
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG2	20	0.11
(1,477)	2:37:B:ALA:HB1	2:38:B:PRO:HG3	20	0.11
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG2	20	0.11
(1,477)	2:37:B:ALA:HB2	2:38:B:PRO:HG3	20	0.11
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG2	20	0.11
(1,477)	2:37:B:ALA:HB3	2:38:B:PRO:HG3	20	0.11
(1,471)	2:36:B:GLU:H	2:37:B:ALA:H	14	0.11
(1,457)	2:35:B:THR:HG21	2:37:B:ALA:H	13	0.11
(1,457)	2:35:B:THR:HG22	2:37:B:ALA:H	13	0.11
(1,457)	2:35:B:THR:HG23	2:37:B:ALA:H	13	0.11
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	1	0.11
(1,452)	2:35:B:THR:HG1	2:37:B:ALA:H	17	0.11
(1,451)	2:35:B:THR:HG1	2:36:B:GLU:H	2	0.11
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	15	0.11
(1,432)	2:34:B:ARG:HA	2:35:B:THR:H	20	0.11
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG21	10	0.11
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	2:34:B:ARG:HA	2:35:B:THR:HG23	10	0.11
(1,430)	2:33:B:ASN:H	2:35:B:THR:HG1	11	0.11
(1,430)	2:33:B:ASN:H	2:35:B:THR:HG1	12	0.11
(1,422)	2:33:B:ASN:HD22	2:34:B:ARG:H	1	0.11
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	2	0.11
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	17	0.11
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	4	0.11
(1,411)	2:32:B:GLU:H	2:32:B:GLU:HA	8	0.11
(1,400)	2:30:B:VAL:H	2:32:B:GLU:H	5	0.11
(1,387)	2:30:B:VAL:HG11	2:32:B:GLU:H	5	0.11
(1,387)	2:30:B:VAL:HG12	2:32:B:GLU:H	5	0.11
(1,387)	2:30:B:VAL:HG13	2:32:B:GLU:H	5	0.11
(1,382)	2:29:B:ASP:H	2:30:B:VAL:H	13	0.11
(1,375)	2:28:B:SER:H	2:30:B:VAL:H	13	0.11
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	2	0.11
(1,366)	2:28:B:SER:HA	2:29:B:ASP:H	9	0.11
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	2	0.11
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	2	0.11
(1,361)	2:27:B:PHE:HE1	2:28:B:SER:H	19	0.11
(1,361)	2:27:B:PHE:HE2	2:28:B:SER:H	19	0.11
(1,356)	2:26:B:GLN:H	2:29:B:ASP:H	17	0.11
(1,337)	2:25:B:SER:H	2:26:B:GLN:HB2	18	0.11
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	7	0.11
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	14	0.11
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	15	0.11
(1,336)	2:25:B:SER:H	2:26:B:GLN:HB3	17	0.11
(1,325)	2:24:B:TRP:HE1	2:123:B:VAL:HG11	19	0.11
(1,325)	2:24:B:TRP:HE1	2:123:B:VAL:HG12	19	0.11
(1,325)	2:24:B:TRP:HE1	2:123:B:VAL:HG13	19	0.11
(1,325)	2:24:B:TRP:HE1	2:123:B:VAL:HG21	19	0.11
(1,325)	2:24:B:TRP:HE1	2:123:B:VAL:HG22	19	0.11
(1,325)	2:24:B:TRP:HE1	2:123:B:VAL:HG23	19	0.11
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG21	14	0.11
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG22	14	0.11
(1,323)	2:24:B:TRP:HD1	2:123:B:VAL:HG23	14	0.11
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	8	0.11
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	8	0.11
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	10	0.11
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	10	0.11
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	12	0.11
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	12	0.11
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	16	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG11	3	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG12	3	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG13	3	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG21	3	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG22	3	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG23	3	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG11	7	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG12	7	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG13	7	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG21	7	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG22	7	0.11
(1,302)	2:22:B:TYR:H	2:112:B:VAL:HG23	7	0.11
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	5	0.11
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	5	0.11
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	14	0.11
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	14	0.11
(1,293)	2:22:B:TYR:HD1	2:112:B:VAL:HG11	2	0.11
(1,293)	2:22:B:TYR:HD1	2:112:B:VAL:HG12	2	0.11
(1,293)	2:22:B:TYR:HD1	2:112:B:VAL:HG13	2	0.11
(1,293)	2:22:B:TYR:HD1	2:112:B:VAL:HG21	2	0.11
(1,293)	2:22:B:TYR:HD1	2:112:B:VAL:HG22	2	0.11
(1,293)	2:22:B:TYR:HD1	2:112:B:VAL:HG23	2	0.11
(1,293)	2:22:B:TYR:HD2	2:112:B:VAL:HG11	2	0.11
(1,293)	2:22:B:TYR:HD2	2:112:B:VAL:HG12	2	0.11
(1,293)	2:22:B:TYR:HD2	2:112:B:VAL:HG13	2	0.11
(1,293)	2:22:B:TYR:HD2	2:112:B:VAL:HG21	2	0.11
(1,293)	2:22:B:TYR:HD2	2:112:B:VAL:HG22	2	0.11
(1,293)	2:22:B:TYR:HD2	2:112:B:VAL:HG23	2	0.11
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	7	0.11
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	7	0.11
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD1	17	0.11
(1,285)	2:20:B:LYS:H	2:22:B:TYR:HD2	17	0.11
(1,271)	2:20:B:LYS:HD2	2:21:B:GLY:H	7	0.11
(1,271)	2:20:B:LYS:HD3	2:21:B:GLY:H	7	0.11
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD2	16	0.11
(1,261)	2:19:B:GLN:H	2:20:B:LYS:HD3	16	0.11
(1,235)	2:18:B:SER:HB2	2:22:B:TYR:H	5	0.11
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	9	0.11
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	17	0.11
(1,229)	2:18:B:SER:HB3	2:20:B:LYS:H	19	0.11
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	10	0.11
(1,224)	2:17:B:LEU:H	2:20:B:LYS:H	15	0.11
(1,211)	2:17:B:LEU:HD11	2:22:B:TYR:H	18	0.11
(1,211)	2:17:B:LEU:HD12	2:22:B:TYR:H	18	0.11
(1,211)	2:17:B:LEU:HD13	2:22:B:TYR:H	18	0.11
(1,211)	2:17:B:LEU:HD21	2:22:B:TYR:H	18	0.11
(1,211)	2:17:B:LEU:HD22	2:22:B:TYR:H	18	0.11
(1,211)	2:17:B:LEU:HD23	2:22:B:TYR:H	18	0.11
(1,211)	2:17:B:LEU:HD11	2:22:B:TYR:H	20	0.11
(1,211)	2:17:B:LEU:HD12	2:22:B:TYR:H	20	0.11
(1,211)	2:17:B:LEU:HD13	2:22:B:TYR:H	20	0.11
(1,211)	2:17:B:LEU:HD21	2:22:B:TYR:H	20	0.11
(1,211)	2:17:B:LEU:HD22	2:22:B:TYR:H	20	0.11
(1,211)	2:17:B:LEU:HD23	2:22:B:TYR:H	20	0.11
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD1	12	0.11
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD2	12	0.11
(1,73)	2:8:B:LEU:HD11	2:50:B:LEU:HD11	12	0.11
(1,73)	2:8:B:LEU:HD11	2:50:B:LEU:HD12	12	0.11
(1,73)	2:8:B:LEU:HD11	2:50:B:LEU:HD13	12	0.11
(1,73)	2:8:B:LEU:HD11	2:50:B:LEU:HD21	12	0.11
(1,73)	2:8:B:LEU:HD11	2:50:B:LEU:HD22	12	0.11
(1,73)	2:8:B:LEU:HD11	2:50:B:LEU:HD23	12	0.11
(1,73)	2:8:B:LEU:HD12	2:50:B:LEU:HD11	12	0.11
(1,73)	2:8:B:LEU:HD12	2:50:B:LEU:HD12	12	0.11
(1,73)	2:8:B:LEU:HD12	2:50:B:LEU:HD13	12	0.11
(1,73)	2:8:B:LEU:HD12	2:50:B:LEU:HD21	12	0.11
(1,73)	2:8:B:LEU:HD12	2:50:B:LEU:HD22	12	0.11
(1,73)	2:8:B:LEU:HD12	2:50:B:LEU:HD23	12	0.11
(1,73)	2:8:B:LEU:HD13	2:50:B:LEU:HD11	12	0.11
(1,73)	2:8:B:LEU:HD13	2:50:B:LEU:HD12	12	0.11
(1,73)	2:8:B:LEU:HD13	2:50:B:LEU:HD13	12	0.11
(1,73)	2:8:B:LEU:HD13	2:50:B:LEU:HD21	12	0.11
(1,73)	2:8:B:LEU:HD13	2:50:B:LEU:HD22	12	0.11
(1,73)	2:8:B:LEU:HD13	2:50:B:LEU:HD23	12	0.11
(1,73)	2:8:B:LEU:HD21	2:50:B:LEU:HD11	12	0.11
(1,73)	2:8:B:LEU:HD21	2:50:B:LEU:HD12	12	0.11
(1,73)	2:8:B:LEU:HD21	2:50:B:LEU:HD13	12	0.11
(1,73)	2:8:B:LEU:HD21	2:50:B:LEU:HD21	12	0.11
(1,73)	2:8:B:LEU:HD21	2:50:B:LEU:HD22	12	0.11
(1,73)	2:8:B:LEU:HD21	2:50:B:LEU:HD23	12	0.11
(1,73)	2:8:B:LEU:HD22	2:50:B:LEU:HD11	12	0.11
(1,73)	2:8:B:LEU:HD22	2:50:B:LEU:HD12	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	2:8:B:LEU:HD22	2:50:B:LEU:HD13	12	0.11
(1,73)	2:8:B:LEU:HD22	2:50:B:LEU:HD21	12	0.11
(1,73)	2:8:B:LEU:HD22	2:50:B:LEU:HD22	12	0.11
(1,73)	2:8:B:LEU:HD22	2:50:B:LEU:HD23	12	0.11
(1,73)	2:8:B:LEU:HD23	2:50:B:LEU:HD11	12	0.11
(1,73)	2:8:B:LEU:HD23	2:50:B:LEU:HD12	12	0.11
(1,73)	2:8:B:LEU:HD23	2:50:B:LEU:HD13	12	0.11
(1,73)	2:8:B:LEU:HD23	2:50:B:LEU:HD21	12	0.11
(1,73)	2:8:B:LEU:HD23	2:50:B:LEU:HD22	12	0.11
(1,73)	2:8:B:LEU:HD23	2:50:B:LEU:HD23	12	0.11
(1,29)	2:4:B:SER:H	2:8:B:LEU:H	8	0.11
(1,9)	2:2:B:SER:H	2:2:B:SER:HB2	13	0.11
(1,9)	2:2:B:SER:H	2:2:B:SER:HB3	13	0.11
(1,5)	2:2:B:SER:HA	2:4:B:SER:H	5	0.11
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD11	5	0.1
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD12	5	0.1
(1,2155)	2:155:B:TYR:HD1	1:318:A:LEU:HD13	5	0.1
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD11	5	0.1
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD12	5	0.1
(1,2155)	2:155:B:TYR:HD2	1:318:A:LEU:HD13	5	0.1
(1,2109)	1:323:A:GLU:H	1:323:A:GLU:HA	5	0.1
(1,2101)	1:323:A:GLU:H	1:321:A:SER:HB3	14	0.1
(1,2073)	1:321:A:SER:H	1:321:A:SER:HB3	9	0.1
(1,2056)	1:320:A:SER:H	1:319:A:TRP:HA	17	0.1
(1,1958)	1:315:A:PHE:HB3	1:314:A:THR:HA	2	0.1
(1,1924)	2:170:B:LEU:H	2:170:B:LEU:HA	12	0.1
(1,1919)	2:169:B:ARG:H	2:170:B:LEU:HA	16	0.1
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	1	0.1
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	1	0.1
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD2	8	0.1
(1,1904)	2:168:B:GLU:H	2:169:B:ARG:HD3	8	0.1
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	3	0.1
(1,1887)	2:167:B:GLN:H	2:167:B:GLN:HE22	6	0.1
(1,1874)	2:166:B:GLY:HA2	2:167:B:GLN:H	8	0.1
(1,1862)	2:165:B:LYS:HD2	2:167:B:GLN:H	5	0.1
(1,1862)	2:165:B:LYS:HD3	2:167:B:GLN:H	5	0.1
(1,1834)	2:162:B:GLU:H	2:162:B:GLU:HA	7	0.1
(1,1788)	2:157:B:ASN:HB2	2:159:B:ALA:HA	18	0.1
(1,1736)	2:152:B:VAL:HG11	2:155:B:TYR:HA	7	0.1
(1,1736)	2:152:B:VAL:HG12	2:155:B:TYR:HA	7	0.1
(1,1736)	2:152:B:VAL:HG13	2:155:B:TYR:HA	7	0.1
(1,1736)	2:152:B:VAL:HG21	2:155:B:TYR:HA	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1736)	2:152:B:VAL:HG22	2:155:B:TYR:HA	7	0.1
(1,1736)	2:152:B:VAL:HG23	2:155:B:TYR:HA	7	0.1
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG11	16	0.1
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG12	16	0.1
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG13	16	0.1
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG21	16	0.1
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG22	16	0.1
(1,1690)	2:150:B:THR:HA	2:152:B:VAL:HG23	16	0.1
(1,1661)	2:146:B:GLY:H	2:149:B:ASP:H	10	0.1
(1,1640)	2:144:B:GLU:H	2:145:B:ASN:HD22	12	0.1
(1,1615)	2:143:B:GLN:HB3	2:144:B:GLU:HA	20	0.1
(1,1598)	2:142:B:ILE:HD11	2:146:B:GLY:H	11	0.1
(1,1598)	2:142:B:ILE:HD12	2:146:B:GLY:H	11	0.1
(1,1598)	2:142:B:ILE:HD13	2:146:B:GLY:H	11	0.1
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD11	1	0.1
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD12	1	0.1
(1,1580)	2:141:B:TRP:HB2	2:142:B:ILE:HD13	1	0.1
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG21	15	0.1
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG22	15	0.1
(1,1574)	2:139:B:GLU:H	2:142:B:ILE:HG23	15	0.1
(1,1565)	2:138:B:LEU:H	2:142:B:ILE:H	15	0.1
(1,1554)	2:138:B:LEU:HG	2:139:B:GLU:H	2	0.1
(1,1531)	2:135:B:ASN:H	2:137:B:HIS:H	7	0.1
(1,1396)	2:120:B:GLN:H	2:120:B:GLN:HE22	9	0.1
(1,1394)	2:120:B:GLN:H	2:120:B:GLN:HB2	14	0.1
(1,1394)	2:120:B:GLN:H	2:120:B:GLN:HB3	14	0.1
(1,1389)	2:119:B:MET:H	2:120:B:GLN:HE22	13	0.1
(1,1361)	2:116:B:ASP:H	2:119:B:MET:H	6	0.1
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG12	20	0.1
(1,1282)	2:111:B:CYS:HB2	2:126:B:ILE:HG13	20	0.1
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG12	20	0.1
(1,1282)	2:111:B:CYS:HB3	2:126:B:ILE:HG13	20	0.1
(1,1237)	2:108:B:GLY:H	2:110:B:LEU:HG	5	0.1
(1,1193)	2:104:B:PHE:HD1	2:107:B:GLY:H	2	0.1
(1,1193)	2:104:B:PHE:HD2	2:107:B:GLY:H	2	0.1
(1,1192)	2:104:B:PHE:HD1	2:106:B:PHE:H	2	0.1
(1,1192)	2:104:B:PHE:HD2	2:106:B:PHE:H	2	0.1
(1,1138)	2:100:B:ILE:HD11	2:142:B:ILE:H	6	0.1
(1,1138)	2:100:B:ILE:HD12	2:142:B:ILE:H	6	0.1
(1,1138)	2:100:B:ILE:HD13	2:142:B:ILE:H	6	0.1
(1,1119)	2:97:B:TRP:H	2:97:B:TRP:HZ3	16	0.1
(1,1114)	2:97:B:TRP:H	2:100:B:ILE:HD11	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	2:97:B:TRP:H	2:100:B:ILE:HD12	19	0.1
(1,1114)	2:97:B:TRP:H	2:100:B:ILE:HD13	19	0.1
(1,1076)	2:95:B:VAL:HG11	2:96:B:ASN:HD22	20	0.1
(1,1076)	2:95:B:VAL:HG12	2:96:B:ASN:HD22	20	0.1
(1,1076)	2:95:B:VAL:HG13	2:96:B:ASN:HD22	20	0.1
(1,1048)	2:92:B:ARG:H	2:93:B:ASP:HA	10	0.1
(1,992)	2:90:B:LEU:HD21	2:102:B:ALA:HB1	2	0.1
(1,992)	2:90:B:LEU:HD21	2:102:B:ALA:HB2	2	0.1
(1,992)	2:90:B:LEU:HD21	2:102:B:ALA:HB3	2	0.1
(1,992)	2:90:B:LEU:HD22	2:102:B:ALA:HB1	2	0.1
(1,992)	2:90:B:LEU:HD22	2:102:B:ALA:HB2	2	0.1
(1,992)	2:90:B:LEU:HD22	2:102:B:ALA:HB3	2	0.1
(1,992)	2:90:B:LEU:HD23	2:102:B:ALA:HB1	2	0.1
(1,992)	2:90:B:LEU:HD23	2:102:B:ALA:HB2	2	0.1
(1,992)	2:90:B:LEU:HD23	2:102:B:ALA:HB3	2	0.1
(1,916)	2:84:B:GLU:HB2	2:86:B:VAL:H	4	0.1
(1,916)	2:84:B:GLU:HB3	2:86:B:VAL:H	4	0.1
(1,889)	2:79:B:ALA:HB1	2:81:B:GLN:HB2	11	0.1
(1,889)	2:79:B:ALA:HB2	2:81:B:GLN:HB2	11	0.1
(1,889)	2:79:B:ALA:HB3	2:81:B:GLN:HB2	11	0.1
(1,861)	2:74:B:ILE:HD11	2:119:B:MET:HB2	12	0.1
(1,861)	2:74:B:ILE:HD11	2:119:B:MET:HB3	12	0.1
(1,861)	2:74:B:ILE:HD12	2:119:B:MET:HB2	12	0.1
(1,861)	2:74:B:ILE:HD12	2:119:B:MET:HB3	12	0.1
(1,861)	2:74:B:ILE:HD13	2:119:B:MET:HB2	12	0.1
(1,861)	2:74:B:ILE:HD13	2:119:B:MET:HB3	12	0.1
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD11	6	0.1
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD12	6	0.1
(1,851)	2:72:B:LEU:HG	2:110:B:LEU:HD13	6	0.1
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD11	18	0.1
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD12	18	0.1
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD13	18	0.1
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD21	18	0.1
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD22	18	0.1
(1,844)	2:72:B:LEU:HD11	2:110:B:LEU:HD23	18	0.1
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD11	18	0.1
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD12	18	0.1
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD13	18	0.1
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD21	18	0.1
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD22	18	0.1
(1,844)	2:72:B:LEU:HD12	2:110:B:LEU:HD23	18	0.1
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD11	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD12	18	0.1
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD13	18	0.1
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD21	18	0.1
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD22	18	0.1
(1,844)	2:72:B:LEU:HD13	2:110:B:LEU:HD23	18	0.1
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD11	18	0.1
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD12	18	0.1
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD13	18	0.1
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD21	18	0.1
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD22	18	0.1
(1,844)	2:72:B:LEU:HD21	2:110:B:LEU:HD23	18	0.1
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD11	18	0.1
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD12	18	0.1
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD13	18	0.1
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD21	18	0.1
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD22	18	0.1
(1,844)	2:72:B:LEU:HD22	2:110:B:LEU:HD23	18	0.1
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD11	18	0.1
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD12	18	0.1
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD13	18	0.1
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD21	18	0.1
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD22	18	0.1
(1,844)	2:72:B:LEU:HD23	2:110:B:LEU:HD23	18	0.1
(1,842)	2:72:B:LEU:HD21	2:86:B:VAL:HB	16	0.1
(1,842)	2:72:B:LEU:HD22	2:86:B:VAL:HB	16	0.1
(1,842)	2:72:B:LEU:HD23	2:86:B:VAL:HB	16	0.1
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD21	14	0.1
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD22	14	0.1
(1,792)	2:67:B:ASP:H	2:68:B:LEU:HD23	14	0.1
(1,774)	2:63:B:ARG:HD3	2:64:B:ALA:H	1	0.1
(1,765)	2:62:B:ARG:HD2	2:63:B:ARG:HA	20	0.1
(1,765)	2:62:B:ARG:HD3	2:63:B:ARG:HA	20	0.1
(1,760)	2:61:B:TYR:H	2:61:B:TYR:HA	15	0.1
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	4	0.1
(1,734)	2:56:B:GLU:H	2:56:B:GLU:HA	16	0.1
(1,721)	2:53:B:ALA:HA	2:56:B:GLU:H	5	0.1
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	5	0.1
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	5	0.1
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	15	0.1
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	15	0.1
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE1	20	0.1
(1,714)	2:52:B:GLU:H	2:155:B:TYR:HE2	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	13	0.1
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	13	0.1
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	13	0.1
(1,673)	2:50:B:LEU:HD11	2:151:B:PHE:H	16	0.1
(1,673)	2:50:B:LEU:HD12	2:151:B:PHE:H	16	0.1
(1,673)	2:50:B:LEU:HD13	2:151:B:PHE:H	16	0.1
(1,672)	2:50:B:LEU:HD11	2:151:B:PHE:HE1	3	0.1
(1,672)	2:50:B:LEU:HD11	2:151:B:PHE:HE2	3	0.1
(1,672)	2:50:B:LEU:HD12	2:151:B:PHE:HE1	3	0.1
(1,672)	2:50:B:LEU:HD12	2:151:B:PHE:HE2	3	0.1
(1,672)	2:50:B:LEU:HD13	2:151:B:PHE:HE1	3	0.1
(1,672)	2:50:B:LEU:HD13	2:151:B:PHE:HE2	3	0.1
(1,666)	2:49:B:ALA:H	2:53:B:ALA:H	19	0.1
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG11	13	0.1
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG12	13	0.1
(1,649)	2:49:B:ALA:HB1	2:152:B:VAL:HG13	13	0.1
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG11	13	0.1
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG12	13	0.1
(1,649)	2:49:B:ALA:HB2	2:152:B:VAL:HG13	13	0.1
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG11	13	0.1
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG12	13	0.1
(1,649)	2:49:B:ALA:HB3	2:152:B:VAL:HG13	13	0.1
(1,628)	2:47:B:LYS:H	2:47:B:LYS:HE2	5	0.1
(1,628)	2:47:B:LYS:H	2:47:B:LYS:HE2	17	0.1
(1,612)	2:47:B:LYS:HB2	2:51:B:ARG:HA	10	0.1
(1,612)	2:47:B:LYS:HB3	2:51:B:ARG:HA	10	0.1
(1,552)	2:43:B:SER:HA	2:44:B:GLU:H	11	0.1
(1,536)	2:41:B:THR:HG1	2:45:B:ALA:H	8	0.1
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	5	0.1
(1,531)	2:41:B:THR:HA	2:42:B:GLU:H	7	0.1
(1,523)	2:40:B:GLY:HA2	2:41:B:THR:H	12	0.1
(1,523)	2:40:B:GLY:HA3	2:41:B:THR:H	12	0.1
(1,496)	2:38:B:PRO:HG2	2:41:B:THR:H	3	0.1
(1,496)	2:38:B:PRO:HG3	2:41:B:THR:H	3	0.1
(1,492)	2:38:B:PRO:HD2	2:39:B:GLU:HG2	1	0.1
(1,492)	2:38:B:PRO:HD2	2:39:B:GLU:HG3	1	0.1
(1,492)	2:38:B:PRO:HD3	2:39:B:GLU:HG2	1	0.1
(1,492)	2:38:B:PRO:HD3	2:39:B:GLU:HG3	1	0.1
(1,486)	2:37:B:ALA:H	2:39:B:GLU:H	19	0.1
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	4	0.1
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	5	0.1
(1,416)	2:33:B:ASN:HA	2:34:B:ARG:H	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	2:24:B:TRP:HD1	2:123:B:VAL:HG11	8	0.1
(1,322)	2:24:B:TRP:HD1	2:123:B:VAL:HG12	8	0.1
(1,322)	2:24:B:TRP:HD1	2:123:B:VAL:HG13	8	0.1
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	3	0.1
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	3	0.1
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE1	5	0.1
(1,306)	2:22:B:TYR:H	2:22:B:TYR:HE2	5	0.1
(1,301)	2:22:B:TYR:HE1	2:26:B:GLN:HG3	11	0.1
(1,301)	2:22:B:TYR:HE2	2:26:B:GLN:HG3	11	0.1
(1,266)	2:20:B:LYS:HB3	2:22:B:TYR:H	4	0.1
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE1	17	0.1
(1,226)	2:17:B:LEU:H	2:22:B:TYR:HE2	17	0.1
(1,211)	2:17:B:LEU:HD11	2:22:B:TYR:H	15	0.1
(1,211)	2:17:B:LEU:HD12	2:22:B:TYR:H	15	0.1
(1,211)	2:17:B:LEU:HD13	2:22:B:TYR:H	15	0.1
(1,211)	2:17:B:LEU:HD21	2:22:B:TYR:H	15	0.1
(1,211)	2:17:B:LEU:HD22	2:22:B:TYR:H	15	0.1
(1,211)	2:17:B:LEU:HD23	2:22:B:TYR:H	15	0.1
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD1	14	0.1
(1,170)	2:14:B:SER:H	2:15:B:TYR:HD2	14	0.1
(1,155)	2:13:B:LEU:HG	2:14:B:SER:H	19	0.1
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG2	6	0.1
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG3	6	0.1
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG2	13	0.1
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG3	13	0.1
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG2	15	0.1
(1,37)	2:5:B:ASN:H	2:6:B:ARG:HG3	15	0.1

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

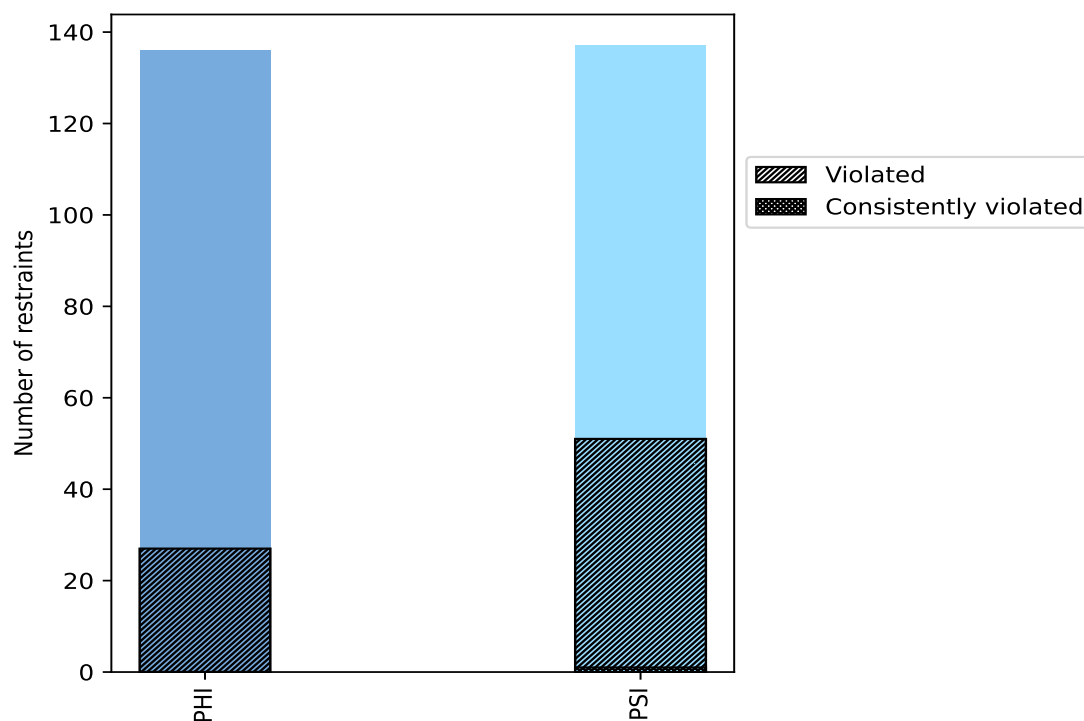
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	136	49.8	27	19.9	9.9	0	0.0	0.0
PSI	137	50.2	51	37.2	18.7	1	0.7	0.4
Total	273	100.0	78	28.6	28.6	1	0.4	0.4

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

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



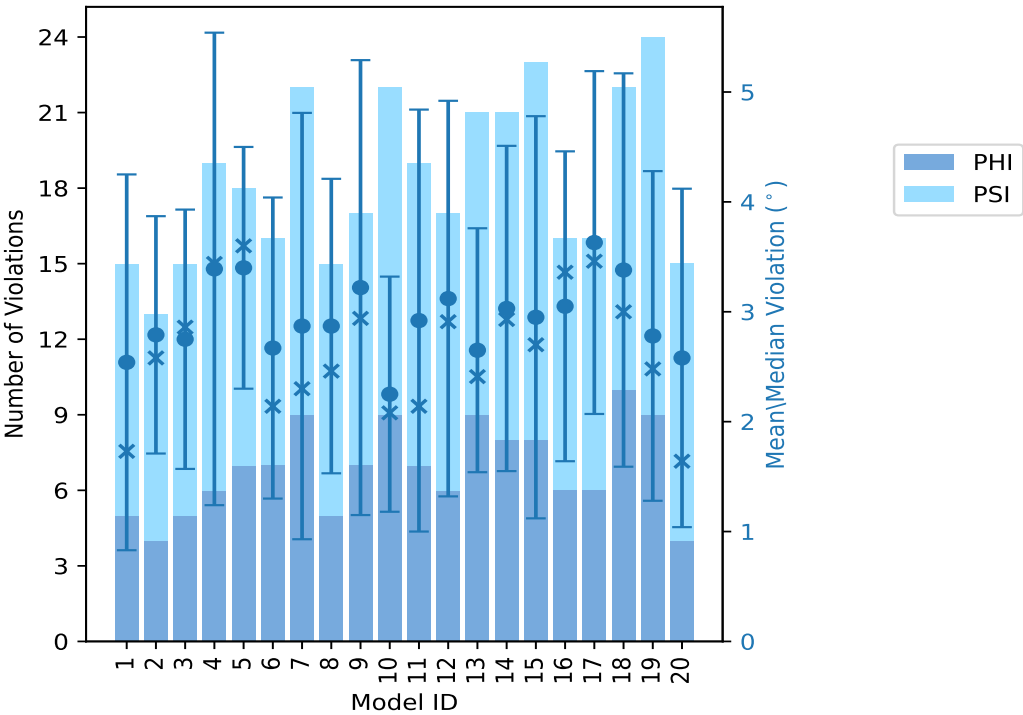
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	5	10	15	2.54	6.15	1.71	1.73
2	4	9	13	2.79	4.78	1.08	2.58
3	5	10	15	2.75	5.13	1.18	2.86
4	6	13	19	3.39	10.87	2.15	3.44
5	7	11	18	3.4	5.67	1.1	3.6
6	7	9	16	2.67	5.57	1.37	2.14
7	9	13	22	2.87	7.43	1.94	2.3
8	5	10	15	2.87	6.17	1.34	2.46
9	7	10	17	3.22	7.82	2.07	2.94
10	9	13	22	2.25	4.83	1.07	2.08
11	7	12	19	2.92	8.49	1.92	2.14
12	6	11	17	3.12	8.29	1.8	2.91
13	9	12	21	2.65	5.6	1.11	2.41
14	8	13	21	3.03	6.69	1.48	2.93
15	8	15	23	2.95	8.47	1.83	2.7
16	6	10	16	3.05	6.45	1.41	3.36
17	6	10	16	3.63	6.66	1.56	3.46
18	10	12	22	3.38	8.84	1.79	3.0
19	9	15	24	2.78	7.86	1.5	2.48
20	4	11	15	2.58	5.95	1.54	1.64

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
9	21	30	1	5.0
4	7	11	2	10.0
1	4	5	3	15.0
3	1	4	4	20.0
1	2	3	5	25.0
1	4	5	6	30.0
1	1	2	7	35.0
0	1	1	8	40.0
1	2	3	9	45.0
2	1	3	10	50.0
0	0	0	11	55.0

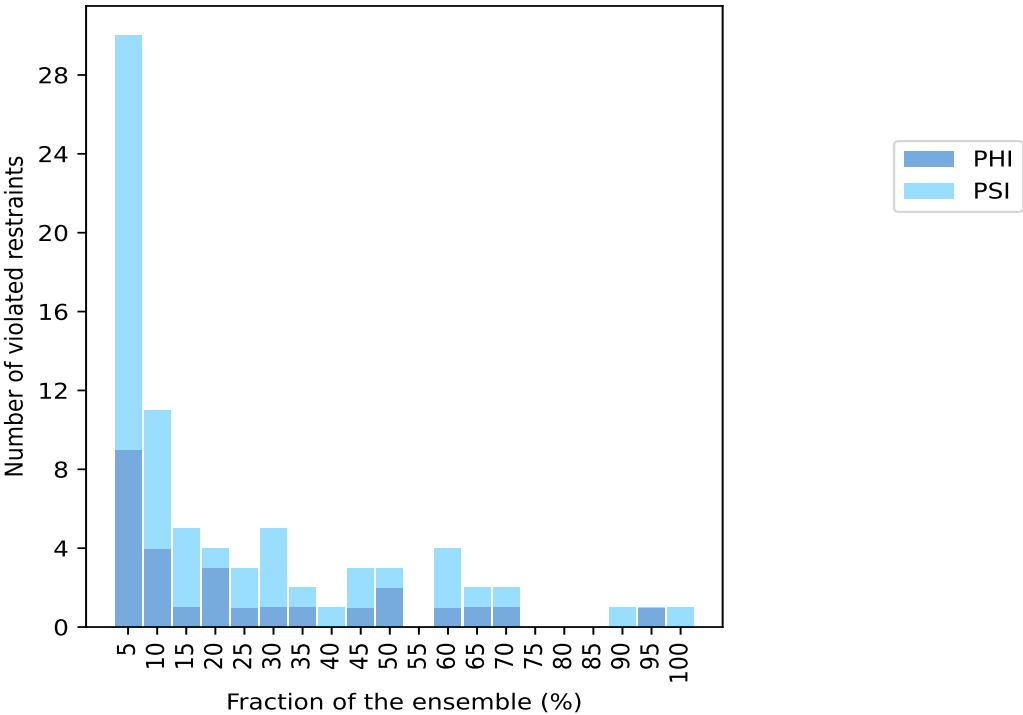
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
1	3	4	12	60.0
1	1	2	13	65.0
1	1	2	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
1	0	1	19	95.0
0	1	1	20	100.0

¹ Number of models with violations

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

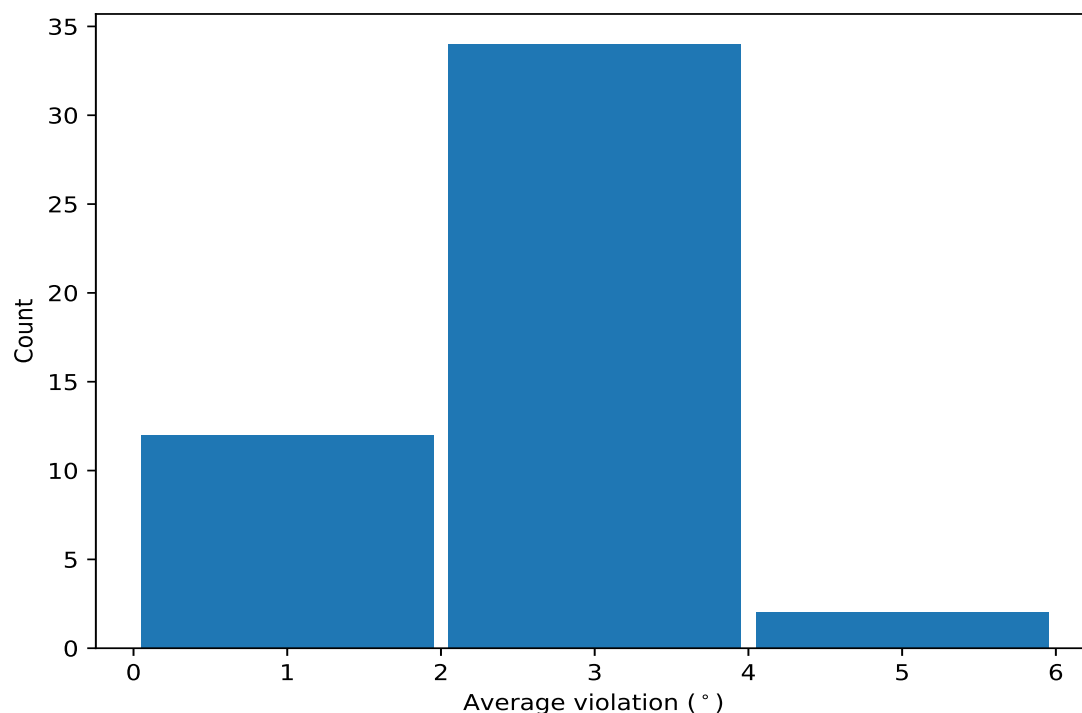


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	20	5.21	2.11	5.02
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	19	3.05	1.26	3.0
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	18	3.69	1.85	3.31
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	14	3.53	1.73	3.23
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	14	3.28	0.98	3.43
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	13	3.9	2.36	3.03
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	13	2.52	1.61	1.97
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	12	3.86	1.35	3.62
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	12	3.21	1.19	2.9
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	12	3.06	1.2	3.16
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	12	2.42	1.16	1.75
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	10	2.95	1.57	2.36
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	10	2.63	0.87	2.94
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	10	2.39	0.98	2.39
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	9	2.7	1.14	2.88
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	9	2.4	0.79	2.53
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	9	2.23	1.38	1.57
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	8	2.92	1.37	2.78
(1,89)	2:61:B:TYR:C	2:62:B:ARG:N	2:62:B:ARG:CA	2:62:B:ARG:C	7	3.26	1.22	3.84
(1,227)	2:141:B:TRP:N	2:141:B:TRP:CA	2:141:B:TRP:C	2:142:B:ILE:N	7	3.13	0.98	3.14

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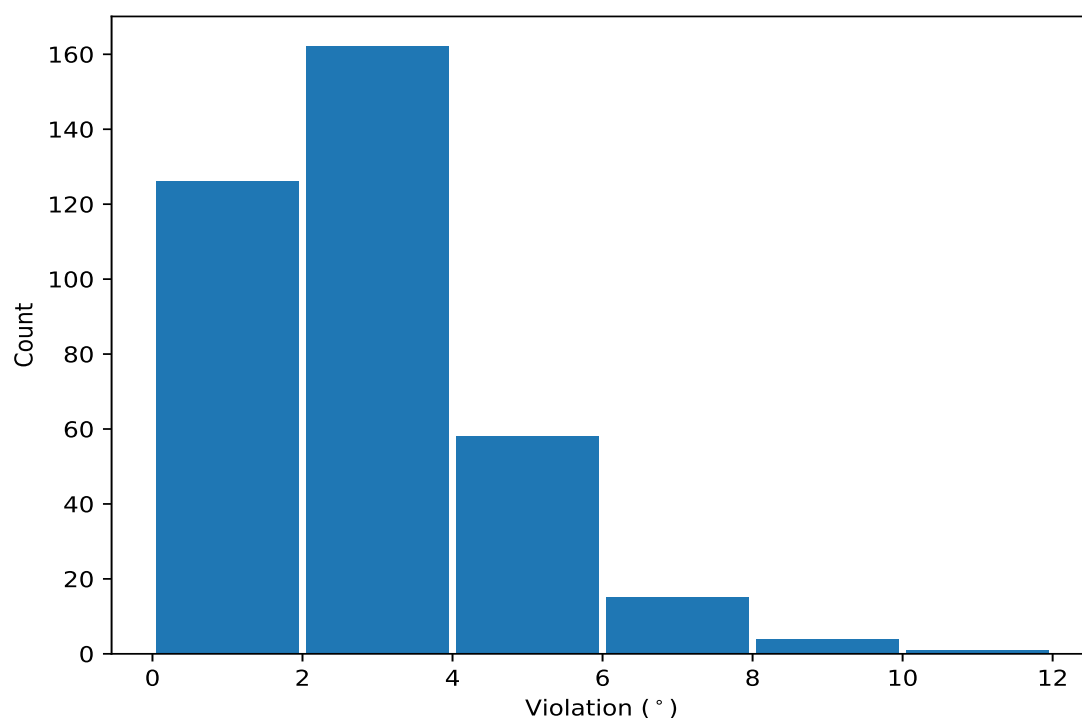
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,82)	2:58:B:GLU:N	2:58:B:GLU:CA	2:58:B:GLU:C	2:59:B:LEU:N	6	3.98	3.23	2.74
(1,26)	2:15:B:TYR:N	2:15:B:TYR:CA	2:15:B:TYR:C	2:16:B:LYS:N	6	3.72	1.9	3.81
(1,233)	2:145:B:ASN:N	2:145:B:ASN:CA	2:145:B:ASN:C	2:146:B:GLY:N	6	3.1	1.44	2.7
(1,141)	2:91:B:PHE:C	2:92:B:ARG:N	2:92:B:ARG:CA	2:92:B:ARG:C	6	2.07	0.8	1.84
(1,217)	2:136:B:ASP:N	2:136:B:ASP:CA	2:136:B:ASP:C	2:137:B:HIS:N	6	1.93	0.81	1.77
(1,54)	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	2:45:B:ALA:N	5	3.04	0.88	3.49
(1,145)	2:94:B:GLY:C	2:95:B:VAL:N	2:95:B:VAL:CA	2:95:B:VAL:C	5	2.82	1.22	3.56
(1,56)	2:45:B:ALA:N	2:45:B:ALA:CA	2:45:B:ALA:C	2:46:B:VAL:N	5	1.64	0.54	1.54
(1,75)	2:54:B:GLY:C	2:55:B:ASP:N	2:55:B:ASP:CA	2:55:B:ASP:C	4	3.16	0.23	3.06
(1,218)	2:136:B:ASP:C	2:137:B:HIS:N	2:137:B:HIS:CA	2:137:B:HIS:C	4	2.64	0.43	2.72
(1,80)	2:57:B:PHE:N	2:57:B:PHE:CA	2:57:B:PHE:C	2:58:B:GLU:N	4	2.26	1.1	2.2
(1,53)	2:43:B:SER:C	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	4	1.43	0.39	1.27
(1,78)	2:56:B:GLU:N	2:56:B:GLU:CA	2:56:B:GLU:C	2:57:B:PHE:N	3	2.04	0.73	2.41
(1,109)	2:74:B:ILE:C	2:75:B:THR:N	2:75:B:THR:CA	2:75:B:THR:C	3	1.83	0.53	2.09
(1,30)	2:17:B:LEU:N	2:17:B:LEU:CA	2:17:B:LEU:C	2:18:B:SER:N	3	1.83	0.4	1.94
(1,36)	2:20:B:LYS:N	2:20:B:LYS:CA	2:20:B:LYS:C	2:21:B:GLY:N	3	1.79	0.38	1.54
(1,70)	2:52:B:GLU:N	2:52:B:GLU:CA	2:52:B:GLU:C	2:53:B:ALA:N	3	1.13	0.06	1.13
(1,160)	2:104:B:PHE:N	2:104:B:PHE:CA	2:104:B:PHE:C	2:105:B:SER:N	2	5.45	1.05	5.45
(1,49)	2:26:B:GLN:C	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2	3.0	1.6	3.0
(1,214)	2:134:B:LEU:N	2:134:B:LEU:CA	2:134:B:LEU:C	2:135:B:ASN:N	2	2.84	0.4	2.84
(1,106)	2:70:B:SER:N	2:70:B:SER:CA	2:70:B:SER:C	2:71:B:GLN:N	2	2.8	0.77	2.8
(1,229)	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	2:143:B:GLN:N	2	2.76	0.45	2.76
(1,65)	2:49:B:ALA:C	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2	2.41	1.08	2.41
(1,234)	2:148:B:TRP:N	2:148:B:TRP:CA	2:148:B:TRP:C	2:149:B:ASP:N	2	1.82	0.64	1.82
(1,178)	2:113:B:GLU:N	2:113:B:GLU:CA	2:113:B:GLU:C	2:114:B:SER:N	2	1.79	0.62	1.79
(1,248)	2:155:B:TYR:N	2:155:B:TYR:CA	2:155:B:TYR:C	2:156:B:GLY:N	2	1.37	0.26	1.37
(1,260)	1:316:A:GLU:C	1:317:A:HIS:N	1:317:A:HIS:CA	1:317:A:HIS:C	2	1.2	0.11	1.2
(1,256)	1:314:A:THR:C	1:315:A:PHE:N	1:315:A:PHE:CA	1:315:A:PHE:C	2	1.13	0.07	1.13

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 (°)
(1,82)	2:58:B:GLU:N	2:58:B:GLU:CA	2:58:B:GLU:C	2:59:B:LEU:N	4	10.87
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	18	8.84
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	11	8.49
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	15	8.47
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	12	8.29
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	19	7.86
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	9	7.82
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	9	7.7
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	7	7.43
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	7	7.42
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	15	6.89
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	14	6.69
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	17	6.66
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	17	6.55
(1,160)	2:104:B:PHE:N	2:104:B:PHE:CA	2:104:B:PHE:C	2:105:B:SER:N	7	6.5
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	16	6.45
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	8	6.17
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	1	6.15
(1,26)	2:15:B:TYR:N	2:15:B:TYR:CA	2:15:B:TYR:C	2:16:B:LYS:N	19	6.05
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	18	6.02
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	20	5.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	20	5.93
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	11	5.81
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	1	5.75
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	14	5.72
(1,26)	2:15:B:TYR:N	2:15:B:TYR:CA	2:15:B:TYR:C	2:16:B:LYS:N	18	5.7
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	5	5.67
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	13	5.6
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	6	5.57
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	6	5.5
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	12	5.25
(1,233)	2:145:B:ASN:N	2:145:B:ASN:CA	2:145:B:ASN:C	2:146:B:GLY:N	17	5.22
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	8	5.18
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	15	5.14
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	3	5.13
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	4	5.03
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	11	4.96
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	4	4.91
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	1	4.88
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	9	4.87
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	10	4.83
(1,26)	2:15:B:TYR:N	2:15:B:TYR:CA	2:15:B:TYR:C	2:16:B:LYS:N	3	4.81
(1,89)	2:61:B:TYR:C	2:62:B:ARG:N	2:62:B:ARG:CA	2:62:B:ARG:C	2	4.78
(1,233)	2:145:B:ASN:N	2:145:B:ASN:CA	2:145:B:ASN:C	2:146:B:GLY:N	18	4.77
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	12	4.75
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	10	4.72
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	18	4.6
(1,227)	2:141:B:TRP:N	2:141:B:TRP:CA	2:141:B:TRP:C	2:142:B:ILE:N	7	4.6
(1,49)	2:26:B:GLN:C	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	5	4.6
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	15	4.59
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	13	4.58
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	17	4.54
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	4	4.52
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	6	4.5
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	9	4.47
(1,160)	2:104:B:PHE:N	2:104:B:PHE:CA	2:104:B:PHE:C	2:105:B:SER:N	14	4.4
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	11	4.39
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	12	4.38
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	19	4.37
(1,82)	2:58:B:GLU:N	2:58:B:GLU:CA	2:58:B:GLU:C	2:59:B:LEU:N	9	4.36
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	11	4.35
(1,74)	2:54:B:GLY:N	2:54:B:GLY:CA	2:54:B:GLY:C	2:55:B:ASP:N	2	4.31
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	17	4.3
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	14	4.3
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	5	4.29
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	5	4.27
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	18	4.23
(1,89)	2:61:B:TYR:C	2:62:B:ARG:N	2:62:B:ARG:CA	2:62:B:ARG:C	5	4.2
(1,54)	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	2:45:B:ALA:N	16	4.16
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	8	4.14
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	17	4.09
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	5	4.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	13	4.04
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	16	4.03
(1,145)	2:94:B:GLY:C	2:95:B:VAL:N	2:95:B:VAL:CA	2:95:B:VAL:C	16	4.02
(1,140)	2:91:B:PHE:N	2:91:B:PHE:CA	2:91:B:PHE:C	2:92:B:ARG:N	16	4.01
(1,89)	2:61:B:TYR:C	2:62:B:ARG:N	2:62:B:ARG:CA	2:62:B:ARG:C	19	4.01
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	14	4.0
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	4	3.98
(1,271)	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	1:323:A:GLU:N	12	3.95
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	5	3.9
(1,227)	2:141:B:TRP:N	2:141:B:TRP:CA	2:141:B:TRP:C	2:142:B:ILE:N	12	3.88
(1,145)	2:94:B:GLY:C	2:95:B:VAL:N	2:95:B:VAL:CA	2:95:B:VAL:C	18	3.86
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	11	3.84
(1,89)	2:61:B:TYR:C	2:62:B:ARG:N	2:62:B:ARG:CA	2:62:B:ARG:C	13	3.84
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	4	3.81
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	20	3.79
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	18	3.78
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	17	3.77
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	16	3.77
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	2	3.77
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	4	3.76
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	4	3.76
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	9	3.76
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	14	3.76
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	14	3.74
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	5	3.73
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	2	3.71
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	14	3.68
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	5	3.64
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	1	3.63
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	15	3.6
(1,80)	2:57:B:PHE:N	2:57:B:PHE:CA	2:57:B:PHE:C	2:58:B:GLU:N	10	3.6
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	15	3.59
(1,106)	2:70:B:SER:N	2:70:B:SER:CA	2:70:B:SER:C	2:71:B:GLN:N	3	3.57
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	17	3.56
(1,145)	2:94:B:GLY:C	2:95:B:VAL:N	2:95:B:VAL:CA	2:95:B:VAL:C	5	3.56
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	18	3.55
(1,75)	2:54:B:GLY:C	2:55:B:ASP:N	2:55:B:ASP:CA	2:55:B:ASP:C	3	3.55
(1,54)	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	2:45:B:ALA:N	14	3.55
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	4	3.52
(1,227)	2:141:B:TRP:N	2:141:B:TRP:CA	2:141:B:TRP:C	2:142:B:ILE:N	15	3.49
(1,77)	2:55:B:ASP:C	2:56:B:GLU:N	2:56:B:GLU:CA	2:56:B:GLU:C	6	3.49
(1,65)	2:49:B:ALA:C	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	7	3.49
(1,54)	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	2:45:B:ALA:N	15	3.49
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	16	3.48
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	12	3.47
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	4	3.44
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	16	3.42
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	18	3.35
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	20	3.35
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	17	3.35
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	3	3.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	16	3.31
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	9	3.27
(1,217)	2:136:B:ASP:N	2:136:B:ASP:CA	2:136:B:ASP:C	2:137:B:HIS:N	7	3.27
(1,214)	2:134:B:LEU:N	2:134:B:LEU:CA	2:134:B:LEU:C	2:135:B:ASN:N	2	3.24
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	7	3.23
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	8	3.23
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	5	3.22
(1,229)	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	2:143:B:GLN:N	10	3.21
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	3	3.18
(1,141)	2:91:B:PHE:C	2:92:B:ARG:N	2:92:B:ARG:CA	2:92:B:ARG:C	14	3.18
(1,227)	2:141:B:TRP:N	2:141:B:TRP:CA	2:141:B:TRP:C	2:142:B:ILE:N	5	3.14
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	6	3.12
(1,218)	2:136:B:ASP:C	2:137:B:HIS:N	2:137:B:HIS:CA	2:137:B:HIS:C	17	3.12
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	18	3.11
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	19	3.09
(1,80)	2:57:B:PHE:N	2:57:B:PHE:CA	2:57:B:PHE:C	2:58:B:GLU:N	13	3.08
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	19	3.07
(1,75)	2:54:B:GLY:C	2:55:B:ASP:N	2:55:B:ASP:CA	2:55:B:ASP:C	11	3.07
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	19	3.06
(1,141)	2:91:B:PHE:C	2:92:B:ARG:N	2:92:B:ARG:CA	2:92:B:ARG:C	9	3.06
(1,75)	2:54:B:GLY:C	2:55:B:ASP:N	2:55:B:ASP:CA	2:55:B:ASP:C	13	3.06
(1,215)	2:134:B:LEU:C	2:135:B:ASN:N	2:135:B:ASN:CA	2:135:B:ASN:C	17	3.04
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	15	3.04
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	8	3.03
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	3	3.03
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	7	3.03
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	12	3.01
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	7	3.0
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	5	3.0
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	8	2.99
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	19	2.98
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	5	2.97
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	11	2.97
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	7	2.96
(1,218)	2:136:B:ASP:C	2:137:B:HIS:N	2:137:B:HIS:CA	2:137:B:HIS:C	13	2.96
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	13	2.94
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	9	2.94
(1,75)	2:54:B:GLY:C	2:55:B:ASP:N	2:55:B:ASP:CA	2:55:B:ASP:C	10	2.94
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	14	2.93
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	4	2.93
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	12	2.91
(1,51)	2:42:B:GLU:C	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	18	2.9
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	15	2.9
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	8	2.88
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	15	2.86
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	3	2.86
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	1	2.84
(1,82)	2:58:B:GLU:N	2:58:B:GLU:CA	2:58:B:GLU:C	2:59:B:LEU:N	17	2.83
(1,26)	2:15:B:TYR:N	2:15:B:TYR:CA	2:15:B:TYR:C	2:16:B:LYS:N	20	2.82
(1,227)	2:141:B:TRP:N	2:141:B:TRP:CA	2:141:B:TRP:C	2:142:B:ILE:N	13	2.81
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	20	2.81

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	1	2.8
(1,84)	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	2:60:B:ARG:N	4	2.8
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	17	2.77
(1,233)	2:145:B:ASN:N	2:145:B:ASN:CA	2:145:B:ASN:C	2:146:B:GLY:N	19	2.76
(1,227)	2:141:B:TRP:N	2:141:B:TRP:CA	2:141:B:TRP:C	2:142:B:ILE:N	18	2.76
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	9	2.76
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	16	2.76
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	10	2.75
(1,89)	2:61:B:TYR:C	2:62:B:ARG:N	2:62:B:ARG:CA	2:62:B:ARG:C	6	2.74
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	9	2.73
(1,78)	2:56:B:GLU:N	2:56:B:GLU:CA	2:56:B:GLU:C	2:57:B:PHE:N	15	2.7
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	14	2.68
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	4	2.67
(1,233)	2:145:B:ASN:N	2:145:B:ASN:CA	2:145:B:ASN:C	2:146:B:GLY:N	10	2.65
(1,217)	2:136:B:ASP:N	2:136:B:ASP:CA	2:136:B:ASP:C	2:137:B:HIS:N	18	2.64
(1,82)	2:58:B:GLU:N	2:58:B:GLU:CA	2:58:B:GLU:C	2:59:B:LEU:N	19	2.64
(1,56)	2:45:B:ALA:N	2:45:B:ALA:CA	2:45:B:ALA:C	2:46:B:VAL:N	16	2.64
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	19	2.63
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2	2.63
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	2	2.58
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	2	2.57
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	2	2.53
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	13	2.51
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	19	2.51
(1,130)	2:86:B:VAL:N	2:86:B:VAL:CA	2:86:B:VAL:C	2:87:B:VAL:N	18	2.51
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	7	2.49
(1,218)	2:136:B:ASP:C	2:137:B:HIS:N	2:137:B:HIS:CA	2:137:B:HIS:C	18	2.48
(1,234)	2:148:B:TRP:N	2:148:B:TRP:CA	2:148:B:TRP:C	2:149:B:ASP:N	8	2.46
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	20	2.46
(1,27)	2:15:B:TYR:C	2:16:B:LYS:N	2:16:B:LYS:CA	2:16:B:LYS:C	19	2.46
(1,214)	2:134:B:LEU:N	2:134:B:LEU:CA	2:134:B:LEU:C	2:135:B:ASN:N	8	2.45
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	10	2.43
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	14	2.42
(1,178)	2:113:B:GLU:N	2:113:B:GLU:CA	2:113:B:GLU:C	2:114:B:SER:N	13	2.41
(1,78)	2:56:B:GLU:N	2:56:B:GLU:CA	2:56:B:GLU:C	2:57:B:PHE:N	8	2.41
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	13	2.37
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	10	2.33
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	8	2.33
(1,36)	2:20:B:LYS:N	2:20:B:LYS:CA	2:20:B:LYS:C	2:21:B:GLY:N	14	2.33
(1,229)	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	2:143:B:GLN:N	19	2.32
(1,109)	2:74:B:ILE:C	2:75:B:THR:N	2:75:B:THR:CA	2:75:B:THR:C	10	2.32
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	14	2.27
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	11	2.27
(1,30)	2:17:B:LEU:N	2:17:B:LEU:CA	2:17:B:LEU:C	2:18:B:SER:N	3	2.26
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	19	2.25
(1,89)	2:61:B:TYR:C	2:62:B:ARG:N	2:62:B:ARG:CA	2:62:B:ARG:C	10	2.23
(1,102)	2:68:B:LEU:N	2:68:B:LEU:CA	2:68:B:LEU:C	2:69:B:THR:N	13	2.22
(1,132)	2:87:B:VAL:N	2:87:B:VAL:CA	2:87:B:VAL:C	2:88:B:ASN:N	6	2.18
(1,1)	2:2:B:SER:C	2:3:B:GLN:N	2:3:B:GLN:CA	2:3:B:GLN:C	15	2.18
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	5	2.17
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	6	2.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	6	2.14
(1,54)	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	2:45:B:ALA:N	11	2.14
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	12	2.12
(1,141)	2:91:B:PHE:C	2:92:B:ARG:N	2:92:B:ARG:CA	2:92:B:ARG:C	7	2.11
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	6	2.1
(1,109)	2:74:B:ILE:C	2:75:B:THR:N	2:75:B:THR:CA	2:75:B:THR:C	6	2.09
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	19	2.08
(1,53)	2:43:B:SER:C	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	12	2.08
(1,116)	2:79:B:ALA:N	2:79:B:ALA:CA	2:79:B:ALA:C	2:80:B:TYR:N	11	2.07
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	5	2.06
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	16	2.05
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	3	2.03
(1,106)	2:70:B:SER:N	2:70:B:SER:CA	2:70:B:SER:C	2:71:B:GLN:N	18	2.02
(1,233)	2:145:B:ASN:N	2:145:B:ASN:CA	2:145:B:ASN:C	2:146:B:GLY:N	6	2.01
(1,218)	2:136:B:ASP:C	2:137:B:HIS:N	2:137:B:HIS:CA	2:137:B:HIS:C	7	2.01
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	13	1.97
(1,144)	2:93:B:ASP:N	2:93:B:ASP:CA	2:93:B:ASP:C	2:94:B:GLY:N	10	1.94
(1,82)	2:58:B:GLU:N	2:58:B:GLU:CA	2:58:B:GLU:C	2:59:B:LEU:N	11	1.94
(1,30)	2:17:B:LEU:N	2:17:B:LEU:CA	2:17:B:LEU:C	2:18:B:SER:N	13	1.94
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	13	1.93
(1,217)	2:136:B:ASP:N	2:136:B:ASP:CA	2:136:B:ASP:C	2:137:B:HIS:N	19	1.89
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	18	1.89
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	2	1.88
(1,54)	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	2:45:B:ALA:N	12	1.88
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	13	1.87
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	19	1.86
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	15	1.86
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	15	1.86
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	11	1.83
(1,50)	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	2:28:B:SER:N	10	1.82
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	14	1.82
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	3	1.8
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	17	1.79
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	4	1.76
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	1	1.76
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	7	1.75
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	2	1.74
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	18	1.74
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	3	1.74
(1,26)	2:15:B:TYR:N	2:15:B:TYR:CA	2:15:B:TYR:C	2:16:B:LYS:N	4	1.74
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	1	1.73
(1,4)	2:4:B:SER:N	2:4:B:SER:CA	2:4:B:SER:C	2:5:B:ASN:N	15	1.73
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	8	1.7
(1,128)	2:85:B:GLN:N	2:85:B:GLN:CA	2:85:B:GLN:C	2:86:B:VAL:N	10	1.68
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	7	1.66
(1,217)	2:136:B:ASP:N	2:136:B:ASP:CA	2:136:B:ASP:C	2:137:B:HIS:N	5	1.65
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	12	1.64
(1,56)	2:45:B:ALA:N	2:45:B:ALA:CA	2:45:B:ALA:C	2:46:B:VAL:N	20	1.64
(1,248)	2:155:B:TYR:N	2:155:B:TYR:CA	2:155:B:TYR:C	2:156:B:GLY:N	3	1.63
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	20	1.63
(1,156)	2:102:B:ALA:N	2:102:B:ALA:CA	2:102:B:ALA:C	2:103:B:PHE:N	15	1.62

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	19	1.62
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	13	1.62
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	8	1.61
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	19	1.61
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	15	1.6
(1,228)	2:141:B:TRP:C	2:142:B:ILE:N	2:142:B:ILE:CA	2:142:B:ILE:C	10	1.6
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	15	1.6
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	13	1.58
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	11	1.57
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	20	1.57
(1,141)	2:91:B:PHE:C	2:92:B:ARG:N	2:92:B:ARG:CA	2:92:B:ARG:C	19	1.56
(1,148)	2:98:B:GLY:N	2:98:B:GLY:CA	2:98:B:GLY:C	2:99:B:ARG:N	10	1.54
(1,56)	2:45:B:ALA:N	2:45:B:ALA:CA	2:45:B:ALA:C	2:46:B:VAL:N	7	1.54
(1,36)	2:20:B:LYS:N	2:20:B:LYS:CA	2:20:B:LYS:C	2:21:B:GLY:N	11	1.54
(1,36)	2:20:B:LYS:N	2:20:B:LYS:CA	2:20:B:LYS:C	2:21:B:GLY:N	20	1.49
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	6	1.47
(1,79)	2:56:B:GLU:C	2:57:B:PHE:N	2:57:B:PHE:CA	2:57:B:PHE:C	14	1.46
(1,254)	2:162:B:GLU:C	2:163:B:SER:N	2:163:B:SER:CA	2:163:B:SER:C	19	1.41
(1,154)	2:101:B:VAL:N	2:101:B:VAL:CA	2:101:B:VAL:C	2:102:B:ALA:N	1	1.4
(1,145)	2:94:B:GLY:C	2:95:B:VAL:N	2:95:B:VAL:CA	2:95:B:VAL:C	8	1.4
(1,49)	2:26:B:GLN:C	2:27:B:PHE:N	2:27:B:PHE:CA	2:27:B:PHE:C	20	1.4
(1,12)	2:8:B:LEU:N	2:8:B:LEU:CA	2:8:B:LEU:C	2:9:B:VAL:N	4	1.4
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	12	1.39
(1,141)	2:91:B:PHE:C	2:92:B:ARG:N	2:92:B:ARG:CA	2:92:B:ARG:C	2	1.38
(1,53)	2:43:B:SER:C	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	16	1.38
(1,28)	2:16:B:LYS:N	2:16:B:LYS:CA	2:16:B:LYS:C	2:17:B:LEU:N	19	1.38
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	9	1.36
(1,185)	2:116:B:ASP:C	2:117:B:LYS:N	2:117:B:LYS:CA	2:117:B:LYS:C	12	1.36
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	12	1.36
(1,67)	2:50:B:LEU:C	2:51:B:ARG:N	2:51:B:ARG:CA	2:51:B:ARG:C	6	1.36
(1,270)	1:321:A:SER:C	1:322:A:LEU:N	1:322:A:LEU:CA	1:322:A:LEU:C	20	1.34
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	15	1.34
(1,32)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:GLN:N	10	1.34
(1,80)	2:57:B:PHE:N	2:57:B:PHE:CA	2:57:B:PHE:C	2:58:B:GLU:N	20	1.33
(1,65)	2:49:B:ALA:C	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	9	1.33
(1,260)	1:316:A:GLU:C	1:317:A:HIS:N	1:317:A:HIS:CA	1:317:A:HIS:C	18	1.31
(1,268)	1:320:A:SER:C	1:321:A:SER:N	1:321:A:SER:CA	1:321:A:SER:C	14	1.3
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	12	1.29
(1,30)	2:17:B:LEU:N	2:17:B:LEU:CA	2:17:B:LEU:C	2:18:B:SER:N	1	1.29
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	19	1.28
(1,145)	2:94:B:GLY:C	2:95:B:VAL:N	2:95:B:VAL:CA	2:95:B:VAL:C	10	1.27
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	17	1.26
(1,56)	2:45:B:ALA:N	2:45:B:ALA:CA	2:45:B:ALA:C	2:46:B:VAL:N	1	1.25
(1,257)	1:315:A:PHE:N	1:315:A:PHE:CA	1:315:A:PHE:C	1:316:A:GLU:N	3	1.24
(1,227)	2:141:B:TRP:N	2:141:B:TRP:CA	2:141:B:TRP:C	2:142:B:ILE:N	6	1.23
(1,82)	2:58:B:GLU:N	2:58:B:GLU:CA	2:58:B:GLU:C	2:59:B:LEU:N	7	1.23
(1,104)	2:69:B:THR:N	2:69:B:THR:CA	2:69:B:THR:C	2:70:B:SER:N	10	1.22
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	16	1.21
(1,70)	2:52:B:GLU:N	2:52:B:GLU:CA	2:52:B:GLU:C	2:53:B:ALA:N	18	1.21
(1,256)	1:314:A:THR:C	1:315:A:PHE:N	1:315:A:PHE:CA	1:315:A:PHE:C	4	1.2
(1,233)	2:145:B:ASN:N	2:145:B:ASN:CA	2:145:B:ASN:C	2:146:B:GLY:N	14	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,164)	2:106:B:PHE:N	2:106:B:PHE:CA	2:106:B:PHE:C	2:107:B:GLY:N	4	1.2
(1,66)	2:50:B:LEU:N	2:50:B:LEU:CA	2:50:B:LEU:C	2:51:B:ARG:N	15	1.2
(1,234)	2:148:B:TRP:N	2:148:B:TRP:CA	2:148:B:TRP:C	2:149:B:ASP:N	7	1.19
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	1	1.18
(1,26)	2:15:B:TYR:N	2:15:B:TYR:CA	2:15:B:TYR:C	2:16:B:LYS:N	13	1.18
(1,265)	1:319:A:TRP:N	1:319:A:TRP:CA	1:319:A:TRP:C	1:320:A:SER:N	1	1.17
(1,178)	2:113:B:GLU:N	2:113:B:GLU:CA	2:113:B:GLU:C	2:114:B:SER:N	17	1.17
(1,138)	2:90:B:LEU:N	2:90:B:LEU:CA	2:90:B:LEU:C	2:91:B:PHE:N	14	1.17
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	4	1.17
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	9	1.17
(1,53)	2:43:B:SER:C	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	7	1.16
(1,10)	2:7:B:GLU:N	2:7:B:GLU:CA	2:7:B:GLU:C	2:8:B:LEU:N	5	1.14
(1,70)	2:52:B:GLU:N	2:52:B:GLU:CA	2:52:B:GLU:C	2:53:B:ALA:N	20	1.13
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	2	1.13
(1,273)	1:323:A:GLU:N	1:323:A:GLU:CA	1:323:A:GLU:C	1:324:A:PRO:N	8	1.12
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	1	1.12
(1,248)	2:155:B:TYR:N	2:155:B:TYR:CA	2:155:B:TYR:C	2:156:B:GLY:N	6	1.11
(1,141)	2:91:B:PHE:C	2:92:B:ARG:N	2:92:B:ARG:CA	2:92:B:ARG:C	1	1.11
(1,56)	2:45:B:ALA:N	2:45:B:ALA:CA	2:45:B:ALA:C	2:46:B:VAL:N	11	1.11
(1,217)	2:136:B:ASP:N	2:136:B:ASP:CA	2:136:B:ASP:C	2:137:B:HIS:N	15	1.1
(1,53)	2:43:B:SER:C	2:44:B:GLU:N	2:44:B:GLU:CA	2:44:B:GLU:C	11	1.1
(1,260)	1:316:A:GLU:C	1:317:A:HIS:N	1:317:A:HIS:CA	1:317:A:HIS:C	9	1.09
(1,109)	2:74:B:ILE:C	2:75:B:THR:N	2:75:B:THR:CA	2:75:B:THR:C	16	1.09
(1,86)	2:60:B:ARG:N	2:60:B:ARG:CA	2:60:B:ARG:C	2:61:B:TYR:N	15	1.09
(1,150)	2:99:B:ARG:N	2:99:B:ARG:CA	2:99:B:ARG:C	2:100:B:ILE:N	18	1.08
(1,118)	2:80:B:TYR:N	2:80:B:TYR:CA	2:80:B:TYR:C	2:81:B:GLN:N	3	1.08
(1,263)	1:318:A:LEU:N	1:318:A:LEU:CA	1:318:A:LEU:C	1:319:A:TRP:N	10	1.06
(1,256)	1:314:A:THR:C	1:315:A:PHE:N	1:315:A:PHE:CA	1:315:A:PHE:C	9	1.06
(1,70)	2:52:B:GLU:N	2:52:B:GLU:CA	2:52:B:GLU:C	2:53:B:ALA:N	16	1.06
(1,230)	2:142:B:ILE:C	2:143:B:GLN:N	2:143:B:GLN:CA	2:143:B:GLN:C	7	1.05
(1,111)	2:76:B:PRO:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	13	1.05
(1,80)	2:57:B:PHE:N	2:57:B:PHE:CA	2:57:B:PHE:C	2:58:B:GLU:N	11	1.05
(1,112)	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	2:78:B:THR:N	11	1.03
(1,89)	2:61:B:TYR:C	2:62:B:ARG:N	2:62:B:ARG:CA	2:62:B:ARG:C	14	1.03
(1,83)	2:58:B:GLU:C	2:59:B:LEU:N	2:59:B:LEU:CA	2:59:B:LEU:C	10	1.03
(1,217)	2:136:B:ASP:N	2:136:B:ASP:CA	2:136:B:ASP:C	2:137:B:HIS:N	9	1.02
(1,78)	2:56:B:GLU:N	2:56:B:GLU:CA	2:56:B:GLU:C	2:57:B:PHE:N	10	1.02
(1,41)	2:22:B:TYR:C	2:23:B:SER:N	2:23:B:SER:CA	2:23:B:SER:C	7	1.01
(1,52)	2:43:B:SER:N	2:43:B:SER:CA	2:43:B:SER:C	2:44:B:GLU:N	7	1.0