



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 01:57 PM UTC

PDB ID : 2MG4 / pdb_00002mg4
BMRB ID : 19585
Title : Computational design and experimental verification of a symmetric protein homodimer
Authors : Mou, Y.; Huang, P.S.; Hsu, F.C.; Huang, S.J.; Mayo, S.L.
Deposited on : 2013-10-26

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

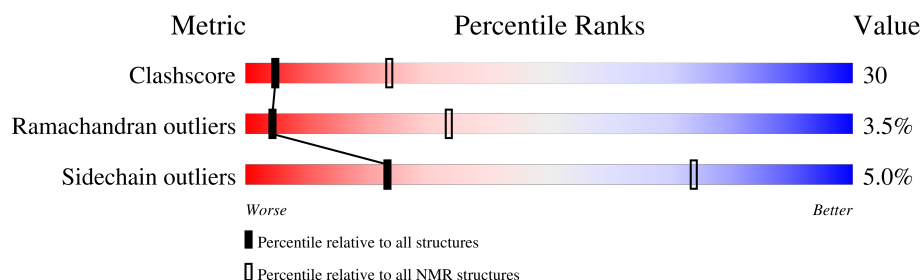
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 35%.

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	66	
1	B	66	

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:64, B:2-B:64 (126)	1.59	8

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, 5, 7, 10
2	3, 6, 8
3	2, 9
Single-model clusters	4

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2362 atoms, of which 1166 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Computational designed homodimer.

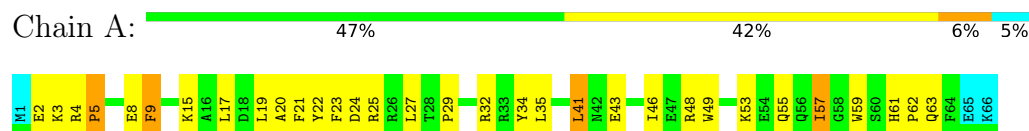
Mol	Chain	Residues	Atoms						Trace
1	A	66	Total	C	H	N	O	S	0
			1181	379	583	113	105	1	
1	B	66	Total	C	H	N	O	S	0
			1181	379	583	113	105	1	

4 Residue-property plots

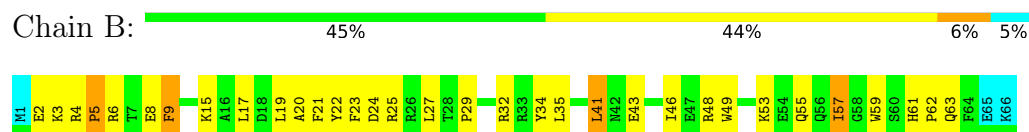
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Computational designed homodimer



- Molecule 1: Computational designed homodimer

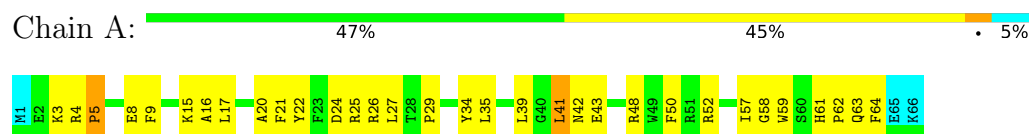


4.2 Scores per residue for each member of the ensemble

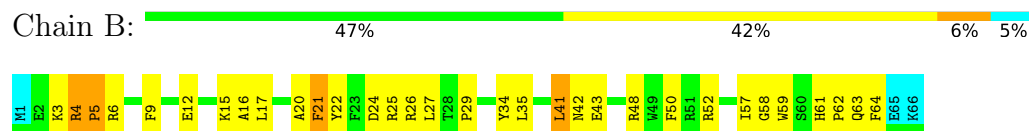
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Computational designed homodimer

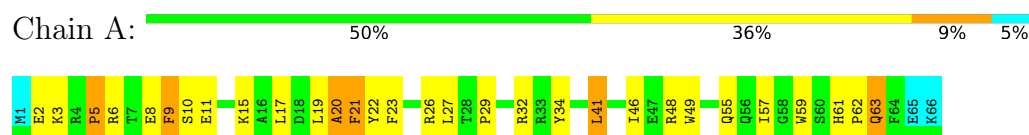


- Molecule 1: Computational designed homodimer

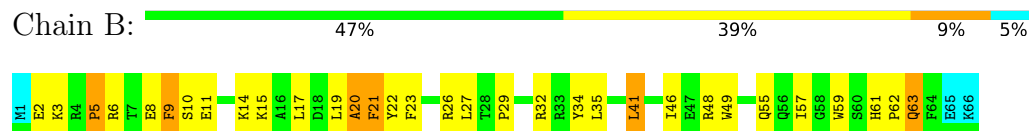


4.2.2 Score per residue for model 2

- Molecule 1: Computational designed homodimer

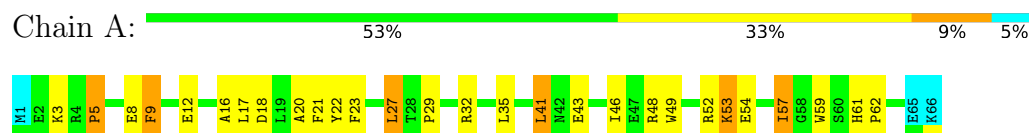


- Molecule 1: Computational designed homodimer

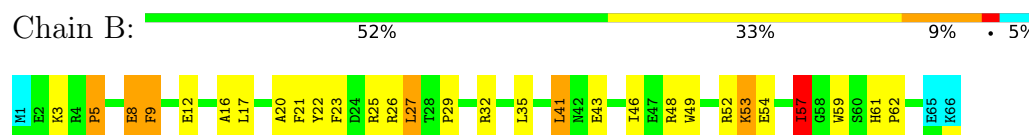


4.2.3 Score per residue for model 3

- Molecule 1: Computational designed homodimer

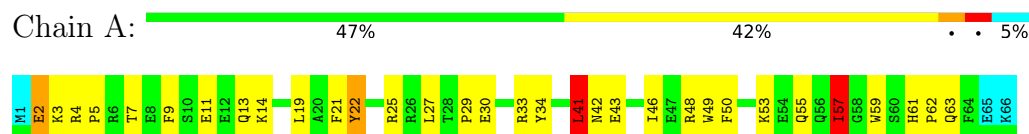


- Molecule 1: Computational designed homodimer

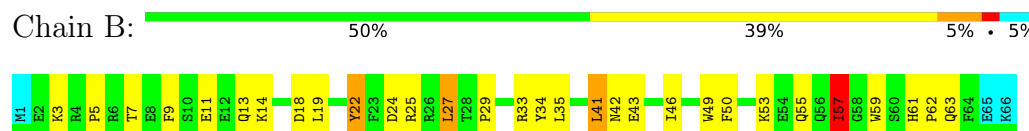


4.2.4 Score per residue for model 4

- Molecule 1: Computational designed homodimer

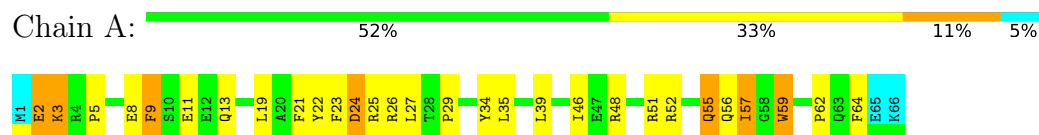


- Molecule 1: Computational designed homodimer

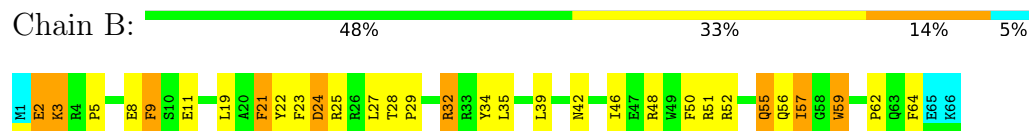


4.2.5 Score per residue for model 5

- Molecule 1: Computational designed homodimer

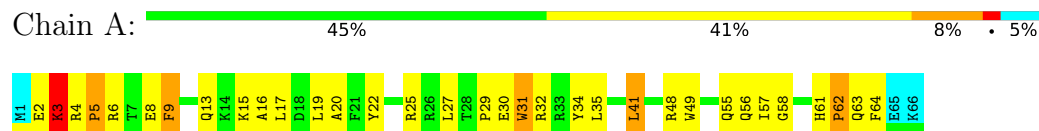


- Molecule 1: Computational designed homodimer

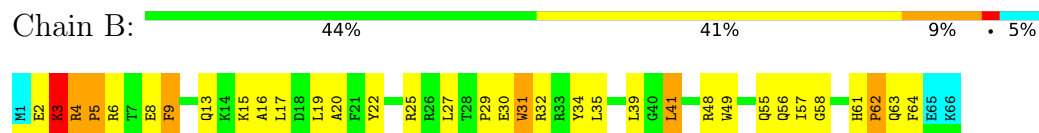


4.2.6 Score per residue for model 6

- Molecule 1: Computational designed homodimer

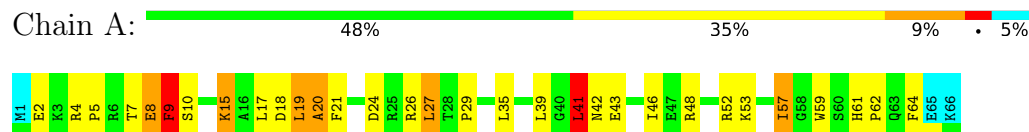


- Molecule 1: Computational designed homodimer

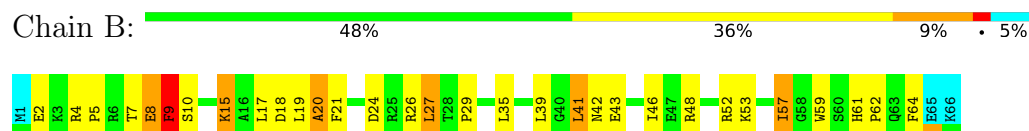


4.2.7 Score per residue for model 7

- Molecule 1: Computational designed homodimer

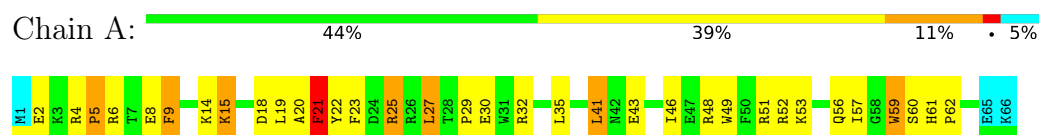


- Molecule 1: Computational designed homodimer

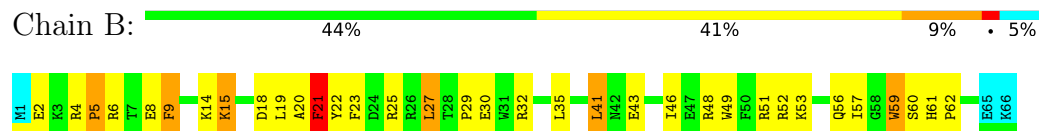


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Computational designed homodimer

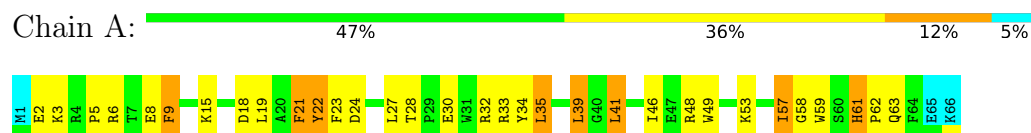


- Molecule 1: Computational designed homodimer

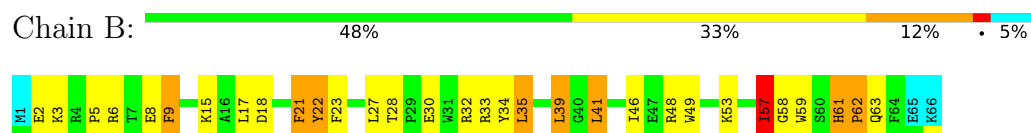


4.2.9 Score per residue for model 9

- Molecule 1: Computational designed homodimer

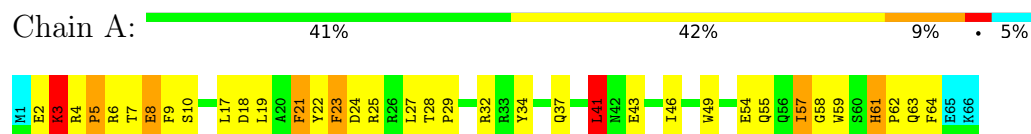


- Molecule 1: Computational designed homodimer

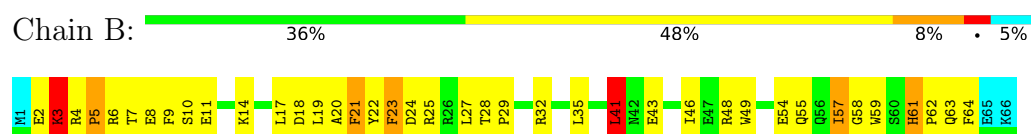


4.2.10 Score per residue for model 10

- Molecule 1: Computational designed homodimer



- Molecule 1: Computational designed homodimer



5 Refinement protocol and experimental data overview

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

Of the 32 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	
ARIA	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	737
Number of shifts mapped to atoms	737
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

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	2.21±0.02	16±3/588 (2.7± 0.6%)	1.48±0.02	2±1/789 (0.2± 0.2%)
1	B	2.22±0.03	16±3/588 (2.7± 0.4%)	1.49±0.02	2±1/789 (0.3± 0.1%)
All	All	2.21	316/11760 (2.7%)	1.48	40/15780 (0.3%)

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	62	PRO	CA-C	-9.79	1.43	1.52	7	10
1	B	62	PRO	CA-C	-9.52	1.43	1.53	7	10
1	A	5	PRO	CA-C	-8.70	1.44	1.52	7	10
1	B	5	PRO	CA-C	-8.66	1.44	1.52	7	10
1	B	22	TYR	CA-C	-7.58	1.46	1.53	8	3
1	A	22	TYR	CA-C	-7.55	1.46	1.53	8	3
1	A	62	PRO	N-CA	-7.44	1.41	1.47	4	5
1	B	62	PRO	N-CA	-7.30	1.41	1.47	4	6
1	A	61	HIS	CA-C	-7.23	1.47	1.53	10	3
1	B	61	HIS	CA-C	-7.19	1.46	1.52	3	3
1	B	23	PHE	CA-C	-7.07	1.46	1.52	8	4
1	A	23	PHE	CA-C	-7.03	1.46	1.52	8	4
1	A	6	ARG	CA-C	-6.68	1.46	1.53	6	3
1	B	6	ARG	CA-C	-6.62	1.46	1.53	6	4
1	A	24	ASP	CA-C	-6.58	1.46	1.53	5	1
1	B	28	THR	N-CA	-6.56	1.41	1.46	9	1
1	A	28	THR	N-CA	-6.52	1.41	1.46	9	1
1	B	53	LYS	CA-C	-6.47	1.46	1.53	7	2
1	B	24	ASP	CA-C	-6.46	1.46	1.53	5	1
1	B	61	HIS	N-CA	-6.40	1.42	1.46	9	3
1	B	63	GLN	CA-C	-6.38	1.46	1.53	2	3
1	A	61	HIS	N-CA	-6.27	1.42	1.46	9	3
1	A	63	GLN	CA-C	-6.26	1.46	1.53	2	3
1	A	53	LYS	CA-C	-6.22	1.46	1.53	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	26	ARG	CA-C	-6.08	1.46	1.53	2	4
1	A	26	ARG	CA-C	-6.05	1.46	1.53	2	4
1	B	64	PHE	CA-C	-6.04	1.46	1.52	1	3
1	A	2	GLU	CA-C	-6.01	1.46	1.52	9	1
1	B	29	PRO	CA-C	-6.01	1.43	1.52	3	9
1	A	20	ALA	CA-C	-6.00	1.45	1.53	1	3
1	B	2	GLU	CA-C	-5.98	1.46	1.52	9	1
1	A	64	PHE	CA-C	-5.98	1.46	1.52	1	3
1	B	20	ALA	CA-C	-5.96	1.46	1.53	1	3
1	A	39	LEU	CA-C	-5.93	1.46	1.52	9	3
1	A	29	PRO	CA-C	-5.93	1.44	1.52	1	9
1	B	5	PRO	N-CA	-5.90	1.41	1.47	7	2
1	B	54	GLU	CA-C	-5.88	1.47	1.53	10	2
1	A	54	GLU	CA-C	-5.86	1.47	1.53	10	2
1	B	39	LEU	CA-C	-5.85	1.46	1.52	9	3
1	A	5	PRO	N-CA	-5.82	1.41	1.47	7	2
1	B	28	THR	CA-C	-5.80	1.46	1.52	9	1
1	A	28	THR	CA-C	-5.77	1.46	1.52	9	1
1	B	57	ILE	CA-C	-5.64	1.46	1.53	8	3
1	A	57	ILE	CA-C	-5.61	1.46	1.53	8	1
1	B	21	PHE	CA-C	-5.61	1.46	1.53	9	2
1	A	21	PHE	CA-C	-5.58	1.46	1.53	9	3
1	B	34	TYR	CA-C	-5.56	1.45	1.52	1	5
1	B	7	THR	CA-C	-5.54	1.47	1.53	7	2
1	A	34	TYR	CA-C	-5.54	1.45	1.52	1	6
1	B	8	GLU	CA-C	-5.54	1.46	1.52	2	5
1	A	7	THR	CA-C	-5.54	1.47	1.53	7	2
1	A	8	GLU	CA-C	-5.53	1.46	1.52	2	6
1	A	46	ILE	CA-C	-5.51	1.46	1.52	4	8
1	B	3	LYS	CA-C	-5.43	1.46	1.52	1	6
1	A	3	LYS	CA-C	-5.37	1.46	1.52	1	6
1	B	16	ALA	CA-C	-5.37	1.46	1.52	1	3
1	B	4	ARG	CA-C	-5.36	1.47	1.52	1	2
1	A	16	ALA	CA-C	-5.36	1.46	1.53	6	3
1	A	35	LEU	CA-C	-5.31	1.46	1.52	7	5
1	B	32	ARG	CA-C	-5.30	1.46	1.52	6	3
1	B	48	ARG	CA-C	-5.30	1.46	1.52	5	9
1	B	52	ARG	CA-C	-5.30	1.46	1.52	8	2
1	B	18	ASP	CA-C	-5.29	1.46	1.52	10	3
1	B	46	ILE	CA-C	-5.29	1.46	1.52	9	8
1	A	10	SER	CA-C	-5.29	1.46	1.53	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	10	SER	CA-C	-5.28	1.46	1.53	7	1
1	A	52	ARG	CA-C	-5.28	1.46	1.52	8	2
1	A	42	ASN	CA-C	-5.28	1.46	1.53	7	3
1	B	42	ASN	CA-C	-5.27	1.46	1.53	1	4
1	B	59	TRP	CA-C	-5.26	1.46	1.53	5	2
1	A	59	TRP	CA-C	-5.25	1.46	1.53	5	2
1	B	14	LYS	CA-C	-5.22	1.46	1.52	8	3
1	B	35	LEU	CA-C	-5.22	1.46	1.52	7	8
1	A	57	ILE	N-CA	-5.22	1.41	1.46	4	1
1	A	48	ARG	CA-C	-5.22	1.46	1.52	8	9
1	A	14	LYS	CA-C	-5.22	1.46	1.52	8	1
1	A	18	ASP	CA-C	-5.21	1.46	1.52	10	3
1	A	15	LYS	CA-C	-5.21	1.46	1.52	8	2
1	A	32	ARG	CA-C	-5.20	1.46	1.52	6	3
1	B	15	LYS	CA-C	-5.16	1.46	1.52	1	2
1	B	50	PHE	CA-C	-5.14	1.46	1.52	1	2
1	A	8	GLU	N-CA	-5.14	1.41	1.46	9	1
1	A	27	LEU	CA-C	-5.12	1.46	1.52	8	2
1	B	41	LEU	CA-C	-5.10	1.46	1.52	10	1
1	A	50	PHE	CA-C	-5.10	1.46	1.52	1	2
1	A	30	GLU	CA-C	-5.08	1.46	1.52	4	1
1	A	41	LEU	CA-C	-5.07	1.46	1.52	10	3
1	B	27	LEU	CA-C	-5.06	1.46	1.53	3	2
1	B	19	LEU	CA-C	-5.06	1.46	1.52	10	1
1	B	57	ILE	N-CA	-5.03	1.41	1.46	4	1
1	A	19	LEU	CA-C	-5.03	1.46	1.52	10	2
1	A	37	GLN	CA-C	-5.03	1.46	1.52	10	1
1	A	25	ARG	CA-C	-5.02	1.46	1.52	8	1
1	B	8	GLU	N-CA	-5.01	1.41	1.46	9	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
1	A	61	HIS	O-C-N	-7.90	117.90	121.53	9	2
1	B	61	HIS	O-C-N	-7.61	118.03	121.53	9	2
1	B	21	PHE	CA-CB-CG	-6.65	107.15	113.80	8	5
1	B	32	ARG	N-CA-C	-6.65	103.86	112.23	2	4
1	A	32	ARG	N-CA-C	-6.62	103.88	112.23	2	3
1	A	21	PHE	CA-CB-CG	-6.62	107.18	113.80	8	4
1	B	18	ASP	CA-CB-CG	-6.04	106.56	112.60	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	PHE	CA-CB-CG	-5.91	107.89	113.80	2	2
1	B	23	PHE	CA-CB-CG	-5.89	107.91	113.80	2	2
1	B	46	ILE	N-CA-C	-5.76	105.24	110.82	2	3
1	A	46	ILE	N-CA-C	-5.69	105.30	110.82	2	2
1	B	9	PHE	CA-CB-CG	-5.61	108.19	113.80	7	1
1	A	9	PHE	CA-CB-CG	-5.60	108.20	113.80	7	1
1	A	24	ASP	N-CA-C	-5.34	107.31	113.88	9	1
1	B	60	SER	N-CA-C	-5.28	106.78	114.12	8	1
1	A	60	SER	N-CA-C	-5.26	106.81	114.12	8	1
1	A	64	PHE	CA-CB-CG	-5.17	108.63	113.80	6	1
1	B	64	PHE	CA-CB-CG	-5.14	108.66	113.80	6	1
1	B	31	TRP	N-CA-C	-5.07	107.27	113.50	6	1
1	B	17	LEU	N-CA-C	-5.02	107.33	113.50	9	1
1	A	31	TRP	N-CA-C	-5.01	107.34	113.50	6	1

There are no chirality outliers.

There are no planarity outliers.

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	571	553	552	33±4
1	B	571	553	552	34±4
All	All	11420	11060	11040	666

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:27:LEU:O	1:B:27:LEU:HD13	1.29	1.25	1	8
1:A:27:LEU:HD13	1:A:27:LEU:O	1.28	1.25	1	9
1:B:22:TYR:CD1	1:B:22:TYR:O	1.23	1.90	3	2
1:A:22:TYR:O	1:A:22:TYR:CD1	1.21	1.94	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:57:ILE:HD12	1:B:57:ILE:O	1.01	1.55	7	6
1:A:57:ILE:HD12	1:A:57:ILE:O	1.00	1.55	7	6
1:A:4:ARG:O	1:A:4:ARG:HD3	0.95	1.60	10	2
1:A:27:LEU:O	1:A:27:LEU:CD1	0.95	2.14	1	9
1:B:27:LEU:O	1:B:27:LEU:CD1	0.94	2.15	10	9
1:A:27:LEU:HD23	1:A:27:LEU:O	0.93	1.64	4	1
1:B:4:ARG:O	1:B:4:ARG:HD3	0.91	1.64	10	2
1:A:9:PHE:CD1	1:A:9:PHE:O	0.87	2.28	7	9
1:B:9:PHE:CD1	1:B:9:PHE:O	0.87	2.27	7	9
1:B:57:ILE:H	1:B:57:ILE:HD13	0.86	1.28	4	1
1:B:27:LEU:HD23	1:B:27:LEU:O	0.85	1.71	4	1
1:A:57:ILE:H	1:A:57:ILE:HD13	0.83	1.29	4	1
1:B:22:TYR:O	1:B:22:TYR:CG	0.83	2.32	3	3
1:A:4:ARG:O	1:A:4:ARG:CD	0.82	2.27	10	2
1:A:43:GLU:H	1:A:43:GLU:CD	0.80	1.82	1	5
1:B:43:GLU:H	1:B:43:GLU:CD	0.80	1.83	7	5
1:B:11:GLU:H	1:B:11:GLU:CD	0.80	1.84	2	2
1:A:22:TYR:O	1:A:22:TYR:CG	0.79	2.34	3	3
1:B:61:HIS:O	1:B:61:HIS:ND1	0.78	2.16	4	1
1:A:11:GLU:CD	1:A:11:GLU:H	0.78	1.84	2	2
1:B:4:ARG:O	1:B:4:ARG:CD	0.77	2.31	10	2
1:B:18:ASP:OD1	1:B:18:ASP:O	0.77	2.02	8	2
1:B:57:ILE:C	1:B:57:ILE:HD12	0.77	2.05	1	2
1:A:57:ILE:HD12	1:A:57:ILE:C	0.77	2.05	1	5
1:A:3:LYS:O	1:A:3:LYS:HD3	0.77	1.78	5	1
1:B:3:LYS:HD3	1:B:3:LYS:O	0.77	1.78	5	1
1:A:18:ASP:O	1:A:18:ASP:OD1	0.77	2.02	8	1
1:B:57:ILE:HD12	1:B:57:ILE:C	0.76	2.05	10	3
1:B:59:TRP:CG	1:B:59:TRP:O	0.74	2.41	1	7
1:A:61:HIS:ND1	1:A:61:HIS:O	0.73	2.21	4	1
1:A:59:TRP:CG	1:A:59:TRP:O	0.73	2.42	3	7
1:A:9:PHE:CD1	1:A:9:PHE:N	0.73	2.54	2	1
1:A:4:ARG:HD2	1:A:4:ARG:O	0.72	1.84	1	1
1:B:9:PHE:CD1	1:B:9:PHE:N	0.72	2.54	2	1
1:A:15:LYS:HB2	1:A:15:LYS:NZ	0.71	2.01	2	4
1:B:15:LYS:HB2	1:B:15:LYS:NZ	0.71	2.01	8	4
1:A:61:HIS:CD2	1:A:61:HIS:O	0.70	2.44	7	4
1:B:4:ARG:HD2	1:B:4:ARG:O	0.70	1.85	1	1
1:A:3:LYS:HE3	1:A:3:LYS:HA	0.70	1.61	6	1
1:B:27:LEU:C	1:B:27:LEU:HD13	0.70	2.11	9	1
1:A:22:TYR:CG	1:A:22:TYR:O	0.70	2.45	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:LYS:HE3	1:B:3:LYS:HA	0.69	1.61	6	1
1:B:61:HIS:O	1:B:61:HIS:CD2	0.69	2.45	7	5
1:A:27:LEU:C	1:A:27:LEU:HD13	0.69	2.11	9	1
1:B:22:TYR:CG	1:B:22:TYR:O	0.68	2.46	5	3
1:A:4:ARG:O	1:A:4:ARG:CG	0.68	2.41	10	1
1:A:59:TRP:O	1:A:59:TRP:CD2	0.68	2.46	1	7
1:B:41:LEU:CD2	1:B:41:LEU:C	0.67	2.67	10	9
1:A:41:LEU:C	1:A:41:LEU:CD2	0.67	2.67	10	9
1:A:33:ARG:HD3	1:A:33:ARG:C	0.67	2.14	4	1
1:B:59:TRP:O	1:B:59:TRP:CD2	0.67	2.46	1	8
1:B:33:ARG:HD3	1:B:33:ARG:C	0.67	2.15	4	1
1:B:9:PHE:O	1:B:9:PHE:HD1	0.67	1.73	5	6
1:A:3:LYS:N	1:A:3:LYS:HE3	0.67	2.05	10	1
1:B:57:ILE:HD13	1:B:57:ILE:N	0.67	2.03	4	1
1:B:6:ARG:N	1:B:6:ARG:HD3	0.67	2.05	9	1
1:A:57:ILE:HD13	1:A:57:ILE:N	0.66	2.04	4	1
1:B:22:TYR:CD1	1:B:22:TYR:C	0.66	2.74	4	1
1:A:6:ARG:N	1:A:6:ARG:HD3	0.66	2.05	9	1
1:A:6:ARG:HD3	1:A:6:ARG:H	0.66	1.50	9	1
1:A:9:PHE:O	1:A:9:PHE:HD1	0.66	1.73	5	6
1:A:15:LYS:HB2	1:A:15:LYS:HZ3	0.65	1.52	2	1
1:B:4:ARG:O	1:B:4:ARG:CG	0.65	2.43	10	1
1:B:6:ARG:HD3	1:B:6:ARG:H	0.65	1.49	9	1
1:B:3:LYS:N	1:B:3:LYS:HE3	0.65	2.06	10	1
1:A:22:TYR:O	1:A:22:TYR:HD1	0.64	1.73	3	1
1:B:3:LYS:HD3	1:B:3:LYS:C	0.64	2.18	5	1
1:A:3:LYS:HD3	1:A:3:LYS:C	0.63	2.18	5	1
1:A:33:ARG:HD3	1:A:33:ARG:O	0.63	1.92	4	1
1:B:53:LYS:HZ3	1:B:53:LYS:HB3	0.62	1.54	3	1
1:A:53:LYS:NZ	1:A:53:LYS:CB	0.62	2.62	3	1
1:A:23:PHE:N	1:A:23:PHE:CD1	0.62	2.68	10	1
1:B:55:GLN:HE21	1:B:55:GLN:HA	0.62	1.55	6	1
1:B:25:ARG:HG3	1:B:25:ARG:O	0.62	1.94	5	3
1:A:22:TYR:CD1	1:A:22:TYR:C	0.61	2.77	4	1
1:B:41:LEU:N	1:B:41:LEU:HD13	0.61	2.10	1	9
1:B:6:ARG:H	1:B:6:ARG:CD	0.61	2.08	9	1
1:A:6:ARG:H	1:A:6:ARG:CD	0.61	2.09	9	1
1:B:63:GLN:HG3	1:B:63:GLN:O	0.61	1.95	2	1
1:B:22:TYR:O	1:B:22:TYR:CD2	0.61	2.54	9	3
1:B:53:LYS:CB	1:B:53:LYS:NZ	0.61	2.63	3	1
1:A:25:ARG:O	1:A:25:ARG:HG3	0.61	1.96	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD13	1:A:41:LEU:N	0.60	2.11	1	9
1:B:41:LEU:H	1:B:41:LEU:HD22	0.60	1.57	3	4
1:A:55:GLN:HE21	1:A:55:GLN:HA	0.60	1.55	6	1
1:B:23:PHE:CD1	1:B:23:PHE:N	0.60	2.68	10	1
1:B:33:ARG:HD3	1:B:33:ARG:O	0.60	1.96	4	1
1:A:24:ASP:CG	1:A:24:ASP:O	0.59	2.41	5	2
1:A:22:TYR:CD2	1:A:22:TYR:O	0.59	2.55	9	1
1:A:27:LEU:HD13	1:A:27:LEU:C	0.59	2.15	10	2
1:A:27:LEU:O	1:A:27:LEU:CD2	0.59	2.47	4	1
1:B:17:LEU:HD12	1:B:17:LEU:N	0.59	2.11	7	3
1:B:24:ASP:CG	1:B:24:ASP:O	0.59	2.41	5	3
1:A:41:LEU:H	1:A:41:LEU:HD22	0.59	1.58	10	5
1:A:17:LEU:N	1:A:17:LEU:HD12	0.59	2.11	7	5
1:A:8:GLU:O	1:A:8:GLU:HG3	0.59	1.97	10	3
1:B:27:LEU:HD13	1:B:27:LEU:C	0.59	2.21	5	2
1:A:59:TRP:CD2	1:A:59:TRP:O	0.59	2.56	5	2
1:A:57:ILE:C	1:A:57:ILE:CD1	0.58	2.76	1	5
1:B:43:GLU:OE1	1:B:43:GLU:N	0.57	2.36	10	1
1:A:63:GLN:O	1:A:63:GLN:HG3	0.57	1.98	2	1
1:B:55:GLN:O	1:B:55:GLN:OE1	0.57	2.23	2	1
1:B:57:ILE:C	1:B:57:ILE:CD1	0.56	2.77	5	5
1:A:53:LYS:HZ3	1:A:53:LYS:HB3	0.56	1.59	3	1
1:A:61:HIS:CG	1:A:61:HIS:O	0.56	2.58	2	2
1:B:11:GLU:CD	1:B:11:GLU:N	0.56	2.63	5	2
1:B:61:HIS:CG	1:B:61:HIS:O	0.56	2.57	2	2
1:B:8:GLU:HG3	1:B:8:GLU:O	0.56	2.00	10	3
1:B:59:TRP:O	1:B:59:TRP:CG	0.56	2.57	5	2
1:B:35:LEU:HD23	1:B:35:LEU:H	0.56	1.60	3	1
1:B:25:ARG:NE	1:B:25:ARG:HA	0.56	2.15	8	2
1:A:43:GLU:N	1:A:43:GLU:OE1	0.56	2.36	10	1
1:A:12:GLU:CD	1:A:12:GLU:N	0.56	2.64	3	1
1:A:2:GLU:HA	1:A:2:GLU:OE1	0.56	2.01	5	2
1:A:25:ARG:NE	1:A:25:ARG:HA	0.56	2.15	8	2
1:B:27:LEU:HD13	1:B:27:LEU:O	0.56	2.01	9	1
1:B:59:TRP:O	1:B:59:TRP:CE3	0.55	2.59	5	2
1:A:3:LYS:HE3	1:A:3:LYS:H	0.55	1.60	10	1
1:B:43:GLU:CD	1:B:43:GLU:N	0.55	2.60	1	5
1:A:59:TRP:O	1:A:59:TRP:CG	0.55	2.57	5	2
1:B:21:PHE:N	1:B:21:PHE:CD1	0.55	2.73	9	2
1:A:59:TRP:O	1:A:59:TRP:CE3	0.55	2.60	5	2
1:A:63:GLN:H	1:A:63:GLN:CD	0.55	2.10	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:2:GLU:OE1	1:B:2:GLU:HA	0.55	2.01	5	2
1:B:13:GLN:NE2	1:B:13:GLN:HA	0.54	2.16	6	1
1:B:61:HIS:O	1:B:61:HIS:CG	0.54	2.58	4	1
1:A:43:GLU:CD	1:A:43:GLU:N	0.54	2.66	3	5
1:B:12:GLU:N	1:B:12:GLU:CD	0.54	2.65	3	1
1:B:4:ARG:HD2	1:B:4:ARG:C	0.54	2.27	6	1
1:A:4:ARG:HD2	1:A:4:ARG:C	0.54	2.28	6	1
1:A:25:ARG:HE	1:A:25:ARG:N	0.54	2.01	1	1
1:B:25:ARG:N	1:B:25:ARG:HE	0.54	2.01	1	1
1:B:41:LEU:C	1:B:41:LEU:HD22	0.54	2.28	1	8
1:B:27:LEU:O	1:B:27:LEU:CD2	0.54	2.52	4	1
1:B:13:GLN:HA	1:B:13:GLN:HE21	0.53	1.62	6	1
1:B:3:LYS:HE3	1:B:3:LYS:H	0.53	1.61	10	1
1:A:2:GLU:N	1:A:2:GLU:CD	0.53	2.67	8	1
1:A:15:LYS:NZ	1:A:15:LYS:CB	0.53	2.72	8	3
1:A:20:ALA:O	1:A:21:PHE:C	0.53	2.52	2	3
1:B:20:ALA:O	1:B:21:PHE:C	0.53	2.52	2	4
1:A:13:GLN:NE2	1:A:13:GLN:HA	0.53	2.18	6	1
1:B:57:ILE:O	1:B:57:ILE:CD1	0.53	2.46	7	4
1:B:27:LEU:C	1:B:27:LEU:CD1	0.53	2.82	9	1
1:B:30:GLU:CD	1:B:30:GLU:N	0.53	2.67	9	1
1:A:6:ARG:N	1:A:6:ARG:CD	0.53	2.71	9	1
1:B:4:ARG:HD3	1:B:4:ARG:C	0.53	2.29	8	1
1:A:30:GLU:CD	1:A:30:GLU:N	0.53	2.67	9	1
1:B:2:GLU:N	1:B:2:GLU:CD	0.52	2.66	8	1
1:A:41:LEU:C	1:A:41:LEU:HD22	0.52	2.28	1	9
1:B:15:LYS:NZ	1:B:15:LYS:CB	0.52	2.72	8	3
1:B:15:LYS:HB2	1:B:15:LYS:HZ2	0.52	1.63	7	1
1:A:17:LEU:N	1:A:17:LEU:CD1	0.52	2.73	1	3
1:B:25:ARG:N	1:B:25:ARG:NE	0.52	2.58	1	1
1:A:3:LYS:O	1:A:3:LYS:CD	0.52	2.55	5	1
1:A:57:ILE:O	1:A:57:ILE:CD1	0.52	2.57	9	4
1:A:9:PHE:N	1:A:9:PHE:HD1	0.52	2.00	2	1
1:B:55:GLN:CD	1:B:55:GLN:C	0.52	2.78	2	3
1:A:61:HIS:O	1:A:61:HIS:HD2	0.52	1.88	7	2
1:A:4:ARG:HD3	1:A:4:ARG:C	0.52	2.29	8	1
1:A:33:ARG:O	1:A:33:ARG:CD	0.51	2.57	4	1
1:A:61:HIS:O	1:A:61:HIS:CG	0.51	2.61	4	1
1:A:13:GLN:HA	1:A:13:GLN:HE21	0.51	1.63	6	1
1:A:25:ARG:N	1:A:25:ARG:NE	0.51	2.58	1	1
1:B:17:LEU:N	1:B:17:LEU:CD1	0.51	2.72	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:19:LEU:N	1:B:19:LEU:CD1	0.51	2.73	4	3
1:B:33:ARG:C	1:B:33:ARG:CD	0.51	2.82	4	1
1:B:12:GLU:CD	1:B:12:GLU:H	0.51	2.14	3	1
1:B:22:TYR:O	1:B:22:TYR:HD1	0.51	1.70	3	1
1:B:11:GLU:HA	1:B:11:GLU:OE1	0.51	2.06	10	2
1:B:63:GLN:CD	1:B:63:GLN:H	0.51	2.13	4	1
1:A:4:ARG:CD	1:A:4:ARG:C	0.51	2.84	8	1
1:A:34:TYR:CD1	1:A:34:TYR:C	0.51	2.89	2	1
1:A:21:PHE:CD2	1:A:21:PHE:O	0.51	2.64	7	2
1:B:2:GLU:OE1	1:B:2:GLU:N	0.51	2.42	10	1
1:B:15:LYS:HB2	1:B:15:LYS:HZ3	0.50	1.66	2	2
1:A:11:GLU:CD	1:A:11:GLU:N	0.50	2.59	2	2
1:B:17:LEU:CD1	1:B:17:LEU:N	0.50	2.74	3	3
1:B:41:LEU:HD22	1:B:41:LEU:N	0.50	2.21	3	2
1:B:21:PHE:CD2	1:B:21:PHE:O	0.50	2.64	7	2
1:B:30:GLU:HA	1:B:30:GLU:OE1	0.50	2.07	8	1
1:A:2:GLU:OE1	1:A:2:GLU:N	0.50	2.42	10	1
1:B:41:LEU:HD22	1:B:41:LEU:O	0.50	2.06	7	7
1:B:57:ILE:N	1:B:57:ILE:CD1	0.50	2.71	4	1
1:A:21:PHE:O	1:A:21:PHE:CG	0.50	2.64	7	2
1:A:15:LYS:HZ3	1:A:15:LYS:CB	0.50	2.18	2	1
1:B:4:ARG:CD	1:B:4:ARG:C	0.50	2.84	8	1
1:B:34:TYR:C	1:B:34:TYR:CD1	0.50	2.89	2	1
1:A:12:GLU:CD	1:A:12:GLU:H	0.50	2.14	3	1
1:A:33:ARG:C	1:A:33:ARG:CD	0.49	2.82	4	1
1:A:21:PHE:CD1	1:A:21:PHE:N	0.49	2.78	9	2
1:A:41:LEU:HD22	1:A:41:LEU:O	0.49	2.07	1	7
1:A:17:LEU:CD1	1:A:17:LEU:N	0.49	2.74	2	3
1:A:15:LYS:HB2	1:A:15:LYS:HZ2	0.49	1.65	8	3
1:B:27:LEU:CD1	1:B:27:LEU:C	0.49	2.79	10	1
1:B:21:PHE:O	1:B:21:PHE:CG	0.49	2.64	7	2
1:A:55:GLN:CD	1:A:55:GLN:C	0.49	2.80	5	3
1:B:49:TRP:HA	1:B:49:TRP:CE3	0.49	2.42	10	6
1:B:3:LYS:O	1:B:3:LYS:CD	0.49	2.56	5	1
1:A:30:GLU:HA	1:A:30:GLU:OE1	0.49	2.07	8	1
1:B:53:LYS:HZ3	1:B:53:LYS:CB	0.49	2.17	3	1
1:A:30:GLU:O	1:A:30:GLU:HG2	0.49	2.08	6	1
1:B:9:PHE:N	1:B:9:PHE:HD1	0.49	2.00	2	1
1:B:56:GLN:HA	1:B:56:GLN:OE1	0.48	2.08	6	2
1:A:11:GLU:HA	1:A:11:GLU:OE1	0.48	2.09	4	1
1:B:30:GLU:O	1:B:30:GLU:HG2	0.48	2.08	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:PHE:CD1	1:B:9:PHE:C	0.48	2.92	7	1
1:A:22:TYR:C	1:A:22:TYR:HD1	0.48	2.15	4	1
1:B:33:ARG:O	1:B:33:ARG:CD	0.48	2.61	4	1
1:B:55:GLN:HA	1:B:55:GLN:OE1	0.48	2.09	4	1
1:B:53:LYS:O	1:B:53:LYS:HD3	0.48	2.08	9	1
1:A:8:GLU:O	1:A:8:GLU:CG	0.48	2.61	10	1
1:A:2:GLU:N	1:A:2:GLU:OE1	0.47	2.47	4	1
1:A:19:LEU:CD1	1:A:19:LEU:N	0.47	2.77	4	2
1:A:56:GLN:HA	1:A:56:GLN:OE1	0.47	2.08	6	2
1:A:31:TRP:CD1	1:A:31:TRP:N	0.47	2.82	6	1
1:A:25:ARG:NE	1:A:25:ARG:CA	0.47	2.77	1	1
1:A:49:TRP:HA	1:A:49:TRP:CE3	0.47	2.43	3	6
1:A:27:LEU:C	1:A:27:LEU:CD1	0.47	2.82	9	1
1:B:13:GLN:HA	1:B:13:GLN:OE1	0.47	2.09	4	1
1:A:35:LEU:H	1:A:35:LEU:HD23	0.47	1.70	3	1
1:A:22:TYR:O	1:A:22:TYR:CD2	0.47	2.67	1	2
1:B:41:LEU:HD22	1:B:41:LEU:H	0.47	1.68	8	2
1:A:19:LEU:N	1:A:19:LEU:HD12	0.47	2.25	9	1
1:A:55:GLN:HA	1:A:55:GLN:OE1	0.47	2.09	4	1
1:A:41:LEU:HD22	1:A:41:LEU:N	0.47	2.21	10	2
1:A:9:PHE:CD1	1:A:9:PHE:C	0.47	2.92	7	1
1:B:14:LYS:CB	1:B:14:LYS:NZ	0.46	2.78	4	1
1:B:22:TYR:C	1:B:22:TYR:HD1	0.46	2.15	4	1
1:A:13:GLN:HA	1:A:13:GLN:OE1	0.46	2.11	4	1
1:B:21:PHE:O	1:B:22:TYR:HB3	0.46	2.10	5	1
1:B:25:ARG:NE	1:B:25:ARG:CA	0.46	2.77	1	1
1:A:27:LEU:CD1	1:A:27:LEU:C	0.46	2.79	10	1
1:A:51:ARG:C	1:A:51:ARG:HD3	0.46	2.35	8	1
1:B:51:ARG:HD3	1:B:51:ARG:C	0.46	2.35	8	1
1:B:53:LYS:CD	1:B:53:LYS:C	0.46	2.89	9	1
1:A:33:ARG:O	1:A:33:ARG:CG	0.46	2.63	4	1
1:A:55:GLN:HA	1:A:55:GLN:NE2	0.46	2.24	6	1
1:B:31:TRP:CD1	1:B:31:TRP:N	0.46	2.82	6	1
1:B:52:ARG:NE	1:B:52:ARG:HA	0.45	2.27	7	3
1:A:3:LYS:C	1:A:3:LYS:CD	0.45	2.88	5	1
1:B:41:LEU:N	1:B:41:LEU:HD22	0.45	2.26	9	2
1:A:61:HIS:O	1:A:61:HIS:CD2	0.45	2.68	1	1
1:A:21:PHE:O	1:A:22:TYR:HB3	0.45	2.11	5	1
1:B:28:THR:O	1:B:32:ARG:N	0.45	2.49	5	2
1:A:8:GLU:O	1:A:9:PHE:C	0.45	2.59	5	3
1:A:19:LEU:HD12	1:A:19:LEU:N	0.45	2.26	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD22	1:A:41:LEU:H	0.45	1.71	6	1
1:B:61:HIS:O	1:B:61:HIS:HD2	0.45	1.94	8	2
1:B:17:LEU:N	1:B:17:LEU:HD12	0.45	2.26	10	3
1:A:14:LYS:NZ	1:A:14:LYS:CB	0.45	2.80	4	1
1:B:8:GLU:O	1:B:9:PHE:C	0.45	2.59	5	3
1:B:15:LYS:N	1:B:15:LYS:HD3	0.45	2.27	7	1
1:A:63:GLN:O	1:A:63:GLN:CG	0.45	2.64	2	1
1:B:35:LEU:O	1:B:39:LEU:N	0.45	2.49	9	1
1:A:53:LYS:O	1:A:53:LYS:HD3	0.45	2.12	9	1
1:B:6:ARG:N	1:B:6:ARG:CD	0.45	2.71	9	1
1:A:57:ILE:N	1:A:57:ILE:CD1	0.45	2.72	4	1
1:B:53:LYS:HB3	1:B:53:LYS:NZ	0.45	2.21	3	1
1:B:19:LEU:HD12	1:B:19:LEU:N	0.45	2.26	8	2
1:A:15:LYS:N	1:A:15:LYS:HD3	0.45	2.26	7	1
1:B:55:GLN:HA	1:B:55:GLN:NE2	0.44	2.24	6	1
1:A:28:THR:O	1:A:32:ARG:N	0.44	2.51	10	1
1:A:35:LEU:O	1:A:39:LEU:N	0.44	2.50	9	1
1:A:4:ARG:NE	1:A:4:ARG:HA	0.44	2.28	4	2
1:A:15:LYS:O	1:A:19:LEU:HD13	0.44	2.12	7	1
1:B:17:LEU:HD11	1:B:39:LEU:HD21	0.44	1.89	7	1
1:A:6:ARG:O	1:A:7:THR:C	0.44	2.61	10	1
1:B:30:GLU:CD	1:B:30:GLU:H	0.44	2.19	9	1
1:B:33:ARG:C	1:B:33:ARG:HD2	0.44	2.38	9	1
1:A:52:ARG:NE	1:A:52:ARG:HA	0.44	2.27	3	3
1:B:33:ARG:O	1:B:33:ARG:CG	0.44	2.66	4	1
1:A:57:ILE:HG23	1:A:58:GLY:N	0.44	2.28	6	1
1:B:57:ILE:HG23	1:B:58:GLY:N	0.43	2.28	6	1
1:A:41:LEU:N	1:A:41:LEU:HD22	0.43	2.27	9	1
1:A:19:LEU:N	1:A:19:LEU:CD1	0.43	2.80	2	2
1:A:18:ASP:O	1:A:18:ASP:CG	0.43	2.61	3	1
1:A:53:LYS:NZ	1:A:53:LYS:HB3	0.43	2.19	3	1
1:A:30:GLU:CD	1:A:30:GLU:H	0.43	2.21	9	1
1:B:58:GLY:O	1:B:59:TRP:HB3	0.43	2.13	10	2
1:B:58:GLY:O	1:B:59:TRP:CB	0.43	2.67	9	1
1:A:10:SER:O	1:A:11:GLU:C	0.43	2.60	2	1
1:A:58:GLY:O	1:A:59:TRP:HB3	0.43	2.13	10	3
1:B:20:ALA:O	1:B:25:ARG:N	0.43	2.51	6	1
1:B:10:SER:O	1:B:11:GLU:C	0.43	2.60	2	2
1:B:25:ARG:O	1:B:25:ARG:CG	0.43	2.63	6	1
1:A:53:LYS:CD	1:A:53:LYS:C	0.43	2.92	9	1
1:B:53:LYS:HD3	1:B:53:LYS:C	0.43	2.39	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:ARG:O	1:B:7:THR:C	0.43	2.61	10	1
1:A:63:GLN:HA	1:A:63:GLN:OE1	0.43	2.14	9	1
1:B:62:PRO:O	1:B:63:GLN:C	0.43	2.62	6	2
1:B:4:ARG:HA	1:B:4:ARG:HE	0.43	1.72	7	1
1:B:41:LEU:HD22	1:B:41:LEU:C	0.42	2.38	3	1
1:A:64:PHE:CD1	1:A:64:PHE:N	0.42	2.87	5	1
1:A:20:ALA:O	1:A:25:ARG:N	0.42	2.51	6	1
1:B:4:ARG:HA	1:B:4:ARG:NE	0.42	2.29	7	1
1:A:4:ARG:HA	1:A:4:ARG:HE	0.42	1.73	7	1
1:B:50:PHE:CD1	1:B:50:PHE:C	0.42	2.98	5	1
1:A:56:GLN:O	1:A:56:GLN:HG3	0.42	2.14	6	2
1:B:56:GLN:O	1:B:56:GLN:HG3	0.42	2.15	8	2
1:A:17:LEU:HD11	1:A:39:LEU:HD21	0.42	1.90	7	1
1:A:51:ARG:HD2	1:A:51:ARG:C	0.42	2.40	5	1
1:A:58:GLY:O	1:A:59:TRP:CB	0.42	2.68	9	1
1:B:20:ALA:O	1:B:22:TYR:N	0.42	2.53	3	1
1:A:33:ARG:HD2	1:A:33:ARG:C	0.42	2.40	9	1
1:B:15:LYS:CB	1:B:15:LYS:HZ3	0.42	2.26	8	1
1:B:41:LEU:N	1:B:41:LEU:CD1	0.41	2.84	2	1
1:B:12:GLU:O	1:B:12:GLU:HG3	0.41	2.15	1	1
1:A:20:ALA:O	1:A:22:TYR:N	0.41	2.54	3	1
1:B:51:ARG:HD2	1:B:51:ARG:C	0.41	2.40	5	1
1:B:64:PHE:CD1	1:B:64:PHE:N	0.41	2.88	5	1
1:A:4:ARG:O	1:A:4:ARG:HG3	0.41	2.13	7	1
1:B:8:GLU:O	1:B:8:GLU:CG	0.41	2.63	10	1
1:B:24:ASP:O	1:B:25:ARG:HB2	0.41	2.16	10	1
1:A:25:ARG:O	1:A:27:LEU:N	0.41	2.54	4	1
1:B:19:LEU:N	1:B:19:LEU:HD12	0.41	2.31	4	1
1:A:62:PRO:O	1:A:63:GLN:C	0.41	2.62	6	1
1:B:15:LYS:O	1:B:19:LEU:HD13	0.41	2.15	7	1
1:A:24:ASP:O	1:A:25:ARG:HB2	0.41	2.16	10	1
1:A:41:LEU:HD13	1:A:41:LEU:H	0.41	1.75	1	1
1:B:63:GLN:CD	1:B:63:GLN:N	0.41	2.79	4	1
1:A:13:GLN:N	1:A:13:GLN:CD	0.40	2.79	5	1
1:A:41:LEU:C	1:A:41:LEU:HD23	0.40	2.40	10	1
1:B:4:ARG:O	1:B:4:ARG:HG2	0.40	2.16	10	1
1:A:41:LEU:N	1:A:41:LEU:CD1	0.40	2.82	1	2
1:B:49:TRP:CE3	1:B:49:TRP:HA	0.40	2.51	2	1
1:B:3:LYS:C	1:B:3:LYS:CD	0.40	2.89	5	1
1:B:21:PHE:CG	1:B:21:PHE:O	0.40	2.73	1	1
1:A:49:TRP:CE3	1:A:49:TRP:HA	0.40	2.51	4	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	63/66 (95%)	52±3 (83±5%)	9±3 (14±5%)	2±1 (3±1%)	5	35
1	B	63/66 (95%)	52±3 (83±5%)	9±3 (14±5%)	2±1 (4±2%)	4	32
All	All	1260/1320 (95%)	1043 (83%)	173 (14%)	44 (3%)	4	33

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	9	PHE	7
1	B	9	PHE	7
1	A	5	PRO	6
1	B	5	PRO	6
1	A	2	GLU	2
1	A	21	PHE	2
1	B	2	GLU	2
1	B	21	PHE	2
1	A	23	PHE	1
1	B	23	PHE	1
1	B	25	ARG	1
1	B	27	LEU	1
1	A	22	TYR	1
1	B	22	TYR	1
1	A	8	GLU	1
1	A	24	ASP	1
1	B	8	GLU	1
1	B	24	ASP	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/62 (95%)	56±1 (95±2%)	3±1 (5±2%)	23	73
1	B	59/62 (95%)	56±1 (95±2%)	3±1 (5±2%)	24	74
All	All	1180/1240 (95%)	1121 (95%)	59 (5%)	23	74

All 22 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	41	LEU	9
1	B	41	LEU	9
1	A	57	ILE	6
1	B	57	ILE	6
1	A	3	LYS	4
1	B	3	LYS	4
1	A	53	LYS	2
1	B	53	LYS	2
1	A	2	GLU	2
1	A	15	LYS	2
1	B	15	LYS	2
1	A	9	PHE	1
1	B	9	PHE	1
1	A	22	TYR	1
1	B	22	TYR	1
1	A	55	GLN	1
1	B	55	GLN	1
1	A	35	LEU	1
1	B	2	GLU	1
1	B	35	LEU	1
1	A	27	LEU	1
1	B	27	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 35% for the well-defined parts and 35% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	737
Number of shifts mapped to atoms	737
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	64	-0.04 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	60	0.64 ± 0.12	Should be checked
$^{13}\text{C}'$	62	-0.06 ± 0.07	None needed (< 0.5 ppm)
^{15}N	63	0.07 ± 0.21	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 35%, i.e. 697 atoms were assigned a chemical shift out of a possible 1972. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	298/622 (48%)	120/250 (48%)	120/252 (48%)	58/120 (48%)
Sidechain	366/1126 (33%)	246/708 (35%)	120/336 (36%)	0/82 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	33/224 (15%)	24/110 (22%)	9/104 (9%)	0/10 (0%)
Overall	697/1972 (35%)	390/1068 (37%)	249/692 (36%)	58/212 (27%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 728 atoms were assigned a chemical shift out of a possible 2062. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	311/652 (48%)	125/262 (48%)	126/264 (48%)	60/126 (48%)
Sidechain	384/1186 (32%)	259/746 (35%)	125/356 (35%)	0/84 (0%)
Aromatic	33/224 (15%)	24/110 (22%)	9/104 (9%)	0/10 (0%)
Overall	728/2062 (35%)	408/1118 (36%)	260/724 (36%)	60/220 (27%)

7.1.4 Statistically unusual chemical shifts [i](#)

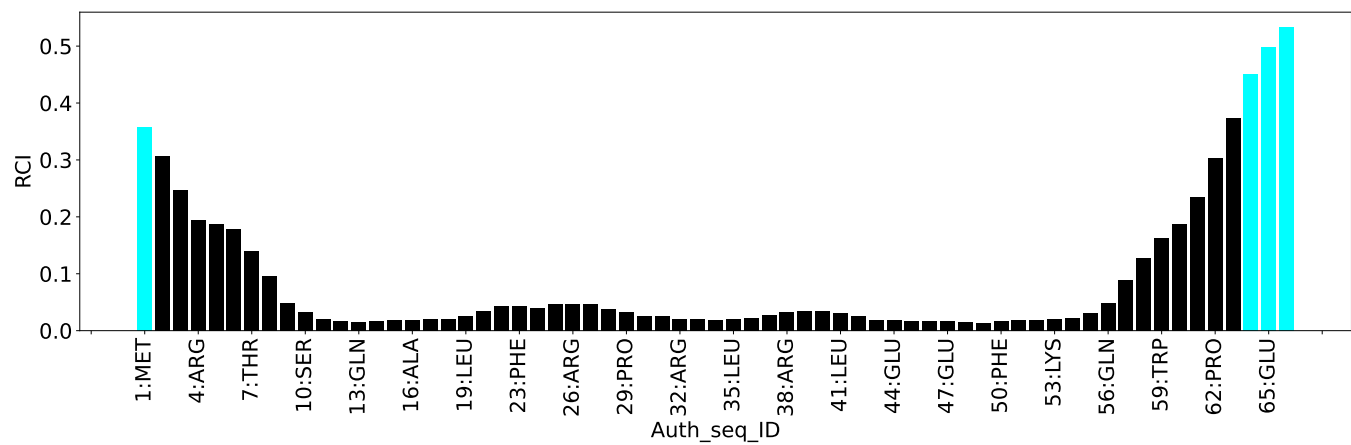
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	7	THR	HG1	4.47	0.08 – 2.19	15.8
1	A	17	LEU	HB2	-0.43	-0.07 – 3.30	-6.1
1	A	53	LYS	HB2	0.36	0.58 – 2.97	-6.0
1	A	53	LYS	HG3	-0.12	0.04 – 2.67	-5.6
1	A	53	LYS	HG2	0.04	0.13 – 2.61	-5.3

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2778
Intra-residue ($ i-j =0$)	1078
Sequential ($ i-j =1$)	608
Medium range ($ i-j >1$ and $ i-j <5$)	472
Long range ($ i-j \geq 5$)	466
Inter-chain	70
Hydrogen bond restraints	84
Disulfide bond restraints	0
Total dihedral-angle restraints	164
Number of unmapped restraints	0
Number of restraints per residue	22.3
Number of long range restraints per residue ¹	3.5

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)	67.4	0.2
0.2-0.5 (Medium)	169.7	0.5
>0.5 (Large)	362.3	5.55

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)	24.1	10.0
10.0-20.0 (Medium)	13.6	19.84
>20.0 (Large)	12.4	45.97

9 Distance violation analysis ⓘ

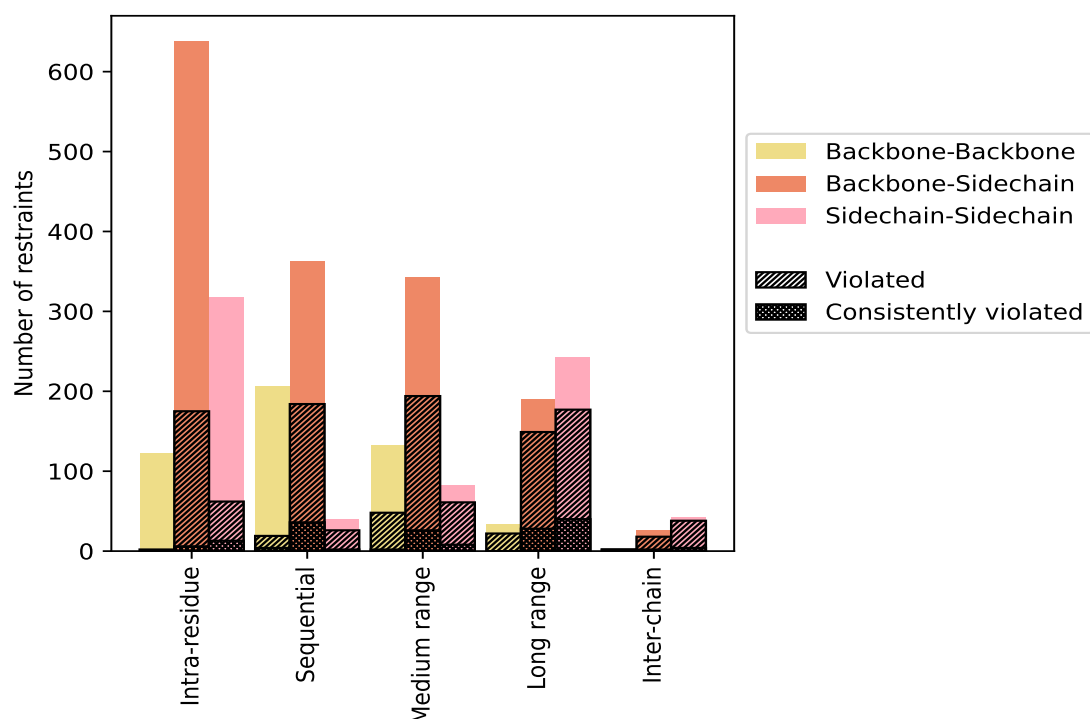
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	1078	38.8	239	22.2	8.6	19	1.8	0.7
Backbone-Backbone	122	4.4	2	1.6	0.1	0	0.0	0.0
Backbone-Sidechain	638	23.0	175	27.4	6.3	6	0.9	0.2
Sidechain-Sidechain	318	11.4	62	19.5	2.2	13	4.1	0.5
Sequential (i-j =1)	608	21.9	229	37.7	8.2	42	6.9	1.5
Backbone-Backbone	206	7.4	19	9.2	0.7	4	1.9	0.1
Backbone-Sidechain	362	13.0	184	50.8	6.6	36	9.9	1.3
Sidechain-Sidechain	40	1.4	26	65.0	0.9	2	5.0	0.1
Medium range (i-j >1 & i-j <5)	472	17.0	267	56.6	9.6	36	7.6	1.3
Backbone-Backbone	132	4.8	48	36.4	1.7	2	1.5	0.1
Backbone-Sidechain	258	9.3	158	61.2	5.7	26	10.1	0.9
Sidechain-Sidechain	82	3.0	61	74.4	2.2	8	9.8	0.3
Long range (i-j ≥5)	466	16.8	348	74.7	12.5	68	14.6	2.4
Backbone-Backbone	34	1.2	22	64.7	0.8	0	0.0	0.0
Backbone-Sidechain	190	6.8	149	78.4	5.4	28	14.7	1.0
Sidechain-Sidechain	242	8.7	177	73.1	6.4	40	16.5	1.4
Inter-chain	70	2.5	58	82.9	2.1	8	11.4	0.3
Backbone-Backbone	2	0.1	2	100.0	0.1	2	100.0	0.1
Backbone-Sidechain	26	0.9	18	69.2	0.6	2	7.7	0.1
Sidechain-Sidechain	42	1.5	38	90.5	1.4	4	9.5	0.1
Hydrogen bond	84	3.0	36	42.9	1.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2778	100.0	1177	42.4	42.4	173	6.2	6.2
Backbone-Backbone	496	17.9	93	18.8	3.3	8	1.6	0.3
Backbone-Sidechain	1558	56.1	720	46.2	25.9	98	6.3	3.5
Sidechain-Sidechain	724	26.1	364	50.3	13.1	67	9.3	2.4

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

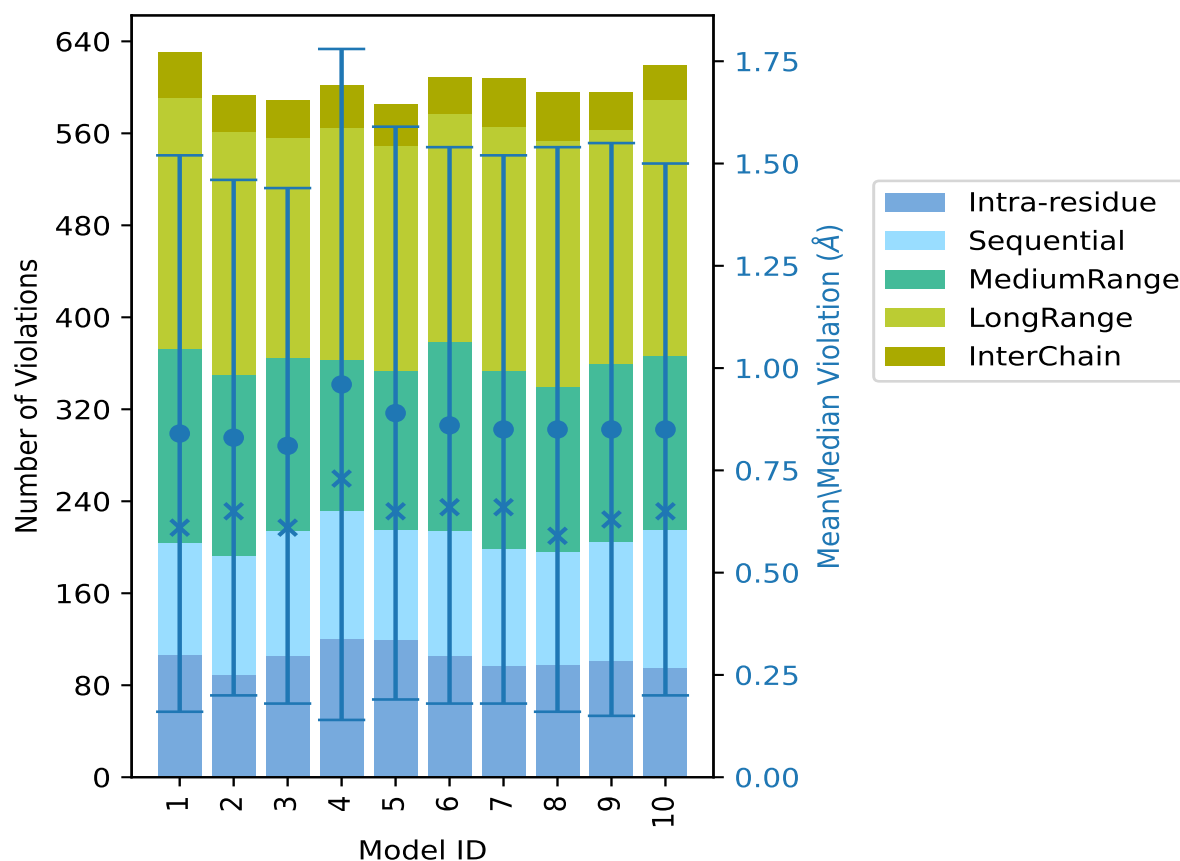
9.2 Distance violation statistics for each model [i](#)

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	106	98	169	218	40	631	0.84	4.09	0.68	0.61
2	89	104	157	211	32	593	0.83	3.64	0.63	0.65
3	106	108	151	191	33	589	0.81	3.56	0.63	0.61
4	120	112	131	202	37	602	0.96	5.55	0.82	0.73
5	120	95	139	195	36	585	0.89	4.13	0.7	0.65
6	106	108	165	198	32	609	0.86	3.67	0.68	0.66
7	97	102	154	213	42	608	0.85	3.84	0.67	0.66
8	98	98	144	214	42	596	0.85	3.46	0.69	0.59
9	101	104	155	203	33	596	0.85	3.88	0.7	0.63
10	95	120	152	222	30	619	0.85	3.37	0.65	0.65

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1553(IR:839, SQ:379, MR:205, LR:118, IC:12) 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	%
61	56	43	36	8	204	1	10.0
39	27	32	41	4	143	2	20.0
30	17	27	26	6	106	3	30.0

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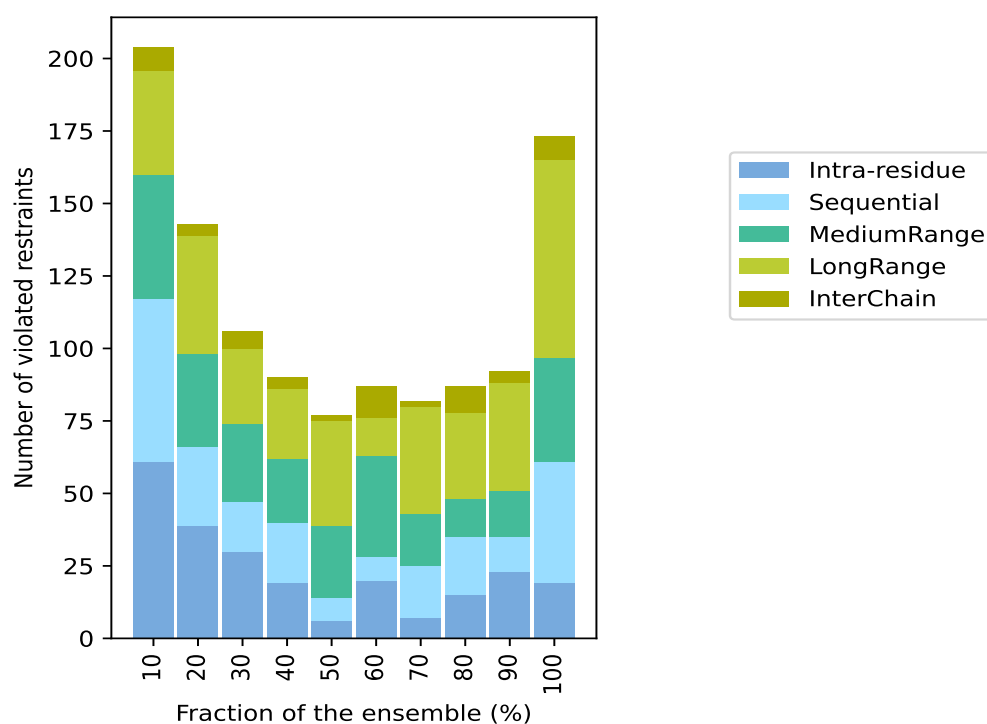
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
19	21	22	24	4	90	4	40.0
6	8	25	36	2	77	5	50.0
20	8	35	13	11	87	6	60.0
7	18	18	37	2	82	7	70.0
15	20	13	30	9	87	8	80.0
23	12	16	37	4	92	9	90.0
19	42	36	68	8	173	10	100.0

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

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

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

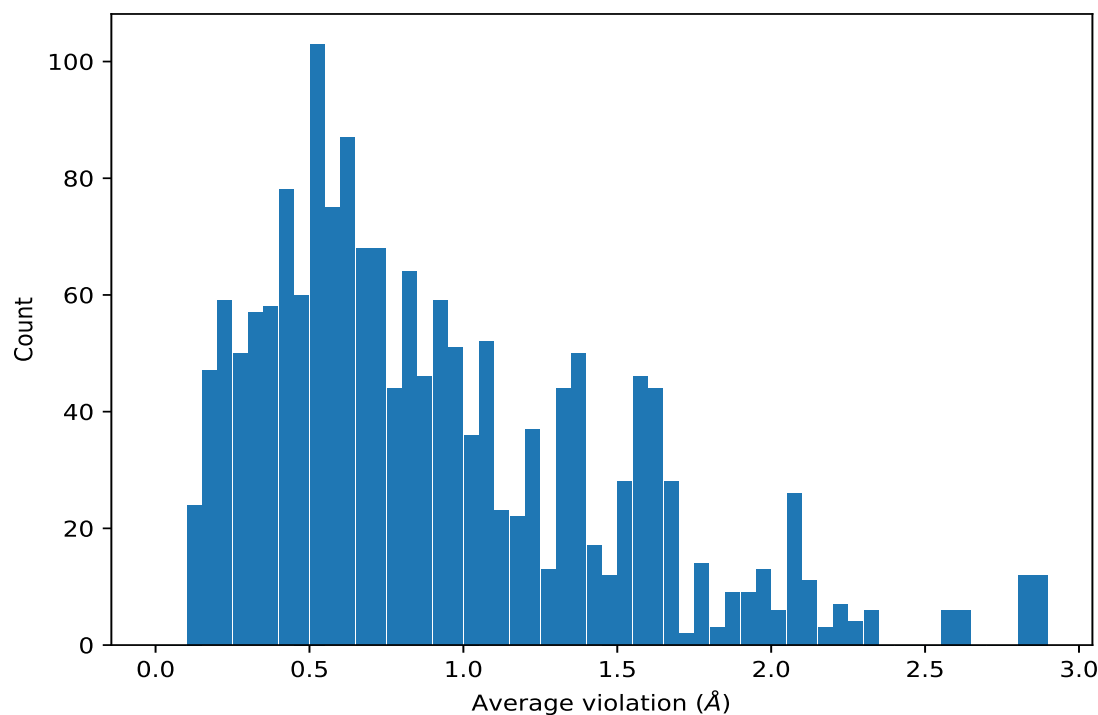


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1092)	1:39:B:LEU:HD21	1:27:B:LEU:HD21	10	2.85	1.0	2.6
(2,1092)	1:39:B:LEU:HD22	1:27:B:LEU:HD23	10	2.85	1.0	2.6
(2,1092)	1:39:B:LEU:HD21	1:27:B:LEU:HD23	10	2.85	1.0	2.6
(2,1092)	1:39:B:LEU:HD21	1:27:B:LEU:HD22	10	2.85	1.0	2.6
(2,1092)	1:39:B:LEU:HD22	1:27:B:LEU:HD22	10	2.85	1.0	2.6
(2,1092)	1:39:B:LEU:HD23	1:27:B:LEU:HD22	10	2.85	1.0	2.6
(2,1091)	1:39:A:LEU:HD21	1:27:A:LEU:HD21	10	2.85	0.99	2.6
(2,1091)	1:39:A:LEU:HD22	1:27:A:LEU:HD23	10	2.85	0.99	2.6
(2,1091)	1:39:A:LEU:HD21	1:27:A:LEU:HD23	10	2.85	0.99	2.6
(2,1091)	1:39:A:LEU:HD21	1:27:A:LEU:HD22	10	2.85	0.99	2.6
(2,1091)	1:39:A:LEU:HD22	1:27:A:LEU:HD22	10	2.85	0.99	2.6
(2,1091)	1:39:A:LEU:HD23	1:27:A:LEU:HD22	10	2.85	0.99	2.6
(2,451)	1:39:A:LEU:HD12	1:39:B:LEU:HD11	10	2.82	0.73	2.57
(2,451)	1:39:A:LEU:HD11	1:39:B:LEU:HD11	10	2.82	0.73	2.57
(2,451)	1:39:A:LEU:HD13	1:39:B:LEU:HD13	10	2.82	0.73	2.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,451)	1:39:A:LEU:HD13	1:39:B:LEU:HD12	10	2.82	0.73	2.57
(2,451)	1:39:A:LEU:HD12	1:39:B:LEU:HD12	10	2.82	0.73	2.57
(2,451)	1:39:A:LEU:HD11	1:39:B:LEU:HD12	10	2.82	0.73	2.57
(2,452)	1:39:B:LEU:HD11	1:39:A:LEU:HD12	10	2.82	0.73	2.57
(2,452)	1:39:B:LEU:HD11	1:39:A:LEU:HD11	10	2.82	0.73	2.57
(2,452)	1:39:B:LEU:HD13	1:39:A:LEU:HD13	10	2.82	0.73	2.57
(2,452)	1:39:B:LEU:HD12	1:39:A:LEU:HD13	10	2.82	0.73	2.57
(2,452)	1:39:B:LEU:HD12	1:39:A:LEU:HD12	10	2.82	0.73	2.57
(2,452)	1:39:B:LEU:HD12	1:39:A:LEU:HD11	10	2.82	0.73	2.57
(2,1224)	1:17:B:LEU:HD21	1:45:B:GLN:HE22	10	2.6	0.55	2.68
(2,1224)	1:17:B:LEU:HD22	1:45:B:GLN:HE22	10	2.6	0.55	2.68
(2,1224)	1:17:B:LEU:HD23	1:45:B:GLN:HE22	10	2.6	0.55	2.68
(2,1223)	1:17:A:LEU:HD21	1:45:A:GLN:HE22	10	2.59	0.5	2.56
(2,1223)	1:17:A:LEU:HD22	1:45:A:GLN:HE22	10	2.59	0.5	2.56
(2,1223)	1:17:A:LEU:HD23	1:45:A:GLN:HE22	10	2.59	0.5	2.56
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD12	10	2.34	0.42	2.34
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD13	10	2.34	0.42	2.34
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD11	10	2.34	0.42	2.34
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD12	10	2.33	0.42	2.32
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD13	10	2.33	0.42	2.32
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD11	10	2.33	0.42	2.32
(2,251)	1:27:A:LEU:HD12	1:44:A:GLU:HA	10	2.21	0.85	2.01
(2,251)	1:27:A:LEU:HD13	1:44:A:GLU:HA	10	2.21	0.85	2.01
(2,251)	1:27:A:LEU:HD11	1:44:A:GLU:HA	10	2.21	0.85	2.01
(2,252)	1:27:B:LEU:HD12	1:44:B:GLU:HA	10	2.17	0.87	1.98
(2,252)	1:27:B:LEU:HD13	1:44:B:GLU:HA	10	2.17	0.87	1.98
(2,252)	1:27:B:LEU:HD11	1:44:B:GLU:HA	10	2.17	0.87	1.98
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE21	10	2.13	0.87	2.16
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE22	10	2.13	0.87	2.16
(2,1624)	1:39:B:LEU:HD13	1:17:B:LEU:HA	10	2.1	0.55	2.35
(2,1624)	1:39:B:LEU:HD12	1:17:B:LEU:HA	10	2.1	0.55	2.35
(2,1624)	1:39:B:LEU:HD11	1:17:B:LEU:HA	10	2.1	0.55	2.35
(2,1623)	1:39:A:LEU:HD13	1:17:A:LEU:HA	10	2.09	0.56	2.36
(2,1623)	1:39:A:LEU:HD12	1:17:A:LEU:HA	10	2.09	0.56	2.36
(2,1623)	1:39:A:LEU:HD11	1:17:A:LEU:HA	10	2.09	0.56	2.36
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	10	2.09	0.51	1.99
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	10	2.09	0.52	2.0
(2,216)	1:27:B:LEU:HD21	1:21:B:PHE:HD1	10	2.09	0.52	2.16
(2,216)	1:27:B:LEU:HD23	1:21:B:PHE:HD1	10	2.09	0.52	2.16
(2,216)	1:27:B:LEU:HD23	1:21:B:PHE:HE1	10	2.09	0.52	2.16
(2,216)	1:27:B:LEU:HD22	1:21:B:PHE:HE1	10	2.09	0.52	2.16
(2,216)	1:27:B:LEU:HD22	1:21:B:PHE:HD1	10	2.09	0.52	2.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,216)	1:27:B:LEU:HD21	1:21:B:PHE:HE1	10	2.09	0.52	2.16
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE21	10	2.06	0.93	2.17
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE22	10	2.06	0.93	2.17
(2,215)	1:27:A:LEU:HD21	1:21:A:PHE:HD1	10	2.06	0.59	2.01
(2,215)	1:27:A:LEU:HD23	1:21:A:PHE:HD1	10	2.06	0.59	2.01
(2,215)	1:27:A:LEU:HD23	1:21:A:PHE:HE1	10	2.06	0.59	2.01
(2,215)	1:27:A:LEU:HD22	1:21:A:PHE:HE1	10	2.06	0.59	2.01
(2,215)	1:27:A:LEU:HD22	1:21:A:PHE:HD1	10	2.06	0.59	2.01
(2,215)	1:27:A:LEU:HD21	1:21:A:PHE:HE1	10	2.06	0.59	2.01
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD11	10	2.0	0.52	1.92
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD12	10	2.0	0.52	1.92
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD13	10	2.0	0.52	1.92
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD11	10	1.96	0.55	1.89
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD12	10	1.96	0.55	1.89
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD13	10	1.96	0.55	1.89
(2,1319)	1:39:A:LEU:HD23	1:9:A:PHE:HD2	10	1.95	0.65	2.0
(2,1319)	1:39:A:LEU:HD21	1:9:A:PHE:HD2	10	1.95	0.65	2.0
(2,1319)	1:39:A:LEU:HD22	1:9:A:PHE:HD2	10	1.95	0.65	2.0
(2,1320)	1:39:B:LEU:HD23	1:9:B:PHE:HD2	10	1.95	0.64	2.0
(2,1320)	1:39:B:LEU:HD21	1:9:B:PHE:HD2	10	1.95	0.64	2.0
(2,1320)	1:39:B:LEU:HD22	1:9:B:PHE:HD2	10	1.95	0.64	2.0
(2,1402)	1:46:B:ILE:HD11	1:43:B:GLU:H	10	1.94	0.2	1.9
(2,1402)	1:46:B:ILE:HD12	1:43:B:GLU:H	10	1.94	0.2	1.9
(2,1402)	1:46:B:ILE:HD13	1:43:B:GLU:H	10	1.94	0.2	1.9
(2,1401)	1:46:A:ILE:HD11	1:43:A:GLU:H	10	1.92	0.17	1.88
(2,1401)	1:46:A:ILE:HD12	1:43:A:GLU:H	10	1.92	0.17	1.88
(2,1401)	1:46:A:ILE:HD13	1:43:A:GLU:H	10	1.92	0.17	1.88
(2,1573)	1:27:A:LEU:HD11	1:46:A:ILE:H	10	1.85	0.81	1.95
(2,1573)	1:27:A:LEU:HD13	1:46:A:ILE:H	10	1.85	0.81	1.95
(2,1573)	1:27:A:LEU:HD12	1:46:A:ILE:H	10	1.85	0.81	1.95
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD23	10	1.76	0.25	1.72
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD22	10	1.76	0.25	1.72
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD21	10	1.76	0.25	1.72
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD23	10	1.76	0.26	1.73
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD22	10	1.76	0.26	1.73
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD21	10	1.76	0.26	1.73
(2,1067)	1:27:A:LEU:HD23	1:32:A:ARG:HB3	10	1.76	0.42	1.73
(2,1067)	1:27:A:LEU:HD22	1:32:A:ARG:HB3	10	1.76	0.42	1.73
(2,1067)	1:27:A:LEU:HD21	1:32:A:ARG:HB3	10	1.76	0.42	1.73
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	10	1.72	0.32	1.65
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	10	1.71	0.34	1.66
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD21	10	1.69	0.79	1.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD23	10	1.69	0.79	1.48
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD22	10	1.69	0.79	1.48
(2,1400)	1:46:B:ILE:HD13	1:44:B:GLU:H	10	1.69	0.08	1.7
(2,1400)	1:46:B:ILE:HD11	1:44:B:GLU:H	10	1.69	0.08	1.7
(2,1400)	1:46:B:ILE:HD12	1:44:B:GLU:H	10	1.69	0.08	1.7
(2,1399)	1:46:A:ILE:HD13	1:44:A:GLU:H	10	1.69	0.07	1.68
(2,1399)	1:46:A:ILE:HD11	1:44:A:GLU:H	10	1.69	0.07	1.68
(2,1399)	1:46:A:ILE:HD12	1:44:A:GLU:H	10	1.69	0.07	1.68
(2,1068)	1:27:B:LEU:HD23	1:32:B:ARG:HB3	10	1.68	0.35	1.64
(2,1068)	1:27:B:LEU:HD22	1:32:B:ARG:HB3	10	1.68	0.35	1.64
(2,1068)	1:27:B:LEU:HD21	1:32:B:ARG:HB3	10	1.68	0.35	1.64
(2,1632)	1:39:B:LEU:HD11	1:9:B:PHE:HB2	10	1.66	0.59	1.92
(2,1632)	1:39:B:LEU:HD13	1:9:B:PHE:HB2	10	1.66	0.59	1.92
(2,1632)	1:39:B:LEU:HD12	1:9:B:PHE:HB2	10	1.66	0.59	1.92
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD21	10	1.66	0.78	1.46
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD23	10	1.66	0.78	1.46
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD22	10	1.66	0.78	1.46
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD21	10	1.65	0.54	1.94
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD22	10	1.65	0.54	1.94
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD23	10	1.65	0.54	1.94
(2,1631)	1:39:A:LEU:HD11	1:9:A:PHE:HB2	10	1.65	0.57	1.88
(2,1631)	1:39:A:LEU:HD13	1:9:A:PHE:HB2	10	1.65	0.57	1.88
(2,1631)	1:39:A:LEU:HD12	1:9:A:PHE:HB2	10	1.65	0.57	1.88
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD21	10	1.64	0.53	1.94
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD22	10	1.64	0.53	1.94
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD23	10	1.64	0.53	1.94
(2,454)	1:39:B:LEU:HD13	1:16:A:ALA:HB3	10	1.63	0.45	1.54
(2,454)	1:39:B:LEU:HD11	1:16:A:ALA:HB2	10	1.63	0.45	1.54
(2,454)	1:39:B:LEU:HD11	1:16:A:ALA:HB1	10	1.63	0.45	1.54
(2,454)	1:39:B:LEU:HD11	1:16:A:ALA:HB3	10	1.63	0.45	1.54
(2,454)	1:39:B:LEU:HD13	1:16:A:ALA:HB2	10	1.63	0.45	1.54
(2,454)	1:39:B:LEU:HD12	1:16:A:ALA:HB1	10	1.63	0.45	1.54
(2,453)	1:39:A:LEU:HD13	1:16:B:ALA:HB3	10	1.62	0.45	1.51
(2,453)	1:39:A:LEU:HD11	1:16:B:ALA:HB2	10	1.62	0.45	1.51
(2,453)	1:39:A:LEU:HD11	1:16:B:ALA:HB1	10	1.62	0.45	1.51
(2,453)	1:39:A:LEU:HD11	1:16:B:ALA:HB3	10	1.62	0.45	1.51
(2,453)	1:39:A:LEU:HD13	1:16:B:ALA:HB2	10	1.62	0.45	1.51
(2,453)	1:39:A:LEU:HD12	1:16:B:ALA:HB1	10	1.62	0.45	1.51
(2,1150)	1:20:B:ALA:HB2	1:35:B:LEU:HD22	10	1.61	0.45	1.54
(2,1150)	1:20:B:ALA:HB1	1:35:B:LEU:HD23	10	1.61	0.45	1.54
(2,1150)	1:20:B:ALA:HB3	1:35:B:LEU:HD23	10	1.61	0.45	1.54
(2,1150)	1:20:B:ALA:HB2	1:35:B:LEU:HD23	10	1.61	0.45	1.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1150)	1:20:B:ALA:HB3	1:35:B:LEU:HD21	10	1.61	0.45	1.54
(2,1150)	1:20:B:ALA:HB3	1:35:B:LEU:HD22	10	1.61	0.45	1.54
(2,1150)	1:20:B:ALA:HB1	1:35:B:LEU:HD22	10	1.61	0.45	1.54
(2,1149)	1:20:A:ALA:HB2	1:35:A:LEU:HD22	10	1.59	0.52	1.52
(2,1149)	1:20:A:ALA:HB1	1:35:A:LEU:HD23	10	1.59	0.52	1.52
(2,1149)	1:20:A:ALA:HB3	1:35:A:LEU:HD23	10	1.59	0.52	1.52
(2,1149)	1:20:A:ALA:HB2	1:35:A:LEU:HD23	10	1.59	0.52	1.52
(2,1149)	1:20:A:ALA:HB3	1:35:A:LEU:HD21	10	1.59	0.52	1.52
(2,1149)	1:20:A:ALA:HB3	1:35:A:LEU:HD22	10	1.59	0.52	1.52
(2,1149)	1:20:A:ALA:HB1	1:35:A:LEU:HD22	10	1.59	0.52	1.52
(2,1615)	1:27:A:LEU:HD11	1:35:A:LEU:HD13	10	1.57	0.9	1.4
(2,1615)	1:27:A:LEU:HD12	1:35:A:LEU:HD13	10	1.57	0.9	1.4
(2,1615)	1:27:A:LEU:HD13	1:35:A:LEU:HD12	10	1.57	0.9	1.4
(2,1615)	1:27:A:LEU:HD12	1:35:A:LEU:HD12	10	1.57	0.9	1.4
(2,1615)	1:27:A:LEU:HD11	1:35:A:LEU:HD11	10	1.57	0.9	1.4
(2,1615)	1:27:A:LEU:HD13	1:35:A:LEU:HD13	10	1.57	0.9	1.4
(2,1616)	1:27:B:LEU:HD11	1:35:B:LEU:HD13	10	1.56	0.89	1.41
(2,1616)	1:27:B:LEU:HD12	1:35:B:LEU:HD13	10	1.56	0.89	1.41
(2,1616)	1:27:B:LEU:HD13	1:35:B:LEU:HD12	10	1.56	0.89	1.41
(2,1616)	1:27:B:LEU:HD12	1:35:B:LEU:HD12	10	1.56	0.89	1.41
(2,1616)	1:27:B:LEU:HD11	1:35:B:LEU:HD11	10	1.56	0.89	1.41
(2,1616)	1:27:B:LEU:HD13	1:35:B:LEU:HD13	10	1.56	0.89	1.41
(2,1622)	1:39:B:LEU:HD11	1:18:B:ASP:H	10	1.55	0.44	1.66
(2,1622)	1:39:B:LEU:HD13	1:18:B:ASP:H	10	1.55	0.44	1.66
(2,1622)	1:39:B:LEU:HD12	1:18:B:ASP:H	10	1.55	0.44	1.66
(2,190)	1:17:B:LEU:HD21	1:53:B:LYS:HE3	10	1.55	0.48	1.5
(2,190)	1:17:B:LEU:HD22	1:53:B:LYS:HE3	10	1.55	0.48	1.5
(2,190)	1:17:B:LEU:HD23	1:53:B:LYS:HE2	10	1.55	0.48	1.5
(2,190)	1:17:B:LEU:HD23	1:13:B:GLN:HG2	10	1.55	0.48	1.5
(2,190)	1:17:B:LEU:HD22	1:13:B:GLN:HG2	10	1.55	0.48	1.5
(2,298)	1:16:B:ALA:H	1:38:A:ARG:HB3	10	1.54	0.28	1.67
(2,298)	1:16:B:ALA:H	1:39:B:LEU:HB2	10	1.54	0.28	1.67
(2,298)	1:16:B:ALA:H	1:39:A:LEU:HB2	10	1.54	0.28	1.67
(2,189)	1:17:A:LEU:HD21	1:53:A:LYS:HE3	10	1.53	0.5	1.5
(2,189)	1:17:A:LEU:HD22	1:53:A:LYS:HE3	10	1.53	0.5	1.5
(2,189)	1:17:A:LEU:HD23	1:53:A:LYS:HE2	10	1.53	0.5	1.5
(2,189)	1:17:A:LEU:HD23	1:13:A:GLN:HG2	10	1.53	0.5	1.5
(2,189)	1:17:A:LEU:HD22	1:13:A:GLN:HG2	10	1.53	0.5	1.5
(2,1621)	1:39:A:LEU:HD11	1:18:A:ASP:H	10	1.53	0.44	1.63
(2,1621)	1:39:A:LEU:HD13	1:18:A:ASP:H	10	1.53	0.44	1.63
(2,1621)	1:39:A:LEU:HD12	1:18:A:ASP:H	10	1.53	0.44	1.63
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	10	1.52	0.61	1.73

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,297)	1:16:A:ALA:H	1:39:B:LEU:HB2	10	1.52	0.28	1.66
(2,297)	1:16:A:ALA:H	1:39:A:LEU:HB2	10	1.52	0.28	1.66
(2,297)	1:16:A:ALA:H	1:38:B:ARG:HB3	10	1.52	0.28	1.66
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	10	1.52	0.36	1.39
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	10	1.51	0.37	1.42
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB1	10	1.51	1.02	1.49
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB3	10	1.51	1.02	1.49
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB2	10	1.51	1.02	1.49
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	10	1.49	0.58	1.72
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB2	10	1.47	0.4	1.35
(2,2)	1:34:B:TYR:HD1	1:20:B:ALA:HB1	10	1.47	0.4	1.35
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB3	10	1.47	0.4	1.35
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB1	10	1.47	0.96	1.49
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB3	10	1.47	0.96	1.49
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB2	10	1.47	0.96	1.49
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB2	10	1.42	0.27	1.47
(2,1)	1:34:A:TYR:HD1	1:20:A:ALA:HB1	10	1.42	0.27	1.47
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB3	10	1.42	0.27	1.47
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD11	10	1.36	0.43	1.21
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD12	10	1.36	0.43	1.21
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD13	10	1.36	0.43	1.21
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB3	10	1.36	0.29	1.32
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB2	10	1.36	0.29	1.32
(2,1575)	1:27:A:LEU:HD12	1:51:A:ARG:H	10	1.36	0.58	1.43
(2,1575)	1:27:A:LEU:HD13	1:51:A:ARG:H	10	1.36	0.58	1.43
(2,1575)	1:27:A:LEU:HD11	1:51:A:ARG:H	10	1.36	0.58	1.43
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB3	10	1.36	0.31	1.3
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB2	10	1.36	0.31	1.3
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	10	1.35	1.06	0.94
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	10	1.33	0.54	1.52
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	10	1.33	0.55	1.52
(2,1323)	1:39:A:LEU:HD22	1:46:A:ILE:H	10	1.33	0.11	1.34
(2,1323)	1:39:A:LEU:HD23	1:46:A:ILE:H	10	1.33	0.11	1.34
(2,1323)	1:39:A:LEU:HD21	1:46:A:ILE:H	10	1.33	0.11	1.34
(2,225)	1:46:A:ILE:HD13	1:9:A:PHE:HB2	10	1.33	0.45	1.23
(2,225)	1:46:A:ILE:HD11	1:9:A:PHE:HB2	10	1.33	0.45	1.23
(2,225)	1:46:A:ILE:HD12	1:9:A:PHE:HB2	10	1.33	0.45	1.23
(2,1324)	1:39:B:LEU:HD22	1:46:B:ILE:H	10	1.32	0.12	1.34
(2,1324)	1:39:B:LEU:HD23	1:46:B:ILE:H	10	1.32	0.12	1.34
(2,1324)	1:39:B:LEU:HD21	1:46:B:ILE:H	10	1.32	0.12	1.34
(2,226)	1:46:B:ILE:HD13	1:9:B:PHE:HB2	10	1.32	0.46	1.23
(2,226)	1:46:B:ILE:HD11	1:9:B:PHE:HB2	10	1.32	0.46	1.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,226)	1:46:B:ILE:HD12	1:9:B:PHE:HB2	10	1.32	0.46	1.23
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD11	10	1.31	0.45	1.18
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD12	10	1.31	0.45	1.18
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD13	10	1.31	0.45	1.18
(2,67)	1:65:A:GLU:HA	1:53:A:LYS:HD2	10	1.31	1.02	1.25
(2,67)	1:25:A:ARG:HA	1:19:B:LEU:HD21	10	1.31	1.02	1.25
(2,67)	1:25:A:ARG:HA	1:19:B:LEU:HD23	10	1.31	1.02	1.25
(2,67)	1:25:A:ARG:HA	1:19:B:LEU:HD22	10	1.31	1.02	1.25
(2,67)	1:65:A:GLU:HA	1:19:A:LEU:HD21	10	1.31	1.02	1.25
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	10	1.26	0.84	1.07
(2,68)	1:65:B:GLU:HA	1:53:B:LYS:HD2	10	1.25	0.92	1.19
(2,68)	1:25:B:ARG:HA	1:19:A:LEU:HD22	10	1.25	0.92	1.19
(2,68)	1:25:B:ARG:HA	1:19:A:LEU:HD21	10	1.25	0.92	1.19
(2,68)	1:25:B:ARG:HA	1:19:A:LEU:HD23	10	1.25	0.92	1.19
(2,68)	1:65:B:GLU:HA	1:19:B:LEU:HD21	10	1.25	0.92	1.19
(2,1398)	1:46:B:ILE:HD11	1:35:B:LEU:H	10	1.22	0.32	1.24
(2,1398)	1:46:B:ILE:HD12	1:35:B:LEU:H	10	1.22	0.32	1.24
(2,1398)	1:46:B:ILE:HD13	1:35:B:LEU:H	10	1.22	0.32	1.24
(2,1397)	1:46:A:ILE:HD11	1:35:A:LEU:H	10	1.21	0.29	1.25
(2,1397)	1:46:A:ILE:HD12	1:35:A:LEU:H	10	1.21	0.29	1.25
(2,1397)	1:46:A:ILE:HD13	1:35:A:LEU:H	10	1.21	0.29	1.25
(2,192)	1:17:B:LEU:HD21	1:14:B:LYS:HB3	10	1.17	0.44	1.08
(2,192)	1:17:B:LEU:HD22	1:14:B:LYS:HB3	10	1.17	0.44	1.08
(2,192)	1:17:B:LEU:HD23	1:14:B:LYS:HB3	10	1.17	0.44	1.08
(2,191)	1:17:A:LEU:HD21	1:14:A:LYS:HB3	10	1.16	0.47	1.07
(2,191)	1:17:A:LEU:HD22	1:14:A:LYS:HB3	10	1.16	0.47	1.07
(2,191)	1:17:A:LEU:HD23	1:14:A:LYS:HB3	10	1.16	0.47	1.07
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	10	1.14	0.6	1.1
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	10	1.14	0.59	1.16
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	10	1.11	0.11	1.1
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	10	1.1	0.1	1.1
(2,305)	1:49:A:TRP:H	1:53:A:LYS:HB3	10	1.07	0.29	1.04
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD12	10	1.07	0.29	1.04
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD13	10	1.07	0.29	1.04
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD11	10	1.07	0.29	1.04
(2,306)	1:49:B:TRP:H	1:53:B:LYS:HB3	10	1.07	0.31	1.02
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD12	10	1.07	0.31	1.02
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD13	10	1.07	0.31	1.02
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD11	10	1.07	0.31	1.02
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	10	1.06	0.22	1.1
(2,1038)	1:51:B:ARG:HG2	1:52:B:ARG:HA	10	1.06	0.22	1.1
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	10	1.06	0.22	1.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1037)	1:51:A:ARG:HG2	1:52:A:ARG:HA	10	1.06	0.22	1.12
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD21	10	1.01	0.33	1.02
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD22	10	1.01	0.33	1.02
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD23	10	1.01	0.33	1.02
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	10	1.01	0.08	1.0
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD21	10	1.0	0.31	1.04
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD22	10	1.0	0.31	1.04
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD23	10	1.0	0.31	1.04
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	10	1.0	0.07	1.0
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	10	0.98	0.31	0.98
(2,219)	1:43:A:GLU:HA	1:47:A:GLU:HG2	10	0.97	0.46	1.17
(2,219)	1:43:A:GLU:HA	1:44:A:GLU:HG2	10	0.97	0.46	1.17
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD22	10	0.97	0.11	1.0
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD23	10	0.97	0.11	1.0
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD21	10	0.97	0.11	1.0
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD22	10	0.96	0.1	0.96
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD23	10	0.96	0.1	0.96
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD21	10	0.96	0.1	0.96
(2,220)	1:43:B:GLU:HA	1:47:B:GLU:HG2	10	0.94	0.44	1.17
(2,220)	1:43:B:GLU:HA	1:44:B:GLU:HG2	10	0.94	0.44	1.17
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	10	0.94	0.33	0.96
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	10	0.93	0.47	0.72
(2,139)	1:55:A:GLN:HB3	1:56:A:GLN:H	10	0.93	0.47	0.72
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	10	0.93	0.46	0.72
(2,140)	1:55:B:GLN:HB3	1:56:B:GLN:H	10	0.93	0.46	0.72
(2,264)	1:39:B:LEU:HD11	1:16:B:ALA:H	10	0.92	0.4	0.86
(2,264)	1:39:B:LEU:HD13	1:16:B:ALA:H	10	0.92	0.4	0.86
(2,264)	1:39:B:LEU:HD12	1:16:B:ALA:H	10	0.92	0.4	0.86
(2,264)	1:39:B:LEU:HD11	1:16:A:ALA:H	10	0.92	0.4	0.86
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	10	0.92	0.39	0.98
(2,263)	1:39:A:LEU:HD11	1:16:A:ALA:H	10	0.9	0.41	0.82
(2,263)	1:39:A:LEU:HD13	1:16:A:ALA:H	10	0.9	0.41	0.82
(2,263)	1:39:A:LEU:HD12	1:16:A:ALA:H	10	0.9	0.41	0.82
(2,263)	1:39:A:LEU:HD11	1:16:B:ALA:H	10	0.9	0.41	0.82
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	10	0.9	0.39	0.94
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG23	10	0.83	0.1	0.88
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG21	10	0.83	0.1	0.88
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG22	10	0.83	0.1	0.88
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG23	10	0.83	0.1	0.87
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG21	10	0.83	0.1	0.87
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG22	10	0.83	0.1	0.87
(2,372)	1:51:B:ARG:H	1:55:B:GLN:HG3	10	0.83	0.17	0.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,372)	1:51:B:ARG:H	1:47:B:GLU:HG2	10	0.83	0.17	0.88
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD13	10	0.82	0.21	0.78
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD12	10	0.82	0.21	0.78
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD11	10	0.82	0.21	0.78
(2,345)	1:36:A:SER:H	1:41:A:LEU:HD13	10	0.82	0.21	0.78
(2,239)	1:49:A:TRP:HB3	1:46:A:ILE:HG12	10	0.82	0.35	0.89
(2,239)	1:49:A:TRP:HB3	1:52:A:ARG:HG2	10	0.82	0.35	0.89
(2,239)	1:59:A:TRP:HB2	1:57:A:ILE:HG12	10	0.82	0.35	0.89
(2,240)	1:49:B:TRP:HB3	1:46:B:ILE:HG12	10	0.82	0.34	0.86
(2,240)	1:49:B:TRP:HB3	1:52:B:ARG:HG2	10	0.82	0.34	0.86
(2,240)	1:59:B:TRP:HB2	1:57:B:ILE:HG12	10	0.82	0.34	0.86
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	10	0.82	0.53	0.71
(2,371)	1:51:A:ARG:H	1:55:A:GLN:HG3	10	0.81	0.17	0.86
(2,371)	1:51:A:ARG:H	1:47:A:GLU:HG2	10	0.81	0.17	0.86
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD13	10	0.81	0.21	0.76
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD12	10	0.81	0.21	0.76
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD11	10	0.81	0.21	0.76
(2,346)	1:36:B:SER:H	1:41:B:LEU:HD13	10	0.81	0.21	0.76
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	10	0.75	0.51	0.57
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	10	0.74	0.2	0.76
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG3	10	0.74	0.2	0.76
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	10	0.74	0.19	0.74
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG3	10	0.74	0.19	0.74
(2,1626)	1:41:B:LEU:HD11	1:36:B:SER:HA	10	0.73	0.39	0.62
(2,1626)	1:41:B:LEU:HD12	1:36:B:SER:HA	10	0.73	0.39	0.62
(2,1626)	1:41:B:LEU:HD13	1:36:B:SER:HA	10	0.73	0.39	0.62
(2,1625)	1:41:A:LEU:HD11	1:36:A:SER:HA	10	0.73	0.38	0.62
(2,1625)	1:41:A:LEU:HD12	1:36:A:SER:HA	10	0.73	0.38	0.62
(2,1625)	1:41:A:LEU:HD13	1:36:A:SER:HA	10	0.73	0.38	0.62
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	10	0.72	0.31	0.74
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	10	0.72	0.31	0.74
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	10	0.69	0.0	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	10	0.69	0.0	0.69
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	10	0.64	0.19	0.7
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	10	0.64	0.24	0.56
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	10	0.64	0.23	0.58
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	10	0.64	0.2	0.7
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	10	0.62	0.28	0.52
(2,1143)	1:46:A:ILE:HG21	1:46:A:ILE:HG12	10	0.62	0.02	0.62
(2,1143)	1:46:A:ILE:HG23	1:46:A:ILE:HG12	10	0.62	0.02	0.62
(2,1143)	1:46:A:ILE:HG22	1:46:A:ILE:HG12	10	0.62	0.02	0.62
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	10	0.62	0.32	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1144)	1:46:B:ILE:HG21	1:46:B:ILE:HG12	10	0.62	0.02	0.62
(2,1144)	1:46:B:ILE:HG23	1:46:B:ILE:HG12	10	0.62	0.02	0.62
(2,1144)	1:46:B:ILE:HG22	1:46:B:ILE:HG12	10	0.62	0.02	0.62
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	10	0.61	0.28	0.49
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	10	0.6	0.29	0.51
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	10	0.6	0.1	0.56
(2,126)	1:48:B:ARG:HB3	1:48:B:ARG:HD2	10	0.6	0.1	0.56
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	10	0.6	0.1	0.55
(2,125)	1:48:A:ARG:HB3	1:48:A:ARG:HD2	10	0.6	0.1	0.55
(2,1388)	1:46:B:ILE:HD13	1:45:B:GLN:HG3	10	0.6	0.11	0.62
(2,1388)	1:46:B:ILE:HD11	1:45:B:GLN:HG3	10	0.6	0.11	0.62
(2,1388)	1:46:B:ILE:HD12	1:45:B:GLN:HG3	10	0.6	0.11	0.62
(2,1387)	1:46:A:ILE:HD13	1:45:A:GLN:HG3	10	0.59	0.13	0.6
(2,1387)	1:46:A:ILE:HD11	1:45:A:GLN:HG3	10	0.59	0.13	0.6
(2,1387)	1:46:A:ILE:HD12	1:45:A:GLN:HG3	10	0.59	0.13	0.6
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD13	10	0.55	0.13	0.56
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD12	10	0.55	0.13	0.56
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD11	10	0.55	0.13	0.56
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD12	10	0.54	0.13	0.55
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD13	10	0.54	0.13	0.55
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD11	10	0.54	0.13	0.55
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	10	0.53	0.18	0.47
(2,1191)	1:16:A:ALA:HB1	1:14:A:LYS:HA	10	0.53	0.22	0.6
(2,1191)	1:16:A:ALA:HB3	1:14:A:LYS:HA	10	0.53	0.22	0.6
(2,1191)	1:16:A:ALA:HB2	1:14:A:LYS:HA	10	0.53	0.22	0.6
(2,1192)	1:16:B:ALA:HB1	1:14:B:LYS:HA	10	0.53	0.23	0.6
(2,1192)	1:16:B:ALA:HB3	1:14:B:LYS:HA	10	0.53	0.23	0.6
(2,1192)	1:16:B:ALA:HB2	1:14:B:LYS:HA	10	0.53	0.23	0.6
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	10	0.53	0.18	0.46
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD22	10	0.52	0.13	0.56
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD23	10	0.52	0.13	0.56
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD21	10	0.52	0.13	0.56
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD11	10	0.52	0.1	0.52
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD12	10	0.52	0.1	0.52
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD13	10	0.52	0.1	0.52
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD22	10	0.51	0.13	0.55
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD23	10	0.51	0.13	0.55
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD21	10	0.51	0.13	0.55
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD11	10	0.5	0.09	0.53
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD12	10	0.5	0.09	0.53
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD13	10	0.5	0.09	0.53
(2,1167)	1:46:A:ILE:HD12	1:46:A:ILE:HB	10	0.5	0.01	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1167)	1:46:A:ILE:HD13	1:46:A:ILE:HB	10	0.5	0.01	0.5
(2,1167)	1:46:A:ILE:HD11	1:46:A:ILE:HB	10	0.5	0.01	0.5
(2,1168)	1:46:B:ILE:HD12	1:46:B:ILE:HB	10	0.5	0.01	0.5
(2,1168)	1:46:B:ILE:HD13	1:46:B:ILE:HB	10	0.5	0.01	0.5
(2,1168)	1:46:B:ILE:HD11	1:46:B:ILE:HB	10	0.5	0.01	0.5
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	10	0.46	0.08	0.49
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	10	0.46	0.04	0.46
(2,1201)	1:17:A:LEU:HD23	1:46:A:ILE:HG12	10	0.46	0.3	0.31
(2,1201)	1:17:A:LEU:HD21	1:46:A:ILE:HG12	10	0.46	0.3	0.31
(2,1201)	1:17:A:LEU:HD22	1:46:A:ILE:HG12	10	0.46	0.3	0.31
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	10	0.46	0.04	0.46
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	10	0.46	0.08	0.49
(2,1202)	1:17:B:LEU:HD23	1:46:B:ILE:HG12	10	0.45	0.28	0.32
(2,1202)	1:17:B:LEU:HD21	1:46:B:ILE:HG12	10	0.45	0.28	0.32
(2,1202)	1:17:B:LEU:HD22	1:46:B:ILE:HG12	10	0.45	0.28	0.32
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	10	0.41	0.04	0.42
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	10	0.41	0.05	0.42
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	10	0.4	0.18	0.36
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	10	0.4	0.19	0.36
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG23	10	0.39	0.07	0.42
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG21	10	0.39	0.07	0.42
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG22	10	0.39	0.07	0.42
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG23	10	0.39	0.08	0.42
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG21	10	0.39	0.08	0.42
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG22	10	0.39	0.08	0.42
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	10	0.38	0.11	0.4
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	10	0.38	0.11	0.4
(2,1189)	1:16:A:ALA:HB1	1:17:A:LEU:HA	10	0.34	0.11	0.34
(2,1189)	1:16:A:ALA:HB3	1:17:A:LEU:HA	10	0.34	0.11	0.34
(2,1189)	1:16:A:ALA:HB2	1:17:A:LEU:HA	10	0.34	0.11	0.34
(2,1190)	1:16:B:ALA:HB1	1:17:B:LEU:HA	10	0.34	0.1	0.34
(2,1190)	1:16:B:ALA:HB3	1:17:B:LEU:HA	10	0.34	0.1	0.34
(2,1190)	1:16:B:ALA:HB2	1:17:B:LEU:HA	10	0.34	0.1	0.34
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	10	0.31	0.08	0.28
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	10	0.31	0.08	0.28
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	10	0.29	0.09	0.32
(2,170)	1:12:B:GLU:HA	1:15:B:LYS:H	10	0.29	0.09	0.32
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	10	0.28	0.08	0.29
(2,169)	1:12:A:GLU:HA	1:15:A:LYS:H	10	0.28	0.08	0.29
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	10	0.28	0.1	0.26
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	10	0.27	0.11	0.26
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	10	0.25	0.04	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	10	0.25	0.04	0.25
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD13	10	0.17	0.02	0.17
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD12	10	0.17	0.02	0.17
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD11	10	0.17	0.02	0.17
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD13	10	0.17	0.01	0.16
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD12	10	0.17	0.01	0.16
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD11	10	0.17	0.01	0.16
(2,1109)	1:41:A:LEU:HD11	1:41:A:LEU:HD22	10	0.14	0.02	0.13
(2,1109)	1:41:A:LEU:HD12	1:41:A:LEU:HD23	10	0.14	0.02	0.13
(2,1109)	1:41:A:LEU:HD11	1:41:A:LEU:HD23	10	0.14	0.02	0.13
(2,1109)	1:41:A:LEU:HD13	1:41:A:LEU:HD21	10	0.14	0.02	0.13
(2,1574)	1:27:B:LEU:HD11	1:46:B:ILE:H	9	2.05	0.6	2.01
(2,1574)	1:27:B:LEU:HD13	1:46:B:ILE:H	9	2.05	0.6	2.01
(2,1574)	1:27:B:LEU:HD12	1:46:B:ILE:H	9	2.05	0.6	2.01
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG22	9	2.01	1.02	2.13
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG21	9	2.01	1.02	2.13
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG23	9	2.01	1.02	2.13
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG22	9	1.99	1.04	2.13
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG21	9	1.99	1.04	2.13
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG23	9	1.99	1.04	2.13
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	9	1.64	0.39	1.6
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	9	1.62	0.42	1.6
(2,179)	1:16:A:ALA:HB2	1:15:B:LYS:HE3	9	1.62	0.69	1.65
(2,179)	1:16:A:ALA:HB1	1:15:B:LYS:HE3	9	1.62	0.69	1.65
(2,179)	1:16:A:ALA:HB2	1:15:A:LYS:HE3	9	1.62	0.69	1.65
(2,179)	1:16:A:ALA:HB1	1:15:A:LYS:HE3	9	1.62	0.69	1.65
(2,179)	1:16:A:ALA:HB3	1:15:B:LYS:HE3	9	1.62	0.69	1.65
(2,1312)	1:39:B:LEU:HD21	1:17:B:LEU:HA	9	1.61	0.25	1.65
(2,1312)	1:39:B:LEU:HD22	1:17:B:LEU:HA	9	1.61	0.25	1.65
(2,1312)	1:39:B:LEU:HD23	1:17:B:LEU:HA	9	1.61	0.25	1.65
(2,1311)	1:39:A:LEU:HD21	1:17:A:LEU:HA	9	1.6	0.26	1.65
(2,1311)	1:39:A:LEU:HD22	1:17:A:LEU:HA	9	1.6	0.26	1.65
(2,1311)	1:39:A:LEU:HD23	1:17:A:LEU:HA	9	1.6	0.26	1.65
(2,180)	1:16:B:ALA:HB2	1:15:A:LYS:HE3	9	1.6	0.71	1.71
(2,180)	1:16:B:ALA:HB3	1:15:A:LYS:HE3	9	1.6	0.71	1.71
(2,180)	1:16:B:ALA:HB1	1:15:A:LYS:HE3	9	1.6	0.71	1.71
(2,180)	1:16:B:ALA:HB2	1:15:B:LYS:HE3	9	1.6	0.71	1.71
(2,180)	1:16:B:ALA:HB1	1:15:B:LYS:HE3	9	1.6	0.71	1.71
(2,442)	1:16:B:ALA:HB2	1:20:A:ALA:H	9	1.56	0.76	1.58
(2,442)	1:16:B:ALA:HB1	1:20:A:ALA:H	9	1.56	0.76	1.58
(2,442)	1:16:B:ALA:HB3	1:20:A:ALA:H	9	1.56	0.76	1.58
(2,441)	1:16:A:ALA:HB2	1:20:B:ALA:H	9	1.56	0.76	1.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,441)	1:16:A:ALA:HB1	1:20:B:ALA:H	9	1.56	0.76	1.55
(2,441)	1:16:A:ALA:HB3	1:20:B:ALA:H	9	1.56	0.76	1.55
(2,1576)	1:27:B:LEU:HD12	1:51:B:ARG:H	9	1.55	0.42	1.72
(2,1576)	1:27:B:LEU:HD13	1:51:B:ARG:H	9	1.55	0.42	1.72
(2,1576)	1:27:B:LEU:HD11	1:51:B:ARG:H	9	1.55	0.42	1.72
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	9	1.52	0.53	1.78
(2,18)	1:60:B:SER:HB2	1:57:B:ILE:HA	9	1.52	0.53	1.78
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	9	1.52	0.54	1.78
(2,17)	1:60:A:SER:HB2	1:57:A:ILE:HA	9	1.52	0.54	1.78
(2,1239)	1:20:A:ALA:HB3	1:39:A:LEU:HD21	9	1.39	0.5	1.29
(2,1239)	1:20:A:ALA:HB1	1:39:A:LEU:HD22	9	1.39	0.5	1.29
(2,1239)	1:20:A:ALA:HB2	1:39:A:LEU:HD22	9	1.39	0.5	1.29
(2,1239)	1:20:A:ALA:HB3	1:39:A:LEU:HD22	9	1.39	0.5	1.29
(2,1239)	1:20:A:ALA:HB2	1:39:A:LEU:HD23	9	1.39	0.5	1.29
(2,1239)	1:20:A:ALA:HB1	1:39:A:LEU:HD21	9	1.39	0.5	1.29
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	9	1.39	0.35	1.47
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	9	1.38	0.35	1.47
(2,1240)	1:20:B:ALA:HB3	1:39:B:LEU:HD21	9	1.37	0.53	1.17
(2,1240)	1:20:B:ALA:HB1	1:39:B:LEU:HD22	9	1.37	0.53	1.17
(2,1240)	1:20:B:ALA:HB2	1:39:B:LEU:HD22	9	1.37	0.53	1.17
(2,1240)	1:20:B:ALA:HB3	1:39:B:LEU:HD22	9	1.37	0.53	1.17
(2,1240)	1:20:B:ALA:HB2	1:39:B:LEU:HD23	9	1.37	0.53	1.17
(2,1240)	1:20:B:ALA:HB1	1:39:B:LEU:HD21	9	1.37	0.53	1.17
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD13	9	1.32	0.82	1.15
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD11	9	1.32	0.82	1.15
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD12	9	1.32	0.82	1.15
(2,1108)	1:39:B:LEU:HD21	1:17:B:LEU:HG	9	1.31	0.52	1.53
(2,1108)	1:39:B:LEU:HD22	1:17:B:LEU:HG	9	1.31	0.52	1.53
(2,1108)	1:39:B:LEU:HD23	1:17:B:LEU:HG	9	1.31	0.52	1.53
(2,1107)	1:39:A:LEU:HD21	1:17:A:LEU:HG	9	1.3	0.52	1.52
(2,1107)	1:39:A:LEU:HD22	1:17:A:LEU:HG	9	1.3	0.52	1.52
(2,1107)	1:39:A:LEU:HD23	1:17:A:LEU:HG	9	1.3	0.52	1.52
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	9	1.23	0.62	1.3
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD13	9	1.23	0.87	0.85
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD11	9	1.23	0.87	0.85
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD12	9	1.23	0.87	0.85
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	9	1.22	0.62	1.29
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	9	1.22	0.08	1.18
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	9	1.21	0.08	1.19
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	9	1.14	0.43	1.17
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	9	1.14	0.42	1.15
(2,1411)	1:46:A:ILE:HG23	1:50:A:PHE:HD1	9	1.08	0.45	1.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1411)	1:46:A:ILE:HG22	1:50:A:PHE:HD1	9	1.08	0.45	1.15
(2,1411)	1:46:A:ILE:HG21	1:50:A:PHE:HD1	9	1.08	0.45	1.15
(2,1411)	1:46:A:ILE:HG22	1:50:A:PHE:HD2	9	1.08	0.45	1.15
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD12	9	1.07	0.45	1.16
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD13	9	1.07	0.45	1.16
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD11	9	1.07	0.45	1.16
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD12	9	1.05	0.44	0.95
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD13	9	1.05	0.44	0.95
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD11	9	1.05	0.44	0.95
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	9	1.05	0.76	0.85
(2,1412)	1:46:B:ILE:HG23	1:50:B:PHE:HD1	9	1.03	0.47	1.09
(2,1412)	1:46:B:ILE:HG22	1:50:B:PHE:HD1	9	1.03	0.47	1.09
(2,1412)	1:46:B:ILE:HG21	1:50:B:PHE:HD1	9	1.03	0.47	1.09
(2,1412)	1:46:B:ILE:HG22	1:50:B:PHE:HD2	9	1.03	0.47	1.09
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	9	1.03	0.69	0.87
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	9	1.01	0.42	0.88
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	9	1.01	0.56	0.88
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	9	1.01	0.44	0.88
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	9	1.01	0.57	0.88
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	9	0.99	0.18	1.05
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	9	0.99	0.18	1.04
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	9	0.97	0.48	0.87
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	9	0.96	0.51	0.86
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD23	9	0.95	0.49	0.78
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD22	9	0.95	0.49	0.78
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD21	9	0.95	0.49	0.78
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD11	9	0.93	0.36	0.92
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD12	9	0.93	0.36	0.92
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD13	9	0.93	0.36	0.92
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD11	9	0.92	0.31	0.9
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD12	9	0.92	0.31	0.9
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD13	9	0.92	0.31	0.9
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD23	9	0.91	0.56	0.77
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD22	9	0.91	0.56	0.77
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD21	9	0.91	0.56	0.77
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	9	0.84	0.21	0.77
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	9	0.84	0.21	0.75
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	9	0.83	0.33	0.71
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	9	0.81	0.32	0.8
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	9	0.8	0.34	0.68
(2,1146)	1:39:B:LEU:HD11	1:16:B:ALA:HB1	9	0.79	0.23	0.85
(2,1146)	1:39:B:LEU:HD11	1:16:B:ALA:HB3	9	0.79	0.23	0.85

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1146)	1:39:B:LEU:HD13	1:16:B:ALA:HB1	9	0.79	0.23	0.85
(2,1146)	1:39:B:LEU:HD12	1:16:B:ALA:HB1	9	0.79	0.23	0.85
(2,1146)	1:39:B:LEU:HD12	1:16:B:ALA:HB2	9	0.79	0.23	0.85
(2,1146)	1:39:B:LEU:HD11	1:16:B:ALA:HB2	9	0.79	0.23	0.85
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	9	0.79	0.32	0.8
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	9	0.78	0.16	0.73
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	9	0.78	0.16	0.73
(2,1145)	1:39:A:LEU:HD11	1:16:A:ALA:HB1	9	0.78	0.23	0.84
(2,1145)	1:39:A:LEU:HD11	1:16:A:ALA:HB3	9	0.78	0.23	0.84
(2,1145)	1:39:A:LEU:HD13	1:16:A:ALA:HB1	9	0.78	0.23	0.84
(2,1145)	1:39:A:LEU:HD12	1:16:A:ALA:HB1	9	0.78	0.23	0.84
(2,1145)	1:39:A:LEU:HD12	1:16:A:ALA:HB2	9	0.78	0.23	0.84
(2,1145)	1:39:A:LEU:HD11	1:16:A:ALA:HB2	9	0.78	0.23	0.84
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	9	0.74	0.28	0.64
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	9	0.72	0.29	0.62
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	9	0.67	0.25	0.7
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	9	0.66	0.28	0.69
(2,1166)	1:46:B:ILE:HD11	1:36:B:SER:H	9	0.62	0.28	0.57
(2,1166)	1:46:B:ILE:HD12	1:36:B:SER:H	9	0.62	0.28	0.57
(2,1166)	1:46:B:ILE:HD13	1:36:B:SER:H	9	0.62	0.28	0.57
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	9	0.6	0.16	0.65
(2,1165)	1:46:A:ILE:HD11	1:36:A:SER:H	9	0.6	0.23	0.62
(2,1165)	1:46:A:ILE:HD12	1:36:A:SER:H	9	0.6	0.23	0.62
(2,1165)	1:46:A:ILE:HD13	1:36:A:SER:H	9	0.6	0.23	0.62
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	9	0.6	0.16	0.65
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	9	0.53	0.21	0.54
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	9	0.5	0.19	0.48
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	9	0.49	0.06	0.48
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	9	0.49	0.07	0.51
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	9	0.49	0.24	0.47
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	9	0.49	0.49	0.3
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	9	0.47	0.24	0.34
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE1	9	0.42	0.05	0.42
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE2	9	0.42	0.05	0.42
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE1	9	0.42	0.05	0.43
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE2	9	0.42	0.05	0.43
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	9	0.41	0.02	0.41
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	9	0.41	0.02	0.41
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	9	0.38	0.18	0.36
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	9	0.37	0.19	0.31
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	9	0.36	0.18	0.32
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	9	0.36	0.17	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD22	9	0.36	0.03	0.35
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD23	9	0.36	0.03	0.35
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD21	9	0.36	0.03	0.35
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD22	9	0.35	0.03	0.35
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD23	9	0.35	0.03	0.35
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD21	9	0.35	0.03	0.35
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	9	0.26	0.06	0.26
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	9	0.25	0.06	0.26
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	9	0.24	0.0	0.24
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	9	0.24	0.0	0.24
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	9	0.24	0.1	0.24
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	9	0.24	0.09	0.25
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	9	0.23	0.05	0.24
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	9	0.23	0.05	0.24
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	9	0.18	0.11	0.13
(2,1511)	1:39:A:LEU:HD21	1:39:A:LEU:HA	9	0.17	0.04	0.17
(2,1511)	1:39:A:LEU:HD22	1:39:A:LEU:HA	9	0.17	0.04	0.17
(2,1511)	1:39:A:LEU:HD23	1:39:A:LEU:HA	9	0.17	0.04	0.17
(2,1110)	1:41:B:LEU:HD11	1:41:B:LEU:HD22	9	0.14	0.01	0.14
(2,1110)	1:41:B:LEU:HD12	1:41:B:LEU:HD23	9	0.14	0.01	0.14
(2,1110)	1:41:B:LEU:HD11	1:41:B:LEU:HD23	9	0.14	0.01	0.14
(2,1110)	1:41:B:LEU:HD13	1:41:B:LEU:HD21	9	0.14	0.01	0.14
(2,164)	1:19:B:LEU:HD21	1:24:A:ASP:HB2	8	2.27	0.83	2.24
(2,164)	1:19:B:LEU:HD23	1:24:A:ASP:HB2	8	2.27	0.83	2.24
(2,164)	1:19:B:LEU:HD22	1:46:A:ILE:HB	8	2.27	0.83	2.24
(2,164)	1:19:B:LEU:HD23	1:46:A:ILE:HB	8	2.27	0.83	2.24
(2,163)	1:19:A:LEU:HD21	1:24:B:ASP:HB2	8	2.21	0.73	2.2
(2,163)	1:19:A:LEU:HD23	1:24:B:ASP:HB2	8	2.21	0.73	2.2
(2,163)	1:19:A:LEU:HD22	1:46:B:ILE:HB	8	2.21	0.73	2.2
(2,163)	1:19:A:LEU:HD23	1:46:B:ILE:HB	8	2.21	0.73	2.2
(2,439)	1:20:A:ALA:HB2	1:20:B:ALA:HB2	8	2.11	1.51	2.56
(2,439)	1:20:A:ALA:HB1	1:20:B:ALA:HB1	8	2.11	1.51	2.56
(2,439)	1:20:A:ALA:HB3	1:20:B:ALA:HB3	8	2.11	1.51	2.56
(2,440)	1:20:B:ALA:HB2	1:20:A:ALA:HB2	8	2.11	1.51	2.56
(2,440)	1:20:B:ALA:HB1	1:20:A:ALA:HB1	8	2.11	1.51	2.56
(2,440)	1:20:B:ALA:HB3	1:20:A:ALA:HB3	8	2.11	1.51	2.56
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	8	1.6	0.9	1.54
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	8	1.59	0.88	1.56
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	8	1.58	0.46	1.56
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	8	1.57	0.44	1.56
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	8	1.5	1.18	1.47
(2,1394)	1:46:B:ILE:HD11	1:36:B:SER:HG	8	1.47	0.65	1.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1394)	1:46:B:ILE:HD12	1:36:B:SER:HG	8	1.47	0.65	1.65
(2,1394)	1:46:B:ILE:HD13	1:36:B:SER:HG	8	1.47	0.65	1.65
(2,1393)	1:46:A:ILE:HD11	1:36:A:SER:HG	8	1.42	0.6	1.61
(2,1393)	1:46:A:ILE:HD12	1:36:A:SER:HG	8	1.42	0.6	1.61
(2,1393)	1:46:A:ILE:HD13	1:36:A:SER:HG	8	1.42	0.6	1.61
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	8	1.39	0.93	1.46
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG22	8	1.39	0.46	1.56
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG23	8	1.39	0.46	1.56
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG21	8	1.39	0.46	1.56
(2,253)	1:27:A:LEU:HD11	1:32:A:ARG:HB2	8	1.38	0.31	1.38
(2,253)	1:27:A:LEU:HD12	1:32:A:ARG:HB2	8	1.38	0.31	1.38
(2,253)	1:27:A:LEU:HD13	1:32:A:ARG:HB2	8	1.38	0.31	1.38
(2,253)	1:27:A:LEU:HD12	1:51:A:ARG:HB3	8	1.38	0.31	1.38
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	8	1.37	0.74	1.08
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG22	8	1.37	0.5	1.57
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG23	8	1.37	0.5	1.57
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG21	8	1.37	0.5	1.57
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	8	1.37	0.74	1.08
(2,254)	1:27:B:LEU:HD11	1:32:B:ARG:HB2	8	1.35	0.32	1.35
(2,254)	1:27:B:LEU:HD12	1:32:B:ARG:HB2	8	1.35	0.32	1.35
(2,254)	1:27:B:LEU:HD11	1:51:B:ARG:HB3	8	1.35	0.32	1.35
(2,254)	1:27:B:LEU:HD13	1:32:B:ARG:HB2	8	1.35	0.32	1.35
(2,254)	1:27:B:LEU:HD12	1:51:B:ARG:HB3	8	1.35	0.32	1.35
(2,236)	1:46:B:ILE:HG21	1:9:B:PHE:HD2	8	1.34	0.25	1.26
(2,236)	1:46:B:ILE:HG23	1:9:B:PHE:HD2	8	1.34	0.25	1.26
(2,236)	1:46:B:ILE:HG22	1:9:B:PHE:HD2	8	1.34	0.25	1.26
(2,236)	1:46:B:ILE:HG22	1:50:B:PHE:HZ	8	1.34	0.25	1.26
(2,235)	1:46:A:ILE:HG21	1:9:A:PHE:HD2	8	1.33	0.25	1.27
(2,235)	1:46:A:ILE:HG23	1:9:A:PHE:HD2	8	1.33	0.25	1.27
(2,235)	1:46:A:ILE:HG22	1:9:A:PHE:HD2	8	1.33	0.25	1.27
(2,235)	1:46:A:ILE:HG22	1:50:A:PHE:HZ	8	1.33	0.25	1.27
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD1	8	1.24	0.31	1.12
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD2	8	1.24	0.31	1.12
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD1	8	1.23	0.28	1.12
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD2	8	1.23	0.28	1.12
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	8	1.22	0.48	1.23
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD23	8	1.21	0.76	1.08
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD22	8	1.21	0.76	1.08
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD21	8	1.21	0.76	1.08
(2,1636)	1:41:B:LEU:HD13	1:13:B:GLN:HG2	8	1.2	0.62	1.31
(2,1636)	1:41:B:LEU:HD12	1:13:B:GLN:HG2	8	1.2	0.62	1.31
(2,1636)	1:41:B:LEU:HD11	1:13:B:GLN:HG2	8	1.2	0.62	1.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1635)	1:41:A:LEU:HD13	1:13:A:GLN:HG2	8	1.2	0.62	1.28
(2,1635)	1:41:A:LEU:HD12	1:13:A:GLN:HG2	8	1.2	0.62	1.28
(2,1635)	1:41:A:LEU:HD11	1:13:A:GLN:HG2	8	1.2	0.62	1.28
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD23	8	1.19	0.77	1.1
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD22	8	1.19	0.77	1.1
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD21	8	1.19	0.77	1.1
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	8	1.18	0.49	1.27
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	8	1.16	0.8	0.96
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	8	1.16	0.78	0.97
(2,468)	1:19:B:LEU:HD22	1:35:A:LEU:HB2	8	1.16	0.93	0.94
(2,468)	1:19:B:LEU:HD21	1:35:A:LEU:HB2	8	1.16	0.93	0.94
(2,468)	1:19:B:LEU:HD23	1:35:A:LEU:HB2	8	1.16	0.93	0.94
(2,467)	1:19:A:LEU:HD22	1:35:B:LEU:HB2	8	1.08	0.84	0.89
(2,467)	1:19:A:LEU:HD21	1:35:B:LEU:HB2	8	1.08	0.84	0.89
(2,467)	1:19:A:LEU:HD23	1:35:B:LEU:HB2	8	1.08	0.84	0.89
(2,351)	1:4:A:ARG:H	1:12:A:GLU:HG3	8	1.06	0.4	1.1
(2,351)	1:4:A:ARG:H	1:12:B:GLU:HG3	8	1.06	0.4	1.1
(2,351)	1:4:A:ARG:H	1:5:A:PRO:HB2	8	1.06	0.4	1.1
(2,352)	1:4:B:ARG:H	1:12:B:GLU:HG3	8	1.04	0.42	1.11
(2,352)	1:4:B:ARG:H	1:12:A:GLU:HG3	8	1.04	0.42	1.11
(2,352)	1:4:B:ARG:H	1:5:B:PRO:HB2	8	1.04	0.42	1.11
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	8	1.03	0.59	0.89
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	8	0.99	0.6	0.82
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD12	8	0.95	0.52	1.04
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD11	8	0.95	0.52	1.04
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD13	8	0.95	0.52	1.04
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	8	0.94	0.39	0.78
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	8	0.94	0.39	0.78
(2,181)	1:16:A:ALA:HB2	1:15:B:LYS:HB3	8	0.93	0.52	0.86
(2,181)	1:16:A:ALA:HB1	1:15:B:LYS:HB3	8	0.93	0.52	0.86
(2,181)	1:16:A:ALA:HB3	1:15:A:LYS:HB3	8	0.93	0.52	0.86
(2,181)	1:16:A:ALA:HB1	1:15:A:LYS:HB3	8	0.93	0.52	0.86
(2,181)	1:16:A:ALA:HB3	1:15:B:LYS:HB3	8	0.93	0.52	0.86
(2,182)	1:16:B:ALA:HB2	1:15:A:LYS:HB3	8	0.93	0.52	0.86
(2,182)	1:16:B:ALA:HB1	1:15:A:LYS:HB3	8	0.93	0.52	0.86
(2,182)	1:16:B:ALA:HB3	1:15:B:LYS:HB3	8	0.93	0.52	0.86
(2,182)	1:16:B:ALA:HB1	1:15:B:LYS:HB3	8	0.93	0.52	0.86
(2,182)	1:16:B:ALA:HB3	1:15:A:LYS:HB3	8	0.93	0.52	0.86
(2,2435)	1:27:A:LEU:HD12	1:47:A:GLU:H	8	0.92	0.52	0.82
(2,2435)	1:27:A:LEU:HD13	1:47:A:GLU:H	8	0.92	0.52	0.82
(2,2435)	1:27:A:LEU:HD11	1:47:A:GLU:H	8	0.92	0.52	0.82
(2,2436)	1:27:B:LEU:HD12	1:47:B:GLU:H	8	0.92	0.53	0.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2436)	1:27:B:LEU:HD13	1:47:B:GLU:H	8	0.92	0.53	0.84
(2,2436)	1:27:B:LEU:HD11	1:47:B:GLU:H	8	0.92	0.53	0.84
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	8	0.91	0.6	0.6
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD12	8	0.89	0.46	1.02
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD11	8	0.89	0.46	1.02
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD13	8	0.89	0.46	1.02
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	8	0.88	0.6	0.6
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	8	0.83	0.34	0.89
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	8	0.81	0.42	0.77
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	8	0.8	0.34	0.9
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	8	0.78	0.41	0.82
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB2	8	0.76	0.28	0.67
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB3	8	0.76	0.28	0.67
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB2	8	0.75	0.29	0.66
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB3	8	0.75	0.29	0.66
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	8	0.73	0.75	0.4
(2,94)	1:32:B:ARG:HD2	1:34:B:TYR:H	8	0.71	0.21	0.75
(2,94)	1:32:B:ARG:HD3	1:45:B:GLN:H	8	0.71	0.21	0.75
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD11	8	0.69	0.32	0.72
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD12	8	0.69	0.32	0.72
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD13	8	0.69	0.32	0.72
(2,10)	1:16:B:ALA:HB3	1:15:A:LYS:HD3	8	0.67	0.53	0.57
(2,10)	1:16:B:ALA:HB1	1:15:A:LYS:HD3	8	0.67	0.53	0.57
(2,10)	1:16:B:ALA:HB2	1:15:A:LYS:HD3	8	0.67	0.53	0.57
(2,10)	1:16:B:ALA:HB1	1:39:A:LEU:HB2	8	0.67	0.53	0.57
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	8	0.66	0.36	0.75
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD11	8	0.66	0.31	0.72
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD12	8	0.66	0.31	0.72
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD13	8	0.66	0.31	0.72
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD12	8	0.64	0.31	0.65
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD11	8	0.64	0.31	0.65
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD13	8	0.64	0.31	0.65
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	8	0.62	0.3	0.63
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	8	0.61	0.29	0.63
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	8	0.58	0.11	0.62
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	8	0.58	0.12	0.6
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD12	8	0.57	0.28	0.44
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD11	8	0.57	0.28	0.44
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD13	8	0.57	0.28	0.44
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	8	0.53	0.21	0.58
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	8	0.53	0.21	0.58
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	8	0.51	0.48	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	8	0.51	0.48	0.32
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	8	0.49	0.22	0.46
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	8	0.49	0.01	0.49
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	8	0.49	0.23	0.45
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	8	0.49	0.01	0.49
(2,149)	1:33:A:ARG:HG3	1:34:A:TYR:HA	8	0.47	0.13	0.54
(2,149)	1:51:A:ARG:HG3	1:51:A:ARG:HA	8	0.47	0.13	0.54
(2,150)	1:33:B:ARG:HG3	1:34:B:TYR:HA	8	0.47	0.14	0.55
(2,150)	1:51:B:ARG:HG3	1:51:B:ARG:HA	8	0.47	0.14	0.55
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	8	0.44	0.01	0.44
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	8	0.44	0.01	0.44
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	8	0.32	0.09	0.34
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	8	0.31	0.08	0.31
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	8	0.31	0.06	0.34
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	8	0.3	0.06	0.34
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD12	8	0.23	0.07	0.21
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD11	8	0.23	0.07	0.21
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD13	8	0.23	0.07	0.21
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD12	8	0.23	0.07	0.2
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD11	8	0.23	0.07	0.2
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD13	8	0.23	0.07	0.2
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	8	0.21	0.04	0.22
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	8	0.21	0.04	0.22
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	8	0.19	0.11	0.14
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	8	0.19	0.01	0.19
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	8	0.18	0.01	0.18
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	8	0.18	0.14	0.11
(2,1512)	1:39:B:LEU:HD21	1:39:B:LEU:HA	8	0.18	0.03	0.18
(2,1512)	1:39:B:LEU:HD22	1:39:B:LEU:HA	8	0.18	0.03	0.18
(2,1512)	1:39:B:LEU:HD23	1:39:B:LEU:HA	8	0.18	0.03	0.18
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	8	0.17	0.06	0.15
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	8	0.17	0.06	0.15
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	8	0.16	0.01	0.16
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	8	0.16	0.01	0.16
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG22	7	1.87	0.83	1.91
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG21	7	1.87	0.83	1.91
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG23	7	1.87	0.83	1.91
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG22	7	1.87	0.81	2.01
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG21	7	1.87	0.81	2.01
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG23	7	1.87	0.81	2.01
(2,1245)	1:20:A:ALA:HB3	1:50:A:PHE:HE1	7	1.56	1.01	1.72
(2,1245)	1:20:A:ALA:HB2	1:50:A:PHE:HE1	7	1.56	1.01	1.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1245)	1:20:A:ALA:HB1	1:50:A:PHE:HE1	7	1.56	1.01	1.72
(2,1246)	1:20:B:ALA:HB3	1:50:B:PHE:HE1	7	1.55	0.96	1.73
(2,1246)	1:20:B:ALA:HB2	1:50:B:PHE:HE1	7	1.55	0.96	1.73
(2,1246)	1:20:B:ALA:HB1	1:50:B:PHE:HE1	7	1.55	0.96	1.73
(2,462)	1:49:B:TRP:HD1	1:14:B:LYS:HE3	7	1.2	0.65	0.95
(2,461)	1:49:A:TRP:HD1	1:14:A:LYS:HE3	7	1.17	0.65	0.95
(2,1496)	1:61:B:HIS:HA	1:54:B:GLU:HB2	7	1.16	1.07	0.89
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD21	7	1.1	0.38	0.99
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD22	7	1.1	0.38	0.99
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD23	7	1.1	0.38	0.99
(2,2255)	1:64:A:PHE:H	1:61:A:HIS:HA	7	1.06	0.31	1.02
(2,1948)	1:61:B:HIS:H	1:60:B:SER:HG	7	1.05	0.37	1.18
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD21	7	1.05	0.42	0.99
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD22	7	1.05	0.42	0.99
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD23	7	1.05	0.42	0.99
(2,1947)	1:61:A:HIS:H	1:60:A:SER:HG	7	1.05	0.37	1.17
(2,2256)	1:64:B:PHE:H	1:61:B:HIS:HA	7	1.04	0.33	1.03
(2,1332)	1:27:B:LEU:HD21	1:50:B:PHE:H	7	1.01	0.88	0.71
(2,1332)	1:27:B:LEU:HD22	1:50:B:PHE:H	7	1.01	0.88	0.71
(2,1332)	1:27:B:LEU:HD23	1:50:B:PHE:H	7	1.01	0.88	0.71
(2,1678)	1:30:B:GLU:HA	1:33:B:ARG:HD3	7	1.0	0.79	0.78
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG22	7	0.99	0.67	1.14
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG21	7	0.99	0.67	1.14
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG23	7	0.99	0.67	1.14
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG22	7	0.98	0.64	1.16
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG21	7	0.98	0.64	1.16
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG23	7	0.98	0.64	1.16
(2,1331)	1:27:A:LEU:HD21	1:50:A:PHE:H	7	0.97	0.93	0.48
(2,1331)	1:27:A:LEU:HD22	1:50:A:PHE:H	7	0.97	0.93	0.48
(2,1331)	1:27:A:LEU:HD23	1:50:A:PHE:H	7	0.97	0.93	0.48
(2,1155)	1:57:A:ILE:HG22	1:58:A:GLY:H	7	0.97	0.43	0.84
(2,1155)	1:57:A:ILE:HG21	1:58:A:GLY:H	7	0.97	0.43	0.84
(2,1155)	1:57:A:ILE:HG23	1:58:A:GLY:H	7	0.97	0.43	0.84
(2,1156)	1:57:B:ILE:HG22	1:58:B:GLY:H	7	0.96	0.42	0.84
(2,1156)	1:57:B:ILE:HG21	1:58:B:GLY:H	7	0.96	0.42	0.84
(2,1156)	1:57:B:ILE:HG23	1:58:B:GLY:H	7	0.96	0.42	0.84
(2,1677)	1:30:A:GLU:HA	1:33:A:ARG:HD3	7	0.95	0.75	0.75
(3,154)	1:11:B:GLU:H	1:13:B:GLN:HG3	7	0.94	0.59	0.58
(3,153)	1:11:A:GLU:H	1:13:A:GLN:HG3	7	0.94	0.6	0.57
(2,1344)	1:41:B:LEU:HD12	1:17:B:LEU:HD23	7	0.87	0.46	0.94
(2,1344)	1:41:B:LEU:HD12	1:17:B:LEU:HD21	7	0.87	0.46	0.94
(2,1344)	1:41:B:LEU:HD12	1:17:B:LEU:HD22	7	0.87	0.46	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1344)	1:41:B:LEU:HD13	1:17:B:LEU:HD21	7	0.87	0.46	0.94
(2,1344)	1:41:B:LEU:HD11	1:17:B:LEU:HD22	7	0.87	0.46	0.94
(2,1344)	1:41:B:LEU:HD11	1:17:B:LEU:HD23	7	0.87	0.46	0.94
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE1	7	0.86	0.88	0.61
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE2	7	0.86	0.88	0.61
(2,19)	1:5:A:PRO:HA	1:4:A:ARG:HG3	7	0.85	0.65	0.77
(2,19)	1:5:A:PRO:HA	1:6:A:ARG:HG3	7	0.85	0.65	0.77
(3,92)	1:27:B:LEU:HA	1:50:B:PHE:HB3	7	0.85	0.41	0.79
(2,20)	1:5:B:PRO:HA	1:4:B:ARG:HG3	7	0.84	0.67	0.74
(2,20)	1:5:B:PRO:HA	1:6:B:ARG:HG3	7	0.84	0.67	0.74
(2,472)	1:19:B:LEU:HD23	1:19:A:LEU:HG	7	0.84	0.66	0.71
(2,472)	1:19:B:LEU:HD21	1:19:A:LEU:HG	7	0.84	0.66	0.71
(2,472)	1:19:B:LEU:HD22	1:19:A:LEU:HG	7	0.84	0.66	0.71
(2,1689)	1:9:A:PHE:HB3	1:14:A:LYS:HG3	7	0.84	0.53	0.73
(2,1901)	1:59:A:TRP:H	1:62:A:PRO:HD2	7	0.83	0.76	0.48
(2,1690)	1:9:B:PHE:HB3	1:14:B:LYS:HG3	7	0.82	0.54	0.7
(2,1343)	1:41:A:LEU:HD12	1:17:A:LEU:HD23	7	0.82	0.47	0.75
(2,1343)	1:41:A:LEU:HD12	1:17:A:LEU:HD21	7	0.82	0.47	0.75
(2,1343)	1:41:A:LEU:HD12	1:17:A:LEU:HD22	7	0.82	0.47	0.75
(2,1343)	1:41:A:LEU:HD13	1:17:A:LEU:HD21	7	0.82	0.47	0.75
(2,1343)	1:41:A:LEU:HD11	1:17:A:LEU:HD22	7	0.82	0.47	0.75
(2,1343)	1:41:A:LEU:HD11	1:17:A:LEU:HD23	7	0.82	0.47	0.75
(3,91)	1:27:A:LEU:HA	1:50:A:PHE:HB3	7	0.82	0.41	0.81
(2,162)	1:39:B:LEU:HG	1:13:B:GLN:H	7	0.77	0.33	0.93
(2,93)	1:32:A:ARG:HD2	1:34:A:TYR:H	7	0.74	0.22	0.81
(2,93)	1:32:A:ARG:HD3	1:45:A:GLN:H	7	0.74	0.22	0.81
(2,9)	1:16:A:ALA:HB3	1:15:B:LYS:HD3	7	0.74	0.51	0.54
(2,9)	1:16:A:ALA:HB1	1:15:B:LYS:HD3	7	0.74	0.51	0.54
(2,9)	1:16:A:ALA:HB2	1:15:B:LYS:HD3	7	0.74	0.51	0.54
(2,9)	1:16:A:ALA:HB1	1:39:B:LEU:HB2	7	0.74	0.51	0.54
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD22	7	0.7	0.58	0.38
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD21	7	0.7	0.58	0.38
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD23	7	0.7	0.58	0.38
(2,328)	1:35:B:LEU:H	1:27:B:LEU:HD23	7	0.7	0.58	0.38
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE1	7	0.7	0.54	0.59
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE2	7	0.7	0.54	0.59
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD22	7	0.69	0.65	0.39
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD21	7	0.69	0.65	0.39
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD23	7	0.69	0.65	0.39
(2,327)	1:35:A:LEU:H	1:27:A:LEU:HD23	7	0.69	0.65	0.39
(2,943)	1:54:A:GLU:HG2	1:21:A:PHE:HZ	7	0.69	0.99	0.24
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB1	7	0.65	0.26	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB3	7	0.65	0.26	0.62
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB2	7	0.65	0.26	0.62
(2,1651)	1:28:A:THR:HB	1:31:A:TRP:HB3	7	0.64	0.32	0.48
(2,1416)	1:46:B:ILE:HG22	1:32:B:ARG:H	7	0.63	0.39	0.58
(2,1416)	1:46:B:ILE:HG21	1:32:B:ARG:H	7	0.63	0.39	0.58
(2,1416)	1:46:B:ILE:HG23	1:32:B:ARG:H	7	0.63	0.39	0.58
(3,186)	1:13:B:GLN:H	1:17:B:LEU:H	7	0.63	0.18	0.75
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB1	7	0.63	0.25	0.63
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB3	7	0.63	0.25	0.63
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB2	7	0.63	0.25	0.63
(3,185)	1:13:A:GLN:H	1:17:A:LEU:H	7	0.62	0.19	0.75
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD21	7	0.6	0.29	0.64
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD22	7	0.6	0.29	0.64
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD23	7	0.6	0.29	0.64
(2,755)	1:43:A:GLU:HA	1:36:A:SER:HB2	7	0.59	0.52	0.35
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD21	7	0.59	0.54	0.23
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD22	7	0.59	0.54	0.23
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD23	7	0.59	0.54	0.23
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD21	7	0.58	0.27	0.59
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD22	7	0.58	0.27	0.59
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD23	7	0.58	0.27	0.59
(2,1696)	1:7:B:THR:HB	1:45:B:GLN:HB2	7	0.58	0.41	0.43
(2,1695)	1:7:A:THR:HB	1:45:A:GLN:HB2	7	0.58	0.4	0.4
(2,2321)	1:6:A:ARG:H	1:5:A:PRO:HB3	7	0.58	0.32	0.52
(3,158)	1:16:B:ALA:H	1:17:B:LEU:HG	7	0.58	0.19	0.47
(2,1553)	1:27:A:LEU:HB3	1:50:A:PHE:HB2	7	0.58	0.35	0.57
(2,2322)	1:6:B:ARG:H	1:5:B:PRO:HB3	7	0.58	0.32	0.51
(3,157)	1:16:A:ALA:H	1:17:A:LEU:HG	7	0.55	0.22	0.46
(2,1415)	1:46:A:ILE:HG22	1:32:A:ARG:H	7	0.55	0.39	0.42
(2,1415)	1:46:A:ILE:HG21	1:32:A:ARG:H	7	0.55	0.39	0.42
(2,1415)	1:46:A:ILE:HG23	1:32:A:ARG:H	7	0.55	0.39	0.42
(2,1063)	1:27:A:LEU:HD22	1:43:A:GLU:HB3	7	0.53	0.33	0.57
(2,1063)	1:27:A:LEU:HD21	1:43:A:GLU:HB3	7	0.53	0.33	0.57
(2,944)	1:54:B:GLU:HG2	1:21:B:PHE:HZ	7	0.52	0.61	0.24
(3,100)	1:59:B:TRP:HB3	1:54:B:GLU:HA	7	0.5	0.27	0.46
(3,99)	1:59:A:TRP:HB3	1:54:A:GLU:HA	7	0.48	0.25	0.44
(2,1195)	1:16:A:ALA:HB1	1:13:A:GLN:HG2	7	0.47	0.28	0.5
(2,1195)	1:16:A:ALA:HB3	1:13:A:GLN:HG2	7	0.47	0.28	0.5
(2,1195)	1:16:A:ALA:HB2	1:13:A:GLN:HG2	7	0.47	0.28	0.5
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HE2	7	0.42	0.21	0.34
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HD2	7	0.42	0.21	0.34
(2,1064)	1:27:B:LEU:HD22	1:43:B:GLU:HB3	7	0.41	0.23	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1064)	1:27:B:LEU:HD21	1:43:B:GLU:HB3	7	0.41	0.23	0.33
(2,2215)	1:36:A:SER:HB2	1:36:A:SER:H	7	0.41	0.02	0.41
(2,55)	1:60:A:SER:HB3	1:61:A:HIS:H	7	0.41	0.06	0.44
(2,55)	1:60:A:SER:HB2	1:61:A:HIS:H	7	0.41	0.06	0.44
(2,56)	1:60:B:SER:HB3	1:61:B:HIS:H	7	0.41	0.05	0.44
(2,56)	1:60:B:SER:HB2	1:61:B:HIS:H	7	0.41	0.05	0.44
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HE2	7	0.4	0.2	0.33
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HD2	7	0.4	0.2	0.33
(2,2216)	1:36:B:SER:HB2	1:36:B:SER:H	7	0.4	0.02	0.4
(2,789)	1:16:A:ALA:HA	1:15:A:LYS:HB3	7	0.26	0.1	0.25
(2,548)	1:57:B:ILE:HA	1:57:B:ILE:HG13	7	0.26	0.21	0.16
(2,547)	1:57:A:ILE:HA	1:57:A:ILE:HG13	7	0.26	0.21	0.16
(2,1890)	1:49:B:TRP:H	1:48:B:ARG:HG3	7	0.24	0.04	0.24
(2,304)	1:59:B:TRP:H	1:62:B:PRO:HD3	7	0.23	0.12	0.2
(2,304)	1:59:B:TRP:H	1:60:B:SER:HB3	7	0.23	0.12	0.2
(2,1889)	1:49:A:TRP:H	1:48:A:ARG:HG3	7	0.23	0.04	0.23
(2,515)	1:62:A:PRO:HA	1:62:A:PRO:HB2	7	0.2	0.14	0.11
(2,590)	1:47:B:GLU:HA	1:46:B:ILE:HB	7	0.15	0.03	0.15
(2,589)	1:47:A:GLU:HA	1:46:A:ILE:HB	7	0.15	0.03	0.15
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG22	7	0.11	0.0	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG23	7	0.11	0.0	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG21	7	0.11	0.0	0.11
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG22	7	0.11	0.0	0.11
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG23	7	0.11	0.0	0.11
(2,104)	1:3:B:LYS:HE3	1:12:A:GLU:HG3	6	2.6	0.49	2.7
(2,104)	1:3:B:LYS:HE2	1:12:A:GLU:HG3	6	2.6	0.49	2.7
(2,104)	1:3:B:LYS:HE2	1:12:B:GLU:HG3	6	2.6	0.49	2.7
(2,103)	1:3:A:LYS:HE3	1:12:B:GLU:HG3	6	2.56	0.43	2.69
(2,103)	1:3:A:LYS:HE2	1:12:B:GLU:HG3	6	2.56	0.43	2.69
(2,103)	1:3:A:LYS:HE2	1:12:A:GLU:HG3	6	2.56	0.43	2.69
(2,438)	1:20:B:ALA:HB1	1:20:A:ALA:H	6	1.9	1.16	2.37
(2,438)	1:20:B:ALA:HB3	1:20:A:ALA:H	6	1.9	1.16	2.37
(2,438)	1:20:B:ALA:HB2	1:20:A:ALA:H	6	1.9	1.16	2.37
(2,437)	1:20:A:ALA:HB1	1:20:B:ALA:H	6	1.77	1.08	2.2
(2,437)	1:20:A:ALA:HB3	1:20:B:ALA:H	6	1.77	1.08	2.2
(2,437)	1:20:A:ALA:HB2	1:20:B:ALA:H	6	1.77	1.08	2.2
(3,1)	1:12:A:GLU:HB2	1:39:B:LEU:HA	6	1.57	0.61	1.54
(3,2)	1:12:B:GLU:HB2	1:39:A:LEU:HA	6	1.54	0.61	1.5
(2,260)	1:45:B:GLN:HG3	1:48:B:ARG:HD3	6	1.42	0.74	1.67
(2,260)	1:54:B:GLU:HG3	1:59:B:TRP:HB2	6	1.42	0.74	1.67
(2,260)	1:54:B:GLU:HG3	1:51:B:ARG:HD2	6	1.42	0.74	1.67
(2,259)	1:45:A:GLN:HG3	1:48:A:ARG:HD3	6	1.39	0.75	1.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,259)	1:54:A:GLU:HG3	1:59:A:TRP:HB2	6	1.39	0.75	1.67
(2,259)	1:54:A:GLU:HG3	1:51:A:ARG:HD2	6	1.39	0.75	1.67
(2,1235)	1:20:A:ALA:HB1	1:26:A:ARG:HD3	6	1.36	0.96	1.18
(2,1235)	1:20:A:ALA:HB3	1:26:A:ARG:HD3	6	1.36	0.96	1.18
(2,1235)	1:20:A:ALA:HB2	1:26:A:ARG:HD3	6	1.36	0.96	1.18
(2,1236)	1:20:B:ALA:HB1	1:26:B:ARG:HD3	6	1.32	0.85	1.19
(2,1236)	1:20:B:ALA:HB3	1:26:B:ARG:HD3	6	1.32	0.85	1.19
(2,1236)	1:20:B:ALA:HB2	1:26:B:ARG:HD3	6	1.32	0.85	1.19
(2,1495)	1:61:A:HIS:HA	1:54:A:GLU:HB2	6	1.31	1.06	0.92
(2,817)	1:62:A:PRO:HD2	1:60:A:SER:HG	6	1.24	0.8	1.43
(2,818)	1:62:B:PRO:HD2	1:60:B:SER:HG	6	1.23	0.78	1.4
(2,16)	1:36:B:SER:HB3	1:46:B:ILE:HD11	6	1.15	0.81	0.87
(2,16)	1:36:B:SER:HB3	1:46:B:ILE:HD13	6	1.15	0.81	0.87
(2,15)	1:36:A:SER:HB3	1:46:A:ILE:HD11	6	1.11	0.88	0.85
(2,15)	1:36:A:SER:HB3	1:46:A:ILE:HD13	6	1.11	0.88	0.85
(2,2103)	1:9:A:PHE:H	1:13:A:GLN:HG2	6	1.08	0.29	1.16
(2,2104)	1:9:B:PHE:H	1:13:B:GLN:HG2	6	1.06	0.3	1.15
(2,2306)	1:58:B:GLY:H	1:60:B:SER:HG	6	1.03	0.55	1.24
(2,2305)	1:58:A:GLY:H	1:60:A:SER:HG	6	1.03	0.55	1.23
(3,159)	1:43:A:GLU:H	1:44:A:GLU:HG2	6	1.0	0.07	1.0
(3,160)	1:43:B:GLU:H	1:44:B:GLU:HG2	6	1.0	0.07	1.0
(2,1909)	1:59:A:TRP:H	1:57:A:ILE:HG12	6	0.95	0.41	0.9
(2,1910)	1:59:B:TRP:H	1:57:B:ILE:HG12	6	0.95	0.38	0.9
(2,471)	1:19:A:LEU:HD23	1:19:B:LEU:HG	6	0.95	0.67	0.8
(2,471)	1:19:A:LEU:HD22	1:19:B:LEU:HG	6	0.95	0.67	0.8
(3,76)	1:57:B:ILE:HG12	1:61:B:HIS:HB2	6	0.88	0.46	0.98
(3,75)	1:57:A:ILE:HG12	1:61:A:HIS:HB2	6	0.87	0.48	0.96
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD22	6	0.86	0.51	0.64
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD21	6	0.86	0.51	0.64
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD23	6	0.86	0.51	0.64
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD22	6	0.86	0.51	0.65
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD21	6	0.86	0.51	0.65
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD23	6	0.86	0.51	0.65
(2,1335)	1:27:A:LEU:HD22	1:47:A:GLU:H	6	0.81	0.29	0.9
(2,1335)	1:27:A:LEU:HD21	1:47:A:GLU:H	6	0.81	0.29	0.9
(2,1335)	1:27:A:LEU:HD23	1:47:A:GLU:H	6	0.81	0.29	0.9
(3,191)	1:44:A:GLU:H	1:36:A:SER:HB2	6	0.77	0.47	0.76
(2,1336)	1:27:B:LEU:HD22	1:47:B:GLU:H	6	0.76	0.35	0.9
(2,1336)	1:27:B:LEU:HD21	1:47:B:GLU:H	6	0.76	0.35	0.9
(2,1336)	1:27:B:LEU:HD23	1:47:B:GLU:H	6	0.76	0.35	0.9
(2,203)	1:28:A:THR:HB	1:32:A:ARG:HB2	6	0.74	0.3	0.85
(2,203)	1:28:A:THR:HB	1:24:A:ASP:HB3	6	0.74	0.3	0.85

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,374)	1:56:B:GLN:H	1:57:B:ILE:HG13	6	0.73	0.47	0.68
(2,204)	1:28:B:THR:HB	1:32:B:ARG:HB2	6	0.73	0.31	0.84
(2,204)	1:28:B:THR:HB	1:24:B:ASP:HB3	6	0.73	0.31	0.84
(2,1652)	1:28:B:THR:HB	1:31:B:TRP:HB3	6	0.72	0.25	0.64
(2,662)	1:52:B:ARG:HA	1:55:B:GLN:HG2	6	0.72	0.25	0.68
(2,2071)	1:55:A:GLN:H	1:55:A:GLN:HB3	6	0.71	0.03	0.72
(2,661)	1:52:A:ARG:HA	1:55:A:GLN:HG2	6	0.71	0.24	0.68
(2,2072)	1:55:B:GLN:H	1:55:B:GLN:HB3	6	0.71	0.03	0.72
(2,373)	1:56:A:GLN:H	1:57:A:ILE:HG13	6	0.7	0.48	0.6
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD21	6	0.66	0.54	0.46
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD22	6	0.66	0.54	0.46
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD23	6	0.66	0.54	0.46
(2,382)	1:34:B:TYR:HD2	1:64:A:PHE:HD2	6	0.65	0.23	0.58
(2,382)	1:34:B:TYR:HD2	1:64:A:PHE:HD1	6	0.65	0.23	0.58
(2,382)	1:34:B:TYR:HD1	1:64:A:PHE:HD1	6	0.65	0.23	0.58
(2,382)	1:34:B:TYR:HD1	1:64:A:PHE:HD2	6	0.65	0.23	0.58
(2,1554)	1:27:B:LEU:HB3	1:50:B:PHE:HB2	6	0.64	0.33	0.7
(2,381)	1:34:A:TYR:HD2	1:64:B:PHE:HD2	6	0.62	0.22	0.55
(2,381)	1:34:A:TYR:HD2	1:64:B:PHE:HD1	6	0.62	0.22	0.55
(2,381)	1:34:A:TYR:HD1	1:64:B:PHE:HD1	6	0.62	0.22	0.55
(2,381)	1:34:A:TYR:HD1	1:64:B:PHE:HD2	6	0.62	0.22	0.55
(3,4)	1:12:B:GLU:HG3	1:12:A:GLU:HB2	6	0.62	0.47	0.42
(3,3)	1:12:A:GLU:HG3	1:12:B:GLU:HB2	6	0.6	0.47	0.36
(2,969)	1:55:A:GLN:HG2	1:55:A:GLN:HB3	6	0.58	0.01	0.59
(2,970)	1:55:B:GLN:HG2	1:55:B:GLN:HB3	6	0.58	0.01	0.59
(2,1850)	1:52:B:ARG:HB3	1:53:B:LYS:H	6	0.56	0.15	0.58
(2,896)	1:42:B:ASN:HB3	1:44:B:GLU:HB3	6	0.56	0.44	0.44
(2,1849)	1:52:A:ARG:HB3	1:53:A:LYS:H	6	0.55	0.15	0.56
(2,895)	1:42:A:ASN:HB3	1:44:A:GLU:HB3	6	0.55	0.44	0.44
(2,87)	1:48:A:ARG:HD3	1:45:A:GLN:HE21	6	0.55	0.42	0.4
(2,321)	1:54:A:GLU:H	1:52:A:ARG:HB2	6	0.54	0.31	0.49
(2,1995)	1:44:A:GLU:H	1:44:A:GLU:HG2	6	0.54	0.01	0.54
(2,1996)	1:44:B:GLU:H	1:44:B:GLU:HG2	6	0.54	0.01	0.54
(2,199)	1:20:A:ALA:HB2	1:17:A:LEU:HB3	6	0.53	0.29	0.48
(2,199)	1:20:A:ALA:HB1	1:17:A:LEU:HB3	6	0.53	0.29	0.48
(2,199)	1:20:A:ALA:HB3	1:17:A:LEU:HB3	6	0.53	0.29	0.48
(3,121)	1:14:A:LYS:HE3	1:49:A:TRP:HB2	6	0.53	0.33	0.48
(2,88)	1:48:B:ARG:HD3	1:45:B:GLN:HE21	6	0.53	0.4	0.38
(3,122)	1:14:B:LYS:HE3	1:49:B:TRP:HB2	6	0.53	0.34	0.46
(2,322)	1:54:B:GLU:H	1:52:B:ARG:HB2	6	0.53	0.29	0.5
(2,1196)	1:16:B:ALA:HB1	1:13:B:GLN:HG2	6	0.53	0.26	0.52
(2,1196)	1:16:B:ALA:HB3	1:13:B:GLN:HG2	6	0.53	0.26	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1196)	1:16:B:ALA:HB2	1:13:B:GLN:HG2	6	0.53	0.26	0.52
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG23	6	0.51	0.5	0.37
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG21	6	0.51	0.5	0.37
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG22	6	0.51	0.5	0.37
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG23	6	0.51	0.49	0.37
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG21	6	0.51	0.49	0.37
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG22	6	0.51	0.49	0.37
(2,688)	1:55:B:GLN:HA	1:55:B:GLN:HB2	6	0.45	0.0	0.45
(2,687)	1:55:A:GLN:HA	1:55:A:GLN:HB2	6	0.45	0.01	0.45
(3,77)	1:37:A:GLN:HB3	1:34:A:TYR:HB2	6	0.44	0.19	0.46
(2,124)	1:15:B:LYS:HB3	1:15:B:LYS:HE3	6	0.44	0.15	0.42
(2,124)	1:14:B:LYS:HB2	1:14:B:LYS:HE3	6	0.44	0.15	0.42
(2,123)	1:15:A:LYS:HB3	1:15:A:LYS:HE3	6	0.43	0.16	0.41
(2,123)	1:14:A:LYS:HB2	1:14:A:LYS:HE3	6	0.43	0.16	0.41
(3,78)	1:37:B:GLN:HB3	1:34:B:TYR:HB2	6	0.42	0.23	0.44
(2,332)	1:14:B:LYS:H	1:12:B:GLU:HA	6	0.39	0.16	0.34
(3,171)	1:17:A:LEU:H	1:14:A:LYS:HG3	6	0.38	0.3	0.28
(3,172)	1:17:B:LEU:H	1:14:B:LYS:HG3	6	0.38	0.3	0.28
(2,14)	1:36:B:SER:HB2	1:32:B:ARG:HB2	6	0.38	0.2	0.33
(2,14)	1:36:B:SER:HB2	1:45:B:GLN:HB2	6	0.38	0.2	0.33
(2,13)	1:36:A:SER:HB2	1:32:A:ARG:HB2	6	0.36	0.21	0.31
(2,13)	1:36:A:SER:HB2	1:45:A:GLN:HB2	6	0.36	0.21	0.31
(2,1087)	1:15:A:LYS:HG3	1:15:A:LYS:HE3	6	0.35	0.22	0.3
(2,1088)	1:15:B:LYS:HG3	1:15:B:LYS:HE3	6	0.35	0.22	0.3
(2,703)	1:64:A:PHE:HA	1:64:A:PHE:HD2	6	0.33	0.23	0.24
(2,703)	1:64:A:PHE:HA	1:64:A:PHE:HD1	6	0.33	0.23	0.24
(2,704)	1:64:B:PHE:HA	1:64:B:PHE:HD2	6	0.32	0.24	0.24
(2,704)	1:64:B:PHE:HA	1:64:B:PHE:HD1	6	0.32	0.24	0.24
(2,790)	1:16:B:ALA:HA	1:15:B:LYS:HB3	6	0.28	0.11	0.29
(2,1084)	1:15:B:LYS:HG3	1:15:B:LYS:HB3	6	0.26	0.02	0.28
(2,1083)	1:15:A:LYS:HG3	1:15:A:LYS:HB3	6	0.26	0.03	0.28
(2,303)	1:59:A:TRP:H	1:62:A:PRO:HD3	6	0.25	0.1	0.22
(2,303)	1:59:A:TRP:H	1:60:A:SER:HB3	6	0.25	0.1	0.22
(2,1466)	1:54:B:GLU:HB2	1:54:B:GLU:H	6	0.22	0.07	0.2
(2,1465)	1:54:A:GLU:HB2	1:54:A:GLU:H	6	0.22	0.07	0.2
(2,957)	1:54:A:GLU:HG2	1:54:A:GLU:HA	6	0.14	0.02	0.14
(2,958)	1:54:B:GLU:HG2	1:54:B:GLU:HA	6	0.14	0.02	0.14
(2,1445)	1:53:A:LYS:HB2	1:21:A:PHE:HZ	5	1.82	1.38	2.24
(2,89)	1:51:A:ARG:HD3	1:59:A:TRP:HD1	5	1.65	0.52	1.56
(2,89)	1:38:A:ARG:HD3	1:64:B:PHE:HD2	5	1.65	0.52	1.56
(2,89)	1:38:A:ARG:HD3	1:64:B:PHE:HD1	5	1.65	0.52	1.56
(2,90)	1:51:B:ARG:HD3	1:59:B:TRP:HD1	5	1.61	0.48	1.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,90)	1:38:B:ARG:HD3	1:64:A:PHE:HD2	5	1.61	0.48	1.57
(2,90)	1:38:B:ARG:HD3	1:64:A:PHE:HD1	5	1.61	0.48	1.57
(2,349)	1:27:A:LEU:H	1:32:A:ARG:HB2	5	1.43	1.26	0.86
(2,349)	1:27:A:LEU:H	1:24:A:ASP:HB3	5	1.43	1.26	0.86
(2,1648)	1:39:B:LEU:HD11	1:13:B:GLN:HG2	5	1.43	0.27	1.35
(2,1648)	1:39:B:LEU:HD12	1:13:B:GLN:HG2	5	1.43	0.27	1.35
(2,1647)	1:39:A:LEU:HD11	1:13:A:GLN:HG2	5	1.41	0.27	1.31
(2,1647)	1:39:A:LEU:HD12	1:13:A:GLN:HG2	5	1.41	0.27	1.31
(2,350)	1:27:B:LEU:H	1:32:B:ARG:HB2	5	1.4	1.23	0.86
(2,350)	1:27:B:LEU:H	1:24:B:ASP:HB3	5	1.4	1.23	0.86
(2,1588)	1:54:B:GLU:HB3	1:59:B:TRP:HB2	5	1.23	0.34	1.27
(2,1587)	1:54:A:GLU:HB3	1:59:A:TRP:HB2	5	1.21	0.32	1.28
(3,61)	1:27:A:LEU:HB2	1:21:A:PHE:H	5	1.15	0.56	0.9
(3,62)	1:27:B:LEU:HB2	1:21:B:PHE:H	5	1.12	0.46	0.93
(2,195)	1:18:A:ASP:HA	1:19:B:LEU:HD21	5	1.1	0.54	1.21
(2,195)	1:18:A:ASP:HA	1:53:A:LYS:HD2	5	1.1	0.54	1.21
(2,195)	1:18:A:ASP:HA	1:19:B:LEU:HD22	5	1.1	0.54	1.21
(3,168)	1:59:B:TRP:H	1:61:B:HIS:HB3	5	1.1	0.48	1.22
(2,196)	1:18:B:ASP:HA	1:19:A:LEU:HD21	5	1.1	0.51	1.21
(2,196)	1:18:B:ASP:HA	1:53:B:LYS:HD2	5	1.1	0.51	1.21
(2,196)	1:18:B:ASP:HA	1:19:A:LEU:HD22	5	1.1	0.51	1.21
(2,85)	1:6:A:ARG:HD3	1:4:A:ARG:HA	5	1.09	0.75	1.37
(2,85)	1:38:A:ARG:HD3	1:64:B:PHE:HA	5	1.09	0.75	1.37
(3,167)	1:59:A:TRP:H	1:61:A:HIS:HB3	5	1.09	0.49	1.22
(2,86)	1:6:B:ARG:HD3	1:4:B:ARG:HA	5	1.08	0.75	1.37
(2,86)	1:38:B:ARG:HD3	1:64:A:PHE:HA	5	1.08	0.75	1.37
(2,1601)	1:53:A:LYS:HG3	1:21:A:PHE:HZ	5	1.07	0.64	1.31
(2,1062)	1:27:B:LEU:HD21	1:50:B:PHE:HB3	5	1.05	0.71	0.95
(2,1062)	1:27:B:LEU:HD22	1:50:B:PHE:HB3	5	1.05	0.71	0.95
(2,1062)	1:27:B:LEU:HD23	1:50:B:PHE:HB3	5	1.05	0.71	0.95
(3,45)	1:6:A:ARG:HD3	1:8:A:GLU:HG3	5	1.02	0.83	0.59
(3,46)	1:6:B:ARG:HD3	1:8:B:GLU:HG3	5	1.01	0.83	0.58
(2,2167)	1:14:A:LYS:H	1:14:A:LYS:HD3	5	0.97	0.08	0.99
(2,2168)	1:14:B:LYS:H	1:14:B:LYS:HD3	5	0.96	0.08	0.98
(2,674)	1:8:B:GLU:HA	1:41:B:LEU:HB2	5	0.91	1.08	0.47
(2,673)	1:8:A:GLU:HA	1:41:A:LEU:HB2	5	0.9	1.08	0.48
(3,192)	1:44:B:GLU:H	1:36:B:SER:HB2	5	0.89	0.41	0.8
(2,1244)	1:20:B:ALA:HB2	1:35:B:LEU:HD12	5	0.89	0.46	1.09
(2,1244)	1:20:B:ALA:HB3	1:35:B:LEU:HD11	5	0.89	0.46	1.09
(2,1244)	1:20:B:ALA:HB1	1:35:B:LEU:HD11	5	0.89	0.46	1.09
(2,1244)	1:20:B:ALA:HB2	1:35:B:LEU:HD13	5	0.89	0.46	1.09
(2,1244)	1:20:B:ALA:HB2	1:35:B:LEU:HD11	5	0.89	0.46	1.09

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1243)	1:20:A:ALA:HB2	1:35:A:LEU:HD12	5	0.87	0.45	1.07
(2,1243)	1:20:A:ALA:HB3	1:35:A:LEU:HD11	5	0.87	0.45	1.07
(2,1243)	1:20:A:ALA:HB1	1:35:A:LEU:HD11	5	0.87	0.45	1.07
(2,1243)	1:20:A:ALA:HB2	1:35:A:LEU:HD13	5	0.87	0.45	1.07
(2,1243)	1:20:A:ALA:HB2	1:35:A:LEU:HD11	5	0.87	0.45	1.07
(1,6)	1:20:A:ALA:H	1:16:A:ALA:O	5	0.85	0.5	0.69
(2,2083)	1:14:A:LYS:H	1:9:A:PHE:HB3	5	0.83	0.37	1.03
(2,1602)	1:53:B:LYS:HG3	1:21:B:PHE:HZ	5	0.83	0.44	0.77
(2,2084)	1:14:B:LYS:H	1:9:B:PHE:HB3	5	0.81	0.36	0.94
(1,48)	1:20:B:ALA:H	1:16:B:ALA:O	5	0.78	0.41	0.69
(2,75)	1:25:A:ARG:HA	1:20:A:ALA:HA	5	0.74	0.52	0.58
(2,75)	1:65:A:GLU:HA	1:15:A:LYS:HA	5	0.74	0.52	0.58
(2,75)	1:3:A:LYS:HA	1:11:A:GLU:HA	5	0.74	0.52	0.58
(3,115)	1:3:A:LYS:HG3	1:1:A:MET:HA	5	0.73	0.63	0.47
(3,116)	1:3:B:LYS:HG3	1:1:B:MET:HA	5	0.73	0.62	0.47
(2,100)	1:51:B:ARG:HD3	1:55:B:GLN:HG3	5	0.7	0.48	0.68
(2,100)	1:51:B:ARG:HD2	1:55:B:GLN:HG3	5	0.7	0.48	0.68
(2,618)	1:12:B:GLU:HA	1:15:B:LYS:HE3	5	0.7	0.28	0.59
(2,317)	1:59:A:TRP:HB2	1:55:A:GLN:H	5	0.7	0.72	0.34
(3,95)	1:59:A:TRP:HB2	1:55:A:GLN:H	5	0.7	0.72	0.34
(2,318)	1:59:B:TRP:HB2	1:55:B:GLN:H	5	0.69	0.72	0.33
(3,96)	1:59:B:TRP:HB2	1:55:B:GLN:H	5	0.69	0.72	0.33
(2,617)	1:12:A:GLU:HA	1:15:A:LYS:HE3	5	0.68	0.27	0.54
(2,99)	1:51:A:ARG:HD3	1:55:A:GLN:HG3	5	0.68	0.48	0.68
(2,99)	1:51:A:ARG:HD2	1:55:A:GLN:HG3	5	0.68	0.48	0.68
(2,1895)	1:65:A:GLU:HB2	1:65:A:GLU:H	5	0.68	0.08	0.68
(2,1896)	1:65:B:GLU:HB2	1:65:B:GLU:H	5	0.68	0.09	0.68
(2,336)	1:15:B:LYS:H	1:15:B:LYS:HD3	5	0.67	0.31	0.71
(2,335)	1:15:A:LYS:H	1:15:A:LYS:HD3	5	0.65	0.3	0.71
(2,1547)	1:27:A:LEU:HB3	1:50:A:PHE:HD2	5	0.63	0.14	0.66
(2,1547)	1:27:A:LEU:HB3	1:50:A:PHE:HD1	5	0.63	0.14	0.66
(2,855)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	5	0.62	0.0	0.62
(2,856)	1:6:B:ARG:HD3	1:6:B:ARG:HG3	5	0.62	0.0	0.62
(2,1339)	1:27:A:LEU:HD21	1:46:A:ILE:H	5	0.6	0.42	0.49
(2,1339)	1:27:A:LEU:HD22	1:46:A:ILE:H	5	0.6	0.42	0.49
(2,1339)	1:27:A:LEU:HD23	1:46:A:ILE:H	5	0.6	0.42	0.49
(2,2006)	1:64:B:PHE:H	1:63:B:GLN:H	5	0.59	0.31	0.52
(2,1614)	1:16:B:ALA:HB2	1:35:B:LEU:HD11	5	0.57	0.31	0.47
(2,1614)	1:16:B:ALA:HB2	1:35:B:LEU:HD13	5	0.57	0.31	0.47
(2,1614)	1:16:B:ALA:HB1	1:35:B:LEU:HD13	5	0.57	0.31	0.47
(2,1614)	1:16:B:ALA:HB3	1:35:B:LEU:HD12	5	0.57	0.31	0.47
(2,1614)	1:16:B:ALA:HB3	1:35:B:LEU:HD11	5	0.57	0.31	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1613)	1:16:A:ALA:HB2	1:35:A:LEU:HD11	5	0.57	0.32	0.44
(2,1613)	1:16:A:ALA:HB2	1:35:A:LEU:HD13	5	0.57	0.32	0.44
(2,1613)	1:16:A:ALA:HB1	1:35:A:LEU:HD13	5	0.57	0.32	0.44
(2,1613)	1:16:A:ALA:HB3	1:35:A:LEU:HD12	5	0.57	0.32	0.44
(2,1613)	1:16:A:ALA:HB3	1:35:A:LEU:HD11	5	0.57	0.32	0.44
(2,2005)	1:64:A:PHE:H	1:63:A:GLN:H	5	0.56	0.33	0.51
(2,1548)	1:27:B:LEU:HB3	1:50:B:PHE:HD2	5	0.54	0.25	0.65
(2,1548)	1:27:B:LEU:HB3	1:50:B:PHE:HD1	5	0.54	0.25	0.65
(2,1608)	1:16:B:ALA:HB2	1:35:B:LEU:HD23	5	0.54	0.55	0.3
(2,1608)	1:16:B:ALA:HB3	1:35:B:LEU:HD23	5	0.54	0.55	0.3
(2,1608)	1:16:B:ALA:HB1	1:35:B:LEU:HD23	5	0.54	0.55	0.3
(2,1608)	1:16:B:ALA:HB3	1:35:B:LEU:HD22	5	0.54	0.55	0.3
(2,1340)	1:27:B:LEU:HD21	1:46:B:ILE:H	5	0.53	0.43	0.2
(2,1340)	1:27:B:LEU:HD22	1:46:B:ILE:H	5	0.53	0.43	0.2
(2,1340)	1:27:B:LEU:HD23	1:46:B:ILE:H	5	0.53	0.43	0.2
(2,1801)	1:65:A:GLU:H	1:64:A:PHE:HD1	5	0.49	0.23	0.47
(2,49)	1:49:A:TRP:HA	1:9:A:PHE:HE2	5	0.47	0.28	0.51
(2,49)	1:49:A:TRP:HA	1:9:A:PHE:HZ	5	0.47	0.28	0.51
(2,49)	1:49:A:TRP:HA	1:9:A:PHE:HE1	5	0.47	0.28	0.51
(2,1781)	1:66:A:LYS:H	1:65:A:GLU:HG2	5	0.47	0.17	0.56
(2,200)	1:20:B:ALA:HB3	1:17:B:LEU:HB3	5	0.45	0.33	0.27
(2,200)	1:20:B:ALA:HB2	1:17:B:LEU:HB3	5	0.45	0.33	0.27
(2,200)	1:20:B:ALA:HB1	1:17:B:LEU:HB3	5	0.45	0.33	0.27
(1,50)	1:34:B:TYR:H	1:30:B:GLU:O	5	0.45	0.29	0.39
(1,8)	1:34:A:TYR:H	1:30:A:GLU:O	5	0.45	0.28	0.39
(2,331)	1:14:A:LYS:H	1:12:A:GLU:HA	5	0.42	0.17	0.34
(2,2245)	1:66:A:LYS:H	1:64:A:PHE:H	5	0.41	0.17	0.46
(2,583)	1:32:A:ARG:HA	1:27:A:LEU:HD11	5	0.4	0.24	0.34
(2,583)	1:32:A:ARG:HA	1:27:A:LEU:HD13	5	0.4	0.24	0.34
(2,2277)	1:9:A:PHE:H	1:41:A:LEU:HA	5	0.4	0.19	0.45
(2,584)	1:32:B:ARG:HA	1:27:B:LEU:HD11	5	0.39	0.25	0.32
(2,584)	1:32:B:ARG:HA	1:27:B:LEU:HD13	5	0.39	0.25	0.32
(2,250)	1:13:B:GLN:HB3	1:9:B:PHE:HD1	5	0.39	0.06	0.35
(2,250)	1:13:B:GLN:HB3	1:41:B:LEU:H	5	0.39	0.06	0.35
(2,1851)	1:53:A:LYS:H	1:52:A:ARG:HG3	5	0.39	0.12	0.38
(2,2278)	1:9:B:PHE:H	1:41:B:LEU:HA	5	0.39	0.19	0.44
(2,1852)	1:53:B:LYS:H	1:52:B:ARG:HG3	5	0.39	0.11	0.38
(2,249)	1:13:A:GLN:HB3	1:9:A:PHE:HD1	5	0.38	0.08	0.34
(2,249)	1:13:A:GLN:HB3	1:41:A:LEU:H	5	0.38	0.08	0.34
(3,222)	1:54:B:GLU:H	1:52:B:ARG:HE	5	0.37	0.11	0.34
(2,2246)	1:66:B:LYS:H	1:64:B:PHE:H	5	0.37	0.17	0.32
(3,64)	1:8:B:GLU:HG3	1:45:B:GLN:HE22	5	0.35	0.19	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,221)	1:54:A:GLU:H	1:52:A:ARG:HE	5	0.32	0.1	0.31
(3,63)	1:8:A:GLU:HG3	1:45:A:GLN:HE22	5	0.31	0.21	0.3
(2,12)	1:36:B:SER:HB2	1:32:B:ARG:HB2	5	0.27	0.11	0.26
(2,12)	1:36:B:SER:HB3	1:45:B:GLN:HB2	5	0.27	0.11	0.26
(2,1446)	1:53:B:LYS:HB2	1:21:B:PHE:HZ	4	1.96	0.99	2.32
(2,1325)	1:40:A:GLY:HA3	1:4:A:ARG:HD3	4	1.82	0.81	1.83
(2,1326)	1:40:B:GLY:HA3	1:4:B:ARG:HD3	4	1.8	0.81	1.8
(2,1061)	1:27:A:LEU:HD22	1:50:A:PHE:HB3	4	1.27	0.74	1.32
(2,1061)	1:27:A:LEU:HD21	1:50:A:PHE:HB3	4	1.27	0.74	1.32
(2,1061)	1:27:A:LEU:HD23	1:50:A:PHE:HB3	4	1.27	0.74	1.32
(2,1605)	1:54:A:GLU:HB3	1:21:A:PHE:HZ	4	1.19	0.26	1.13
(3,68)	1:63:B:GLN:HG2	1:54:B:GLU:HA	4	1.13	0.55	1.14
(3,67)	1:63:A:GLN:HG2	1:54:A:GLU:HA	4	1.08	0.57	1.03
(2,1002)	1:44:B:GLU:HB3	1:45:B:GLN:H	4	0.98	0.24	1.0
(3,74)	1:39:B:LEU:HG	1:15:A:LYS:HE3	4	0.97	0.88	0.66
(2,1001)	1:44:A:GLU:HB3	1:45:A:GLN:H	4	0.97	0.25	0.98
(3,73)	1:39:A:LEU:HG	1:15:B:LYS:HE3	4	0.93	0.85	0.62
(2,76)	1:65:B:GLU:HA	1:15:B:LYS:HA	4	0.92	0.59	0.98
(2,76)	1:25:B:ARG:HA	1:20:B:ALA:HA	4	0.92	0.59	0.98
(2,76)	1:3:B:LYS:HA	1:11:B:GLU:HA	4	0.92	0.59	0.98
(2,107)	1:9:A:PHE:HB2	1:4:A:ARG:HB2	4	0.86	0.57	0.88
(2,107)	1:9:A:PHE:HB2	1:8:A:GLU:HB3	4	0.86	0.57	0.88
(2,108)	1:9:B:PHE:HB2	1:4:B:ARG:HB2	4	0.86	0.57	0.86
(2,108)	1:9:B:PHE:HB2	1:8:B:GLU:HB3	4	0.86	0.57	0.86
(2,1665)	1:57:A:ILE:HG12	1:60:A:SER:H	4	0.81	0.51	0.76
(2,1666)	1:57:B:ILE:HG12	1:60:B:SER:H	4	0.8	0.5	0.75
(1,1)	1:15:A:LYS:H	1:11:A:GLU:O	4	0.74	0.4	0.68
(3,181)	1:64:A:PHE:H	1:62:A:PRO:HB3	4	0.73	0.36	0.7
(2,807)	1:4:A:ARG:HA	1:4:A:ARG:HG3	4	0.73	0.09	0.75
(2,808)	1:4:B:ARG:HA	1:4:B:ARG:HG3	4	0.72	0.09	0.74
(2,1824)	1:8:B:GLU:H	1:9:B:PHE:HB3	4	0.72	0.15	0.66
(2,1823)	1:8:A:GLU:H	1:9:A:PHE:HB3	4	0.72	0.15	0.65
(1,43)	1:15:B:LYS:H	1:11:B:GLU:O	4	0.72	0.33	0.68
(2,637)	1:53:A:LYS:HA	1:53:A:LYS:HD2	4	0.7	0.31	0.55
(2,600)	1:50:B:PHE:HA	1:53:B:LYS:HB3	4	0.7	0.7	0.38
(2,599)	1:50:A:PHE:HA	1:53:A:LYS:HB3	4	0.7	0.72	0.36
(2,638)	1:53:B:LYS:HA	1:53:B:LYS:HD2	4	0.7	0.3	0.55
(2,177)	1:16:A:ALA:HB3	1:20:A:ALA:H	4	0.68	0.19	0.72
(2,177)	1:16:A:ALA:HB2	1:20:A:ALA:H	4	0.68	0.19	0.72
(3,182)	1:64:B:PHE:H	1:62:B:PRO:HB3	4	0.68	0.37	0.6
(2,2293)	1:60:A:SER:H	1:57:A:ILE:HG22	4	0.66	0.53	0.52
(2,2293)	1:60:A:SER:H	1:57:A:ILE:HG21	4	0.66	0.53	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2293)	1:60:A:SER:H	1:57:A:ILE:HG23	4	0.66	0.53	0.52
(2,1607)	1:16:A:ALA:HB3	1:35:A:LEU:HD23	4	0.66	0.63	0.36
(2,1607)	1:16:A:ALA:HB3	1:35:A:LEU:HD22	4	0.66	0.63	0.36
(2,1607)	1:16:A:ALA:HB2	1:35:A:LEU:HD23	4	0.66	0.63	0.36
(2,1607)	1:16:A:ALA:HB1	1:35:A:LEU:HD23	4	0.66	0.63	0.36
(2,477)	1:19:A:LEU:HD21	1:19:B:LEU:HA	4	0.66	0.64	0.38
(2,477)	1:19:A:LEU:HD22	1:19:B:LEU:HA	4	0.66	0.64	0.38
(2,2294)	1:60:B:SER:H	1:57:B:ILE:HG22	4	0.65	0.51	0.52
(2,2294)	1:60:B:SER:H	1:57:B:ILE:HG21	4	0.65	0.51	0.52
(2,2294)	1:60:B:SER:H	1:57:B:ILE:HG23	4	0.65	0.51	0.52
(2,43)	1:53:A:LYS:HA	1:53:A:LYS:HD3	4	0.65	0.24	0.65
(2,478)	1:19:B:LEU:HD21	1:19:A:LEU:HA	4	0.65	0.62	0.38
(2,478)	1:19:B:LEU:HD22	1:19:A:LEU:HA	4	0.65	0.62	0.38
(2,44)	1:53:B:LYS:HA	1:53:B:LYS:HD3	4	0.64	0.24	0.64
(2,178)	1:16:B:ALA:HB3	1:20:B:ALA:H	4	0.62	0.16	0.64
(2,178)	1:16:B:ALA:HB2	1:20:B:ALA:H	4	0.62	0.16	0.64
(2,873)	1:14:A:LYS:HE3	1:14:A:LYS:HG3	4	0.62	0.22	0.5
(2,874)	1:14:B:LYS:HE3	1:14:B:LYS:HG3	4	0.62	0.22	0.5
(2,528)	1:57:B:ILE:HA	1:57:B:ILE:HG23	4	0.6	0.28	0.54
(2,528)	1:57:B:ILE:HA	1:57:B:ILE:HG21	4	0.6	0.28	0.54
(2,528)	1:57:B:ILE:HA	1:57:B:ILE:HG22	4	0.6	0.28	0.54
(2,527)	1:57:A:ILE:HA	1:57:A:ILE:HG23	4	0.58	0.28	0.52
(2,527)	1:57:A:ILE:HA	1:57:A:ILE:HG21	4	0.58	0.28	0.52
(2,527)	1:57:A:ILE:HA	1:57:A:ILE:HG22	4	0.58	0.28	0.52
(2,50)	1:49:B:TRP:HA	1:9:B:PHE:HE1	4	0.58	0.21	0.62
(2,50)	1:49:B:TRP:HA	1:9:B:PHE:HZ	4	0.58	0.21	0.62
(2,50)	1:49:B:TRP:HA	1:9:B:PHE:HE2	4	0.58	0.21	0.62
(2,1804)	1:65:B:GLU:H	1:64:B:PHE:HB3	4	0.57	0.12	0.6
(2,1803)	1:65:A:GLU:H	1:64:A:PHE:HB3	4	0.57	0.12	0.6
(3,145)	1:4:A:ARG:H	1:12:A:GLU:H	4	0.56	0.1	0.57
(3,146)	1:4:B:ARG:H	1:12:B:GLU:H	4	0.56	0.11	0.56
(2,1514)	1:9:B:PHE:HA	1:17:B:LEU:HD22	4	0.56	0.23	0.54
(2,1514)	1:9:B:PHE:HA	1:17:B:LEU:HD23	4	0.56	0.23	0.54
(2,1514)	1:9:B:PHE:HA	1:17:B:LEU:HD21	4	0.56	0.23	0.54
(2,1123)	1:20:A:ALA:HB2	1:21:A:PHE:H	4	0.56	0.12	0.56
(2,1123)	1:20:A:ALA:HB1	1:21:A:PHE:H	4	0.56	0.12	0.56
(2,1123)	1:20:A:ALA:HB3	1:21:A:PHE:H	4	0.56	0.12	0.56
(2,119)	1:47:A:GLU:HG2	1:27:A:LEU:HD23	4	0.55	0.49	0.34
(2,119)	1:47:A:GLU:HG2	1:27:A:LEU:HD22	4	0.55	0.49	0.34
(2,119)	1:47:A:GLU:HG2	1:27:A:LEU:HD21	4	0.55	0.49	0.34
(2,1782)	1:66:B:LYS:H	1:65:B:GLU:HG2	4	0.55	0.03	0.56
(3,150)	1:2:B:GLU:H	1:4:B:ARG:HA	4	0.55	0.13	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,149)	1:2:A:GLU:H	1:4:A:ARG:HA	4	0.55	0.13	0.55
(2,105)	1:9:A:PHE:HB3	1:4:A:ARG:HB2	4	0.53	0.17	0.6
(2,105)	1:9:A:PHE:HB3	1:8:A:GLU:HB3	4	0.53	0.17	0.6
(2,1048)	1:57:B:ILE:HG13	1:57:B:ILE:H	4	0.53	0.29	0.46
(2,106)	1:9:B:PHE:HB3	1:4:B:ARG:HB2	4	0.52	0.17	0.59
(2,106)	1:9:B:PHE:HB3	1:8:B:GLU:HB3	4	0.52	0.17	0.59
(2,1210)	1:49:B:TRP:HB3	1:17:B:LEU:HD12	4	0.52	0.28	0.5
(2,1210)	1:49:B:TRP:HB3	1:17:B:LEU:HD13	4	0.52	0.28	0.5
(2,1513)	1:9:A:PHE:HA	1:17:A:LEU:HD22	4	0.52	0.27	0.52
(2,1513)	1:9:A:PHE:HA	1:17:A:LEU:HD23	4	0.52	0.27	0.52
(2,1513)	1:9:A:PHE:HA	1:17:A:LEU:HD21	4	0.52	0.27	0.52
(2,1124)	1:20:B:ALA:HB2	1:21:B:PHE:H	4	0.51	0.2	0.56
(2,1124)	1:20:B:ALA:HB1	1:21:B:PHE:H	4	0.51	0.2	0.56
(2,1124)	1:20:B:ALA:HB3	1:21:B:PHE:H	4	0.51	0.2	0.56
(2,1047)	1:57:A:ILE:HG13	1:57:A:ILE:H	4	0.5	0.32	0.46
(2,341)	1:60:A:SER:H	1:59:A:TRP:HA	4	0.5	0.1	0.47
(2,342)	1:60:B:SER:H	1:59:B:TRP:HA	4	0.5	0.09	0.46
(2,1209)	1:49:A:TRP:HB3	1:17:A:LEU:HD12	4	0.5	0.29	0.48
(2,1209)	1:49:A:TRP:HB3	1:17:A:LEU:HD13	4	0.5	0.29	0.48
(2,1474)	1:58:B:GLY:HA3	1:57:B:ILE:HB	4	0.48	0.2	0.53
(2,1473)	1:58:A:GLY:HA3	1:57:A:ILE:HB	4	0.47	0.19	0.52
(2,2128)	1:55:B:GLN:H	1:53:B:LYS:HB2	4	0.46	0.19	0.51
(2,2127)	1:55:A:GLN:H	1:53:A:LYS:HB2	4	0.45	0.19	0.5
(1,62)	1:56:B:GLN:H	1:52:B:ARG:O	4	0.44	0.17	0.42
(2,101)	1:19:A:LEU:HB3	1:16:A:ALA:HA	4	0.44	0.2	0.44
(2,101)	1:19:A:LEU:HB3	1:16:B:ALA:HA	4	0.44	0.2	0.44
(1,20)	1:56:A:GLN:H	1:52:A:ARG:O	4	0.44	0.16	0.42
(2,799)	1:42:A:ASN:HA	1:43:A:GLU:HG3	4	0.44	0.16	0.4
(2,800)	1:42:B:ASN:HA	1:43:B:GLU:HG3	4	0.44	0.17	0.4
(2,1193)	1:16:A:ALA:HB2	1:13:A:GLN:HB3	4	0.43	0.29	0.44
(2,1193)	1:16:A:ALA:HB3	1:13:A:GLN:HB3	4	0.43	0.29	0.44
(2,1193)	1:16:A:ALA:HB1	1:13:A:GLN:HB3	4	0.43	0.29	0.44
(2,1927)	1:6:A:ARG:H	1:6:A:ARG:HG3	4	0.42	0.15	0.4
(2,1928)	1:6:B:ARG:H	1:6:B:ARG:HG3	4	0.42	0.16	0.4
(2,102)	1:19:B:LEU:HB3	1:16:B:ALA:HA	4	0.42	0.21	0.4
(2,102)	1:19:B:LEU:HB3	1:16:A:ALA:HA	4	0.42	0.21	0.4
(2,1802)	1:65:B:GLU:H	1:64:B:PHE:HD1	4	0.36	0.12	0.4
(2,353)	1:47:A:GLU:H	1:45:A:GLN:HB3	4	0.35	0.09	0.36
(2,353)	1:47:A:GLU:H	1:44:A:GLU:HG3	4	0.35	0.09	0.36
(2,1943)	1:61:A:HIS:HB3	1:61:A:HIS:H	4	0.34	0.09	0.34
(2,354)	1:47:B:GLU:H	1:45:B:GLN:HB3	4	0.34	0.08	0.34
(2,354)	1:47:B:GLU:H	1:44:B:GLU:HG3	4	0.34	0.08	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1944)	1:61:B:HIS:HB3	1:61:B:HIS:H	4	0.34	0.09	0.34
(2,11)	1:36:A:SER:HB2	1:32:A:ARG:HB2	4	0.31	0.09	0.28
(2,11)	1:36:A:SER:HB3	1:45:A:GLN:HB2	4	0.31	0.09	0.28
(2,1853)	1:16:A:ALA:H	1:15:A:LYS:HB3	4	0.3	0.2	0.27
(2,186)	1:17:B:LEU:HD22	1:50:B:PHE:HA	4	0.28	0.17	0.22
(2,186)	1:17:B:LEU:HD21	1:50:B:PHE:HA	4	0.28	0.17	0.22
(3,120)	1:9:B:PHE:HB3	1:45:B:GLN:HA	4	0.26	0.1	0.28
(2,449)	1:9:A:PHE:HD1	1:10:A:SER:H	4	0.24	0.03	0.26
(2,450)	1:9:B:PHE:HD1	1:10:B:SER:H	4	0.24	0.04	0.25
(3,118)	1:39:B:LEU:HG	1:9:B:PHE:H	4	0.24	0.07	0.26
(3,117)	1:39:A:LEU:HG	1:9:A:PHE:H	4	0.23	0.07	0.22
(2,2105)	1:54:A:GLU:HB3	1:54:A:GLU:H	4	0.22	0.03	0.24
(2,2106)	1:54:B:GLU:HB3	1:54:B:GLU:H	4	0.22	0.03	0.24
(2,185)	1:17:A:LEU:HD22	1:50:A:PHE:HA	4	0.2	0.09	0.19
(2,185)	1:17:A:LEU:HD21	1:50:A:PHE:HA	4	0.2	0.09	0.19
(2,274)	1:44:B:GLU:HA	1:48:B:ARG:HD3	4	0.17	0.03	0.17
(2,273)	1:44:A:GLU:HA	1:48:A:ARG:HD3	4	0.16	0.01	0.16
(2,1509)	1:65:A:GLU:HG2	1:65:A:GLU:HA	4	0.14	0.02	0.14
(2,647)	1:53:A:LYS:HA	1:63:A:GLN:HG3	3	1.79	0.72	2.29
(2,648)	1:53:B:LYS:HA	1:63:B:GLN:HG3	3	1.77	0.71	2.24
(2,778)	1:9:B:PHE:HA	1:4:B:ARG:HB2	3	1.54	1.03	1.99
(2,777)	1:9:A:PHE:HA	1:4:A:ARG:HB2	3	1.54	1.01	1.97
(2,1606)	1:54:B:GLU:HB3	1:21:B:PHE:HZ	3	1.24	0.27	1.22
(2,1060)	1:27:B:LEU:HD22	1:50:B:PHE:HB2	3	1.15	0.83	0.88
(3,136)	1:27:B:LEU:H	1:31:B:TRP:HA	3	1.14	0.31	1.04
(3,135)	1:27:A:LEU:H	1:31:A:TRP:HA	3	1.12	0.36	1.04
(2,248)	1:63:B:GLN:HG2	1:57:B:ILE:H	3	0.99	0.47	0.96
(2,248)	1:63:B:GLN:HG2	1:56:B:GLN:H	3	0.99	0.47	0.96
(2,247)	1:63:A:GLN:HG2	1:57:A:ILE:H	3	0.98	0.45	0.96
(2,247)	1:63:A:GLN:HG2	1:56:A:GLN:H	3	0.98	0.45	0.96
(2,1699)	1:12:A:GLU:HB3	1:13:A:GLN:H	3	0.98	0.17	0.97
(2,1700)	1:12:B:GLU:HB3	1:13:B:GLN:H	3	0.97	0.17	0.95
(3,65)	1:55:A:GLN:HG2	1:54:A:GLU:HA	3	0.94	0.11	0.96
(3,66)	1:55:B:GLN:HG2	1:54:B:GLU:HA	3	0.92	0.12	0.96
(2,981)	1:33:A:ARG:HB2	1:33:A:ARG:HD3	3	0.8	0.03	0.79
(2,1580)	1:27:B:LEU:HD12	1:47:B:GLU:HG3	3	0.8	0.34	1.03
(2,1580)	1:27:B:LEU:HD13	1:47:B:GLU:HG3	3	0.8	0.34	1.03
(2,982)	1:33:B:ARG:HB2	1:33:B:ARG:HD3	3	0.8	0.02	0.79
(2,1579)	1:27:A:LEU:HD12	1:47:A:GLU:HG3	3	0.78	0.37	1.03
(2,1497)	1:63:A:GLN:HG2	1:64:A:PHE:HD1	3	0.77	0.48	0.52
(2,1497)	1:63:A:GLN:HG2	1:64:A:PHE:HD2	3	0.77	0.48	0.52
(2,1498)	1:63:B:GLN:HG2	1:64:B:PHE:HD1	3	0.77	0.49	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1498)	1:63:B:GLN:HG2	1:64:B:PHE:HD2	3	0.77	0.49	0.52
(2,294)	1:53:B:LYS:H	1:54:B:GLU:HB3	3	0.76	0.47	1.01
(2,294)	1:53:B:LYS:H	1:55:B:GLN:HG3	3	0.76	0.47	1.01
(2,1935)	1:61:A:HIS:H	1:57:A:ILE:HG22	3	0.75	0.48	0.7
(2,1935)	1:61:A:HIS:H	1:57:A:ILE:HG21	3	0.75	0.48	0.7
(2,1935)	1:61:A:HIS:H	1:57:A:ILE:HG23	3	0.75	0.48	0.7
(3,184)	1:13:B:GLN:H	1:4:B:ARG:HA	3	0.73	0.19	0.62
(3,183)	1:13:A:GLN:H	1:4:A:ARG:HA	3	0.73	0.22	0.59
(2,1936)	1:61:B:HIS:H	1:57:B:ILE:HG22	3	0.71	0.47	0.7
(2,1936)	1:61:B:HIS:H	1:57:B:ILE:HG21	3	0.71	0.47	0.7
(2,1936)	1:61:B:HIS:H	1:57:B:ILE:HG23	3	0.71	0.47	0.7
(2,120)	1:47:B:GLU:HG2	1:27:B:LEU:HD23	3	0.69	0.48	0.39
(2,120)	1:47:B:GLU:HG2	1:27:B:LEU:HD22	3	0.69	0.48	0.39
(2,120)	1:47:B:GLU:HG2	1:27:B:LEU:HD21	3	0.69	0.48	0.39
(1,49)	1:33:B:ARG:H	1:29:B:PRO:O	3	0.67	0.2	0.54
(2,224)	1:45:B:GLN:HG3	1:41:B:LEU:HA	3	0.67	0.71	0.21
(2,223)	1:45:A:GLN:HG3	1:41:A:LEU:HA	3	0.66	0.71	0.19
(2,1599)	1:53:A:LYS:HG2	1:21:A:PHE:HZ	3	0.65	0.35	0.52
(2,1876)	1:63:B:GLN:H	1:63:B:GLN:HB2	3	0.64	0.15	0.72
(1,7)	1:33:A:ARG:H	1:29:A:PRO:O	3	0.64	0.21	0.5
(2,1875)	1:63:A:GLN:H	1:63:A:GLN:HB2	3	0.64	0.14	0.72
(2,2393)	1:7:A:THR:H	1:4:A:ARG:HG3	3	0.64	0.23	0.52
(2,1181)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	3	0.62	0.29	0.47
(2,2394)	1:7:B:THR:H	1:4:B:ARG:HG3	3	0.62	0.23	0.52
(2,1182)	1:6:B:ARG:HD3	1:6:B:ARG:HB2	3	0.62	0.3	0.47
(2,2397)	1:42:A:ASN:H	1:36:A:SER:HB2	3	0.62	0.03	0.63
(2,2398)	1:42:B:ASN:H	1:36:B:SER:HB2	3	0.6	0.04	0.63
(2,991)	1:11:A:GLU:HB3	1:11:A:GLU:H	3	0.58	0.02	0.57
(2,992)	1:11:B:GLU:HB3	1:11:B:GLU:H	3	0.58	0.02	0.57
(2,1194)	1:16:B:ALA:HB2	1:13:B:GLN:HB3	3	0.53	0.23	0.67
(2,1194)	1:16:B:ALA:HB3	1:13:B:GLN:HB3	3	0.53	0.23	0.67
(2,1147)	1:16:A:ALA:HB3	1:19:B:LEU:HD23	3	0.52	0.28	0.7
(2,1147)	1:16:A:ALA:HB3	1:19:B:LEU:HD22	3	0.52	0.28	0.7
(2,1147)	1:16:A:ALA:HB2	1:19:B:LEU:HD23	3	0.52	0.28	0.7
(2,1148)	1:16:B:ALA:HB3	1:19:A:LEU:HD23	3	0.5	0.26	0.69
(2,1148)	1:16:B:ALA:HB3	1:19:A:LEU:HD22	3	0.5	0.26	0.69
(2,1148)	1:16:B:ALA:HB2	1:19:A:LEU:HD23	3	0.5	0.26	0.69
(2,1023)	1:12:A:GLU:HB2	1:12:A:GLU:HA	3	0.49	0.18	0.61
(2,443)	1:16:A:ALA:HB3	1:16:B:ALA:H	3	0.45	0.31	0.28
(2,443)	1:16:A:ALA:HB2	1:16:B:ALA:H	3	0.45	0.31	0.28
(2,444)	1:16:B:ALA:HB3	1:16:A:ALA:H	3	0.45	0.3	0.29
(2,444)	1:16:B:ALA:HB2	1:16:A:ALA:H	3	0.45	0.3	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2348)	1:16:B:ALA:H	1:17:B:LEU:HD22	3	0.45	0.24	0.53
(2,2348)	1:16:B:ALA:H	1:17:B:LEU:HD21	3	0.45	0.24	0.53
(2,1891)	1:65:A:GLU:HG2	1:65:A:GLU:H	3	0.44	0.13	0.39
(2,1892)	1:65:B:GLU:HG2	1:65:B:GLU:H	3	0.44	0.13	0.38
(2,2420)	1:51:B:ARG:H	1:54:B:GLU:HG3	3	0.44	0.41	0.18
(2,2347)	1:16:A:ALA:H	1:17:A:LEU:HD22	3	0.43	0.2	0.53
(2,2347)	1:16:A:ALA:H	1:17:A:LEU:HD21	3	0.43	0.2	0.53
(2,72)	1:16:B:ALA:HA	1:19:A:LEU:HD22	3	0.43	0.09	0.44
(2,72)	1:16:B:ALA:HA	1:19:B:LEU:HD23	3	0.43	0.09	0.44
(2,1735)	1:64:A:PHE:H	1:64:A:PHE:HD1	3	0.43	0.26	0.31
(2,257)	1:54:A:GLU:HG2	1:59:A:TRP:HB2	3	0.42	0.14	0.38
(2,257)	1:54:A:GLU:HG2	1:21:A:PHE:HB3	3	0.42	0.14	0.38
(2,2030)	1:32:B:ARG:H	1:32:B:ARG:HD3	3	0.42	0.1	0.44
(2,258)	1:54:B:GLU:HG2	1:59:B:TRP:HB2	3	0.42	0.14	0.35
(2,258)	1:54:B:GLU:HG2	1:21:B:PHE:HB3	3	0.42	0.14	0.35
(2,2029)	1:32:A:ARG:H	1:32:A:ARG:HD3	3	0.42	0.09	0.42
(2,1539)	1:13:A:GLN:HB3	1:41:A:LEU:HD22	3	0.41	0.04	0.4
(2,1539)	1:13:A:GLN:HB3	1:41:A:LEU:HD23	3	0.41	0.04	0.4
(2,1540)	1:13:B:GLN:HB3	1:41:B:LEU:HD22	3	0.41	0.03	0.39
(2,1540)	1:13:B:GLN:HB3	1:41:B:LEU:HD23	3	0.41	0.03	0.39
(2,2441)	1:14:A:LYS:H	1:17:A:LEU:HD22	3	0.4	0.25	0.32
(2,2441)	1:14:A:LYS:H	1:17:A:LEU:HD23	3	0.4	0.25	0.32
(2,2441)	1:14:A:LYS:H	1:17:A:LEU:HD21	3	0.4	0.25	0.32
(1,74)	1:33:B:ARG:N	1:29:B:PRO:O	3	0.39	0.21	0.26
(1,3)	1:17:A:LEU:H	1:13:A:GLN:O	3	0.38	0.06	0.36
(2,1854)	1:16:B:ALA:H	1:15:B:LYS:HB3	3	0.38	0.16	0.41
(1,32)	1:33:A:ARG:N	1:29:A:PRO:O	3	0.36	0.23	0.21
(2,71)	1:16:A:ALA:HA	1:19:B:LEU:HD22	3	0.35	0.11	0.42
(2,71)	1:16:A:ALA:HA	1:19:B:LEU:HD23	3	0.35	0.11	0.42
(2,71)	1:16:A:ALA:HA	1:19:A:LEU:HD23	3	0.35	0.11	0.42
(2,1137)	1:17:A:LEU:HA	1:20:A:ALA:HB3	3	0.35	0.15	0.43
(2,1137)	1:17:A:LEU:HA	1:20:A:ALA:HB1	3	0.35	0.15	0.43
(2,1268)	1:10:B:SER:HB2	1:12:B:GLU:H	3	0.35	0.24	0.18
(2,1267)	1:10:A:SER:HB2	1:12:A:GLU:H	3	0.34	0.24	0.18
(2,1691)	1:7:A:THR:HB	1:42:A:ASN:HB2	3	0.34	0.21	0.31
(2,1692)	1:7:B:THR:HB	1:42:B:ASN:HB2	3	0.34	0.2	0.31
(1,45)	1:17:B:LEU:H	1:13:B:GLN:O	3	0.34	0.02	0.35
(2,320)	1:9:B:PHE:H	1:45:B:GLN:HB2	3	0.33	0.2	0.22
(2,1138)	1:17:B:LEU:HA	1:20:B:ALA:HB3	3	0.33	0.15	0.37
(2,1138)	1:17:B:LEU:HA	1:20:B:ALA:HB1	3	0.33	0.15	0.37
(3,177)	1:49:A:TRP:H	1:45:A:GLN:H	3	0.31	0.14	0.23
(2,130)	1:33:B:ARG:HB2	1:33:B:ARG:H	3	0.31	0.04	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1861)	1:53:A:LYS:H	1:55:A:GLN:H	3	0.31	0.13	0.35
(2,1862)	1:53:B:LYS:H	1:55:B:GLN:H	3	0.31	0.13	0.35
(3,119)	1:9:A:PHE:HB3	1:45:A:GLN:HA	3	0.31	0.07	0.32
(2,129)	1:33:A:ARG:HB2	1:33:A:ARG:H	3	0.31	0.04	0.31
(2,129)	1:65:A:GLU:HB2	1:65:A:GLU:H	3	0.31	0.04	0.31
(3,178)	1:49:B:TRP:H	1:45:B:GLN:H	3	0.31	0.12	0.28
(2,309)	1:42:A:ASN:H	1:45:A:GLN:HA	3	0.3	0.22	0.17
(2,311)	1:17:A:LEU:H	1:14:A:LYS:HB3	3	0.29	0.14	0.2
(2,2197)	1:60:A:SER:H	1:58:A:GLY:HA2	3	0.29	0.11	0.23
(2,2198)	1:60:B:SER:H	1:58:B:GLY:HA2	3	0.29	0.11	0.23
(2,1786)	1:66:B:LYS:H	1:64:B:PHE:HB3	3	0.28	0.12	0.35
(2,1785)	1:66:A:LYS:H	1:64:A:PHE:HB3	3	0.28	0.12	0.35
(2,312)	1:17:B:LEU:H	1:14:B:LYS:HB3	3	0.27	0.16	0.18
(2,2173)	1:17:A:LEU:HG	1:17:A:LEU:H	3	0.26	0.15	0.21
(2,362)	1:55:B:GLN:HB3	1:58:B:GLY:H	3	0.25	0.02	0.27
(2,362)	1:55:B:GLN:HB2	1:58:B:GLY:H	3	0.25	0.02	0.27
(2,2174)	1:17:B:LEU:HG	1:17:B:LEU:H	3	0.25	0.13	0.22
(2,727)	1:36:A:SER:HB3	1:36:A:SER:H	3	0.25	0.0	0.25
(2,728)	1:36:B:SER:HB3	1:36:B:SER:H	3	0.25	0.0	0.25
(2,366)	1:14:B:LYS:H	1:17:B:LEU:HB2	3	0.24	0.03	0.26
(2,366)	1:14:B:LYS:H	1:39:B:LEU:HD12	3	0.24	0.03	0.26
(2,361)	1:55:A:GLN:HB3	1:58:A:GLY:H	3	0.24	0.05	0.26
(2,361)	1:55:A:GLN:HB2	1:58:A:GLY:H	3	0.24	0.05	0.26
(3,42)	1:61:B:HIS:HA	1:60:B:SER:HG	3	0.22	0.07	0.27
(3,41)	1:61:A:HIS:HA	1:60:A:SER:HG	3	0.22	0.09	0.28
(1,42)	1:54:A:GLU:N	1:50:A:PHE:O	3	0.22	0.03	0.21
(1,84)	1:54:B:GLU:N	1:50:B:PHE:O	3	0.21	0.04	0.19
(2,365)	1:14:A:LYS:H	1:17:A:LEU:HB2	3	0.21	0.04	0.19
(2,365)	1:14:A:LYS:H	1:39:A:LEU:HD12	3	0.21	0.04	0.19
(3,56)	1:57:B:ILE:HB	1:58:B:GLY:HA2	3	0.2	0.07	0.18
(3,55)	1:57:A:ILE:HB	1:58:A:GLY:HA2	3	0.19	0.06	0.18
(2,714)	1:3:B:LYS:HA	1:4:B:ARG:H	3	0.18	0.07	0.14
(2,1965)	1:13:A:GLN:HB3	1:13:A:GLN:H	3	0.18	0.03	0.2
(2,1966)	1:13:B:GLN:HB3	1:13:B:GLN:H	3	0.18	0.02	0.19
(2,713)	1:3:A:LYS:HA	1:4:A:ARG:H	3	0.17	0.07	0.13
(2,1762)	1:36:B:SER:H	1:36:B:SER:HG	3	0.17	0.04	0.18
(2,1025)	1:52:A:ARG:HD2	1:52:A:ARG:HG3	3	0.16	0.0	0.16
(2,1026)	1:52:B:ARG:HD2	1:52:B:ARG:HG3	3	0.16	0.0	0.16
(2,1761)	1:36:A:SER:H	1:36:A:SER:HG	3	0.16	0.04	0.13
(2,1079)	1:13:A:GLN:HB2	1:13:A:GLN:HG2	3	0.15	0.0	0.15
(2,1080)	1:13:B:GLN:HB2	1:13:B:GLN:HG2	3	0.15	0.0	0.15
(2,1510)	1:65:B:GLU:HG2	1:65:B:GLU:HA	3	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,724)	1:10:B:SER:HB2	1:11:B:GLU:H	3	0.12	0.01	0.12
(2,665)	1:48:A:ARG:HA	1:51:A:ARG:HG2	2	2.08	0.57	2.08
(2,665)	1:48:A:ARG:HA	1:51:A:ARG:HG3	2	2.08	0.57	2.08
(2,666)	1:48:B:ARG:HA	1:51:B:ARG:HG2	2	2.06	0.56	2.06
(2,666)	1:48:B:ARG:HA	1:51:B:ARG:HG3	2	2.06	0.56	2.06
(2,1059)	1:27:A:LEU:HD22	1:50:A:PHE:HB2	2	1.66	0.77	1.66
(2,847)	1:51:A:ARG:HD2	1:52:A:ARG:HA	2	1.48	0.6	1.48
(2,848)	1:51:B:ARG:HD2	1:52:B:ARG:HA	2	1.48	0.6	1.48
(2,1057)	1:47:A:GLU:HA	1:27:A:LEU:HD22	2	1.36	0.24	1.36
(2,1058)	1:47:B:GLU:HA	1:27:B:LEU:HD22	2	1.31	0.29	1.31
(2,2077)	1:48:A:ARG:H	1:51:A:ARG:HG2	2	1.25	0.17	1.25
(2,2077)	1:48:A:ARG:H	1:51:A:ARG:HG3	2	1.25	0.17	1.25
(2,2187)	1:54:A:GLU:H	1:21:A:PHE:HE2	2	1.25	0.72	1.25
(2,2187)	1:54:A:GLU:H	1:21:A:PHE:HE1	2	1.25	0.72	1.25
(2,1151)	1:46:A:ILE:HG21	1:27:A:LEU:HD22	2	1.24	0.9	1.24
(2,1152)	1:46:B:ILE:HG21	1:27:B:LEU:HD22	2	1.24	0.9	1.24
(2,2078)	1:48:B:ARG:H	1:51:B:ARG:HG2	2	1.23	0.18	1.23
(2,2078)	1:48:B:ARG:H	1:51:B:ARG:HG3	2	1.23	0.18	1.23
(2,956)	1:8:B:GLU:HG3	1:9:B:PHE:H	2	1.1	0.48	1.1
(2,947)	1:54:A:GLU:HG2	1:21:A:PHE:HE2	2	1.09	0.67	1.09
(2,947)	1:54:A:GLU:HG2	1:21:A:PHE:HE1	2	1.09	0.67	1.09
(2,955)	1:8:A:GLU:HG3	1:9:A:PHE:H	2	1.09	0.47	1.09
(2,293)	1:53:A:LYS:H	1:54:A:GLU:HB3	2	1.09	0.08	1.09
(2,293)	1:53:A:LYS:H	1:55:A:GLN:HG3	2	1.09	0.08	1.09
(2,1232)	1:18:B:ASP:HA	1:49:B:TRP:HE1	2	1.04	0.44	1.04
(2,2437)	1:53:A:LYS:H	1:21:A:PHE:HE1	2	1.02	0.78	1.02
(2,480)	1:19:B:LEU:HD22	1:17:A:LEU:HD13	2	1.0	0.01	1.0
(2,480)	1:19:B:LEU:HD23	1:17:A:LEU:HD13	2	1.0	0.01	1.0
(2,1020)	1:57:B:ILE:HG12	1:57:B:ILE:HG23	2	0.94	0.02	0.94
(2,1019)	1:57:A:ILE:HG12	1:57:A:ILE:HG23	2	0.94	0.02	0.94
(2,2199)	1:33:A:ARG:H	1:33:A:ARG:HD3	2	0.92	0.0	0.92
(2,2200)	1:33:B:ARG:H	1:33:B:ARG:HD3	2	0.91	0.01	0.91
(2,1231)	1:18:A:ASP:HA	1:49:A:TRP:HE1	2	0.88	0.54	0.88
(2,391)	1:34:A:TYR:HD2	1:35:A:LEU:HD23	2	0.88	0.45	0.88
(2,392)	1:34:B:TYR:HD2	1:35:B:LEU:HD23	2	0.86	0.46	0.86
(2,1337)	1:27:A:LEU:HD21	1:50:A:PHE:HD1	2	0.85	0.47	0.85
(2,1337)	1:27:A:LEU:HD23	1:50:A:PHE:HD2	2	0.85	0.47	0.85
(2,1338)	1:27:B:LEU:HD21	1:50:B:PHE:HD1	2	0.85	0.47	0.85
(2,1338)	1:27:B:LEU:HD23	1:50:B:PHE:HD2	2	0.85	0.47	0.85
(2,1603)	1:53:A:LYS:HB3	1:21:A:PHE:HZ	2	0.84	0.7	0.84
(2,1939)	1:61:A:HIS:H	1:54:A:GLU:HB2	2	0.82	0.49	0.82
(2,1600)	1:53:B:LYS:HG2	1:21:B:PHE:HZ	2	0.82	0.31	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1940)	1:61:B:HIS:H	1:54:B:GLU:HB2	2	0.81	0.49	0.81
(2,436)	1:16:B:ALA:HB2	1:39:A:LEU:HD11	2	0.78	0.43	0.78
(2,436)	1:16:B:ALA:HB3	1:39:A:LEU:HD11	2	0.78	0.43	0.78
(2,435)	1:16:A:ALA:HB2	1:39:B:LEU:HD11	2	0.78	0.44	0.78
(2,435)	1:16:A:ALA:HB3	1:39:B:LEU:HD11	2	0.78	0.44	0.78
(2,479)	1:19:A:LEU:HD22	1:17:B:LEU:HD13	2	0.78	0.15	0.78
(2,479)	1:19:A:LEU:HD23	1:17:B:LEU:HD13	2	0.78	0.15	0.78
(2,1447)	1:53:A:LYS:HB2	1:21:A:PHE:HE1	2	0.76	0.62	0.76
(2,2149)	1:52:A:ARG:HB3	1:56:A:GLN:H	2	0.71	0.51	0.71
(2,491)	1:61:A:HIS:HD1	1:61:A:HIS:H	2	0.7	0.16	0.7
(2,492)	1:61:B:HIS:HD1	1:61:B:HIS:H	2	0.69	0.16	0.69
(2,2150)	1:52:B:ARG:HB3	1:56:B:GLN:H	2	0.68	0.52	0.68
(2,2419)	1:51:A:ARG:H	1:54:A:GLU:HG3	2	0.67	0.31	0.67
(3,53)	1:9:A:PHE:HB2	1:39:A:LEU:HG	2	0.66	0.5	0.66
(2,2152)	1:15:B:LYS:HG3	1:15:B:LYS:H	2	0.63	0.29	0.63
(3,54)	1:9:B:PHE:HB2	1:39:B:LEU:HG	2	0.63	0.51	0.63
(2,1997)	1:44:A:GLU:H	1:44:A:GLU:HB3	2	0.62	0.01	0.62
(2,1998)	1:44:B:GLU:H	1:44:B:GLU:HB3	2	0.62	0.01	0.62
(2,2151)	1:15:A:LYS:HG3	1:15:A:LYS:H	2	0.62	0.3	0.62
(2,1024)	1:12:B:GLU:HB2	1:12:B:GLU:HA	2	0.62	0.01	0.62
(3,27)	1:2:A:GLU:HA	1:12:A:GLU:H	2	0.62	0.18	0.62
(2,1485)	1:60:A:SER:HB2	1:60:A:SER:HA	2	0.6	0.01	0.6
(2,1486)	1:60:B:SER:HB2	1:60:B:SER:HA	2	0.6	0.01	0.6
(3,28)	1:2:B:GLU:HA	1:12:B:GLU:H	2	0.6	0.22	0.6
(2,188)	1:17:B:LEU:HD23	1:13:B:GLN:HB3	2	0.55	0.42	0.55
(2,188)	1:17:B:LEU:HD23	1:45:B:GLN:HB3	2	0.55	0.42	0.55
(2,2442)	1:14:B:LYS:H	1:17:B:LEU:HD22	2	0.55	0.24	0.55
(2,2442)	1:14:B:LYS:H	1:17:B:LEU:HD21	2	0.55	0.24	0.55
(2,1836)	1:53:B:LYS:H	1:53:B:LYS:HD2	2	0.53	0.16	0.53
(2,458)	1:49:B:TRP:HD1	1:17:B:LEU:HD12	2	0.53	0.18	0.53
(2,1835)	1:53:A:LYS:H	1:53:A:LYS:HD2	2	0.52	0.16	0.52
(2,679)	1:63:A:GLN:HA	1:63:A:GLN:HG2	2	0.52	0.03	0.52
(2,680)	1:63:B:GLN:HA	1:63:B:GLN:HG2	2	0.52	0.03	0.52
(2,2119)	1:28:A:THR:H	1:32:A:ARG:HE	2	0.51	0.26	0.51
(2,457)	1:49:A:TRP:HD1	1:17:A:LEU:HD12	2	0.5	0.18	0.5
(2,484)	1:50:B:PHE:HD2	1:27:B:LEU:HD11	2	0.5	0.22	0.5
(2,484)	1:50:B:PHE:HD1	1:27:B:LEU:HD13	2	0.5	0.22	0.5
(2,282)	1:7:B:THR:HB	1:41:B:LEU:H	2	0.5	0.09	0.5
(2,281)	1:7:A:THR:HB	1:41:A:LEU:H	2	0.48	0.08	0.48
(2,1960)	1:34:B:TYR:H	1:33:B:ARG:HG3	2	0.48	0.24	0.48
(2,1932)	1:49:B:TRP:H	1:52:B:ARG:HB2	2	0.47	0.01	0.47
(3,215)	1:7:A:THR:H	1:4:A:ARG:HA	2	0.47	0.02	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1620)	1:13:B:GLN:HA	1:39:B:LEU:HD11	2	0.46	0.08	0.46
(2,1959)	1:34:A:TYR:H	1:33:A:ARG:HG3	2	0.46	0.3	0.46
(2,1931)	1:49:A:TRP:H	1:52:A:ARG:HB2	2	0.46	0.0	0.46
(3,216)	1:7:B:THR:H	1:4:B:ARG:HA	2	0.46	0.02	0.46
(2,2188)	1:54:B:GLU:H	1:21:B:PHE:HE2	2	0.45	0.11	0.45
(2,2188)	1:54:B:GLU:H	1:21:B:PHE:HE1	2	0.45	0.11	0.45
(1,39)	1:20:A:ALA:N	1:16:A:ALA:O	2	0.44	0.03	0.44
(2,2179)	1:51:A:ARG:H	1:51:A:ARG:HG2	2	0.43	0.11	0.43
(2,2180)	1:51:B:ARG:H	1:51:B:ARG:HG2	2	0.43	0.11	0.43
(2,1619)	1:13:A:GLN:HA	1:39:A:LEU:HD11	2	0.42	0.04	0.42
(2,1228)	1:17:B:LEU:HD23	1:49:B:TRP:HE1	2	0.42	0.13	0.42
(2,1228)	1:17:B:LEU:HD21	1:49:B:TRP:HE1	2	0.42	0.13	0.42
(2,319)	1:9:A:PHE:H	1:45:A:GLN:HB2	2	0.42	0.19	0.42
(2,1609)	1:35:A:LEU:HB2	1:39:A:LEU:HD22	2	0.4	0.1	0.4
(2,310)	1:42:B:ASN:H	1:45:B:GLN:HA	2	0.4	0.22	0.4
(2,993)	1:12:A:GLU:HB3	1:12:A:GLU:H	2	0.38	0.04	0.38
(1,65)	1:15:B:LYS:N	1:11:B:GLU:O	2	0.38	0.27	0.38
(2,994)	1:12:B:GLU:HB3	1:12:B:GLU:H	2	0.38	0.04	0.38
(2,2260)	1:6:B:ARG:H	1:6:B:ARG:HD3	2	0.37	0.19	0.37
(2,2259)	1:6:A:ARG:H	1:6:A:ARG:HD3	2	0.36	0.19	0.36
(2,1610)	1:35:B:LEU:HB2	1:39:B:LEU:HD22	2	0.35	0.14	0.35
(2,485)	1:50:A:PHE:HB2	1:50:A:PHE:HE1	2	0.34	0.0	0.34
(2,486)	1:50:B:PHE:HB2	1:50:B:PHE:HE1	2	0.34	0.0	0.34
(2,2224)	1:57:B:ILE:HG12	1:58:B:GLY:H	2	0.34	0.06	0.34
(2,926)	1:36:B:SER:HB2	1:43:B:GLU:HG3	2	0.34	0.1	0.34
(2,948)	1:54:B:GLU:HG2	1:21:B:PHE:HE2	2	0.34	0.1	0.34
(2,948)	1:54:B:GLU:HG2	1:21:B:PHE:HE1	2	0.34	0.1	0.34
(2,615)	1:15:A:LYS:HA	1:18:A:ASP:HB2	2	0.34	0.06	0.34
(2,2223)	1:57:A:ILE:HG12	1:58:A:GLY:H	2	0.34	0.05	0.34
(2,925)	1:36:A:SER:HB2	1:43:A:GLU:HG3	2	0.33	0.1	0.33
(1,81)	1:20:B:ALA:N	1:16:B:ALA:O	2	0.32	0.08	0.32
(2,1926)	1:6:B:ARG:H	1:5:B:PRO:HB2	2	0.32	0.05	0.32
(2,1925)	1:6:A:ARG:H	1:5:A:PRO:HB2	2	0.32	0.05	0.32
(2,827)	1:62:A:PRO:HD3	1:62:A:PRO:HB3	2	0.3	0.02	0.3
(2,828)	1:62:B:PRO:HD3	1:62:B:PRO:HB3	2	0.3	0.02	0.3
(2,576)	1:14:B:LYS:HA	1:17:B:LEU:HD22	2	0.3	0.05	0.3
(2,576)	1:14:B:LYS:HA	1:17:B:LEU:HD21	2	0.3	0.05	0.3
(2,1053)	1:12:A:GLU:HB3	1:12:A:GLU:HG3	2	0.29	0.01	0.29
(3,205)	1:57:A:ILE:H	1:54:A:GLU:HB2	2	0.29	0.03	0.29
(2,1054)	1:12:B:GLU:HB3	1:12:B:GLU:HG3	2	0.29	0.0	0.29
(2,1629)	1:41:A:LEU:HD11	1:9:A:PHE:HB2	2	0.29	0.01	0.29
(2,1629)	1:41:A:LEU:HD12	1:9:A:PHE:HB2	2	0.29	0.01	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1630)	1:41:B:LEU:HD11	1:9:B:PHE:HB2	2	0.29	0.0	0.29
(2,1630)	1:41:B:LEU:HD12	1:9:B:PHE:HB2	2	0.29	0.0	0.29
(2,1924)	1:63:B:GLN:HG2	1:63:B:GLN:H	2	0.28	0.09	0.28
(3,206)	1:57:B:ILE:H	1:54:B:GLU:HB2	2	0.28	0.02	0.28
(2,575)	1:14:A:LYS:HA	1:17:A:LEU:HD22	2	0.28	0.07	0.28
(2,575)	1:14:A:LYS:HA	1:17:A:LEU:HD21	2	0.28	0.07	0.28
(2,737)	1:60:A:SER:HB3	1:60:A:SER:H	2	0.26	0.1	0.26
(2,738)	1:60:B:SER:HB3	1:60:B:SER:H	2	0.26	0.1	0.26
(2,529)	1:50:A:PHE:HA	1:53:A:LYS:HB2	2	0.25	0.02	0.25
(2,1604)	1:53:B:LYS:HB3	1:21:B:PHE:HZ	2	0.25	0.07	0.25
(2,1736)	1:64:B:PHE:H	1:64:B:PHE:HD1	2	0.24	0.08	0.24
(2,530)	1:50:B:PHE:HA	1:53:B:LYS:HB2	2	0.24	0.04	0.24
(2,1816)	1:4:B:ARG:H	1:10:B:SER:HB3	2	0.24	0.13	0.24
(2,1923)	1:63:A:GLN:HG2	1:63:A:GLN:H	2	0.24	0.13	0.24
(2,1815)	1:4:A:ARG:H	1:10:A:SER:HB3	2	0.23	0.13	0.23
(2,2317)	1:4:A:ARG:H	1:4:A:ARG:HD3	2	0.23	0.02	0.23
(2,2318)	1:4:B:ARG:H	1:4:B:ARG:HD3	2	0.23	0.02	0.23
(2,109)	1:3:A:LYS:HE3	1:4:A:ARG:HA	2	0.22	0.07	0.22
(2,109)	1:3:A:LYS:HE2	1:4:A:ARG:HA	2	0.22	0.07	0.22
(2,110)	1:3:B:LYS:HE3	1:4:B:ARG:HA	2	0.22	0.06	0.22
(2,110)	1:3:B:LYS:HE2	1:4:B:ARG:HA	2	0.22	0.06	0.22
(2,2429)	1:57:A:ILE:H	1:56:A:GLN:HB3	2	0.22	0.02	0.22
(2,2074)	1:55:B:GLN:H	1:53:B:LYS:HA	2	0.21	0.07	0.21
(2,905)	1:18:A:ASP:HB2	1:19:A:LEU:H	2	0.21	0.0	0.21
(2,2430)	1:57:B:ILE:H	1:56:B:GLN:HB3	2	0.21	0.03	0.21
(2,2073)	1:55:A:GLN:H	1:53:A:LYS:HA	2	0.2	0.08	0.2
(3,102)	1:42:B:ASN:HB3	1:36:B:SER:HB2	2	0.2	0.01	0.2
(2,2093)	1:54:A:GLU:H	1:53:A:LYS:HG3	2	0.2	0.02	0.2
(3,101)	1:42:A:ASN:HB3	1:36:A:SER:HB2	2	0.2	0.01	0.2
(2,2089)	1:28:A:THR:H	1:27:A:LEU:HD21	2	0.19	0.01	0.19
(2,2090)	1:28:B:THR:H	1:27:B:LEU:HD21	2	0.19	0.01	0.19
(2,906)	1:18:B:ASP:HB2	1:19:B:LEU:H	2	0.18	0.02	0.18
(2,2094)	1:54:B:GLU:H	1:53:B:LYS:HG3	2	0.18	0.02	0.18
(2,2326)	1:7:B:THR:H	1:4:B:ARG:HD3	2	0.18	0.04	0.18
(2,2325)	1:7:A:THR:H	1:4:A:ARG:HD3	2	0.18	0.04	0.18
(3,22)	1:3:B:LYS:HA	1:2:B:GLU:HG3	2	0.17	0.02	0.17
(2,815)	1:61:A:HIS:HA	1:62:A:PRO:HD2	2	0.16	0.04	0.16
(2,816)	1:61:B:HIS:HA	1:62:B:PRO:HD2	2	0.16	0.04	0.16
(3,231)	1:60:A:SER:H	1:57:A:ILE:HA	2	0.16	0.06	0.16
(3,232)	1:60:B:SER:H	1:57:B:ILE:HA	2	0.15	0.05	0.15
(2,2053)	1:47:A:GLU:H	1:44:A:GLU:H	2	0.14	0.01	0.14
(2,723)	1:10:A:SER:HB2	1:11:A:GLU:H	2	0.12	0.02	0.12

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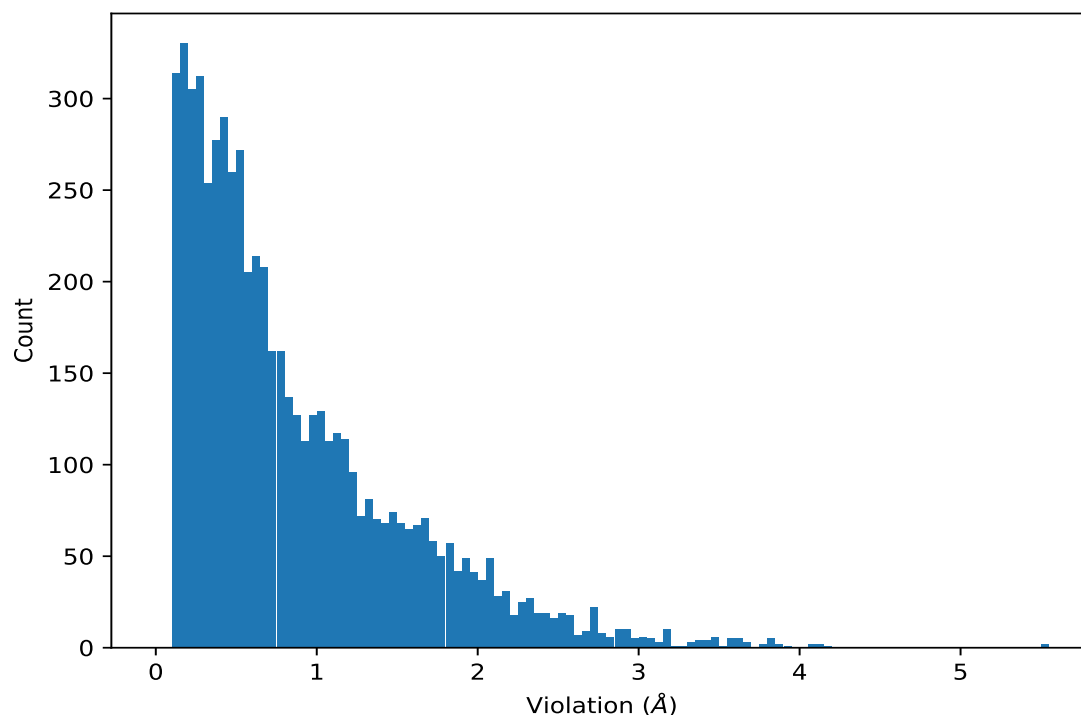
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1952)	1:49:B:TRP:H	1:52:B:ARG:H	2	0.12	0.02	0.12
(2,1349)	1:42:A:ASN:HA	1:42:A:ASN:HD21	2	0.11	0.01	0.11
(2,1350)	1:42:B:ASN:HA	1:42:B:ASN:HD21	2	0.11	0.01	0.11
(2,1951)	1:49:A:TRP:H	1:52:A:ARG:H	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1092)	1:39:B:LEU:HD21	1:27:B:LEU:HD22	4	5.55
(2,1091)	1:39:A:LEU:HD21	1:27:A:LEU:HD22	4	5.5
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	4	4.17
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE21	5	4.13
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE21	5	4.11
(2,452)	1:39:B:LEU:HD11	1:39:A:LEU:HD12	1	4.09
(2,451)	1:39:A:LEU:HD12	1:39:B:LEU:HD11	1	4.09
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB3	4	3.9
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	9	3.88
(2,349)	1:27:A:LEU:H	1:24:A:ASP:HB3	9	3.85
(2,452)	1:39:B:LEU:HD11	1:39:A:LEU:HD12	7	3.84
(2,451)	1:39:A:LEU:HD12	1:39:B:LEU:HD11	7	3.84
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD22	4	3.82
(2,252)	1:27:B:LEU:HD12	1:44:B:GLU:HA	1	3.8
(2,251)	1:27:A:LEU:HD12	1:44:A:GLU:HA	1	3.8
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD22	4	3.76
(2,350)	1:27:B:LEU:H	1:24:B:ASP:HB3	9	3.75
(2,1495)	1:61:A:HIS:HA	1:54:A:GLU:HB2	6	3.67
(2,1496)	1:61:B:HIS:HA	1:54:B:GLU:HB2	6	3.66
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB3	4	3.66
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG21	2	3.64
(2,440)	1:20:B:ALA:HB1	1:20:A:ALA:HB1	9	3.62
(2,439)	1:20:A:ALA:HB1	1:20:B:ALA:HB1	9	3.62
(2,440)	1:20:B:ALA:HB2	1:20:A:ALA:HB2	5	3.6
(2,439)	1:20:A:ALA:HB2	1:20:B:ALA:HB2	5	3.6
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG21	2	3.59
(2,1445)	1:53:A:LYS:HB2	1:21:A:PHE:HZ	4	3.59
(2,440)	1:20:B:ALA:HB3	1:20:A:ALA:HB3	6	3.58
(2,439)	1:20:A:ALA:HB3	1:20:B:ALA:HB3	6	3.58
(2,1615)	1:27:A:LEU:HD13	1:35:A:LEU:HD12	3	3.56
(2,468)	1:19:B:LEU:HD21	1:35:A:LEU:HB2	9	3.51
(2,1616)	1:27:B:LEU:HD13	1:35:B:LEU:HD12	3	3.49
(2,440)	1:20:B:ALA:HB1	1:20:A:ALA:HB1	4	3.49
(2,439)	1:20:A:ALA:HB1	1:20:B:ALA:HB1	4	3.49
(2,164)	1:19:B:LEU:HD22	1:46:A:ILE:HB	4	3.48
(2,1092)	1:39:B:LEU:HD23	1:27:B:LEU:HD22	8	3.46
(2,1091)	1:39:A:LEU:HD23	1:27:A:LEU:HD22	8	3.46
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	9	3.43
(2,452)	1:39:B:LEU:HD12	1:39:A:LEU:HD12	6	3.4
(2,451)	1:39:A:LEU:HD12	1:39:B:LEU:HD12	6	3.4
(2,438)	1:20:B:ALA:HB1	1:20:A:ALA:H	9	3.4
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	5	3.38
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG21	2	3.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1224)	1:17:B:LEU:HD23	1:45:B:GLN:HE22	10	3.37
(2,215)	1:27:A:LEU:HD23	1:21:A:PHE:HD1	4	3.37
(2,1223)	1:17:A:LEU:HD23	1:45:A:GLN:HE22	10	3.33
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	5	3.31
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG21	2	3.3
(2,1235)	1:20:A:ALA:HB3	1:26:A:ARG:HD3	9	3.26
(2,216)	1:27:B:LEU:HD23	1:21:B:PHE:HD1	4	3.23
(2,467)	1:19:A:LEU:HD21	1:35:B:LEU:HB2	9	3.19
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	6	3.18
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	6	3.18
(2,252)	1:27:B:LEU:HD12	1:44:B:GLU:HA	8	3.18
(2,251)	1:27:A:LEU:HD12	1:44:A:GLU:HA	8	3.18
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	4	3.17
(2,452)	1:39:B:LEU:HD12	1:39:A:LEU:HD13	5	3.16
(2,451)	1:39:A:LEU:HD13	1:39:B:LEU:HD12	5	3.16
(2,164)	1:19:B:LEU:HD23	1:46:A:ILE:HB	7	3.16
(2,104)	1:3:B:LYS:HE2	1:12:B:GLU:HG3	10	3.15
(2,179)	1:16:A:ALA:HB2	1:15:A:LYS:HE3	7	3.14
(2,180)	1:16:B:ALA:HB2	1:15:B:LYS:HE3	7	3.12
(2,437)	1:20:A:ALA:HB1	1:20:B:ALA:H	9	3.1
(2,1224)	1:17:B:LEU:HD22	1:45:B:GLN:HE22	8	3.06
(2,1223)	1:17:A:LEU:HD22	1:45:A:GLN:HE22	8	3.06
(2,943)	1:54:A:GLU:HG2	1:21:A:PHE:HZ	4	3.06
(2,163)	1:19:A:LEU:HD23	1:46:B:ILE:HB	7	3.06
(2,674)	1:8:B:GLU:HA	1:41:B:LEU:HB2	5	3.05
(2,673)	1:8:A:GLU:HA	1:41:A:LEU:HB2	5	3.04
(2,163)	1:19:A:LEU:HD22	1:46:B:ILE:HB	4	3.03
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD11	1	3.02
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD11	1	3.02
(2,1224)	1:17:B:LEU:HD21	1:45:B:GLN:HE22	1	3.01
(2,1223)	1:17:A:LEU:HD21	1:45:A:GLN:HE22	1	3.01
(2,1574)	1:27:B:LEU:HD11	1:46:B:ILE:H	1	2.97
(2,1573)	1:27:A:LEU:HD11	1:46:A:ILE:H	1	2.97
(2,67)	1:25:A:ARG:HA	1:19:B:LEU:HD21	4	2.97
(2,104)	1:3:B:LYS:HE3	1:12:A:GLU:HG3	8	2.96
(2,103)	1:3:A:LYS:HE3	1:12:B:GLU:HG3	8	2.95
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG22	1	2.94
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG22	1	2.94
(2,1236)	1:20:B:ALA:HB3	1:26:B:ARG:HD3	9	2.93
(2,1091)	1:39:A:LEU:HD23	1:27:A:LEU:HD22	7	2.93
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD12	3	2.92
(2,1574)	1:27:B:LEU:HD11	1:46:B:ILE:H	8	2.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1331)	1:27:A:LEU:HD22	1:50:A:PHE:H	4	2.91
(2,1092)	1:39:B:LEU:HD23	1:27:B:LEU:HD22	7	2.91
(2,1573)	1:27:A:LEU:HD11	1:46:A:ILE:H	8	2.9
(2,103)	1:3:A:LYS:HE2	1:12:A:GLU:HG3	10	2.9
(2,1446)	1:53:B:LYS:HB2	1:21:B:PHE:HZ	7	2.89
(2,441)	1:16:A:ALA:HB3	1:20:B:ALA:H	9	2.89
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD13	3	2.89
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE1	4	2.88
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	4	2.87
(2,1224)	1:17:B:LEU:HD21	1:45:B:GLN:HE22	6	2.87
(2,1092)	1:39:B:LEU:HD21	1:27:B:LEU:HD23	3	2.87
(2,442)	1:16:B:ALA:HB3	1:20:A:ALA:H	9	2.86
(2,1445)	1:53:A:LYS:HB2	1:21:A:PHE:HZ	7	2.85
(2,1223)	1:17:A:LEU:HD21	1:45:A:GLN:HE22	6	2.85
(2,1326)	1:40:B:GLY:HA3	1:4:B:ARG:HD3	5	2.84
(2,1325)	1:40:A:GLY:HA3	1:4:A:ARG:HD3	5	2.84
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD12	10	2.84
(2,1091)	1:39:A:LEU:HD21	1:27:A:LEU:HD23	3	2.83
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD12	10	2.81
(2,454)	1:39:B:LEU:HD11	1:16:A:ALA:HB3	6	2.8
(2,453)	1:39:A:LEU:HD11	1:16:B:ALA:HB3	6	2.79
(2,251)	1:27:A:LEU:HD13	1:44:A:GLU:HA	5	2.79
(2,1332)	1:27:B:LEU:HD22	1:50:B:PHE:H	4	2.78
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	4	2.77
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE22	2	2.77
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD22	8	2.76
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD22	8	2.76
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD11	7	2.75
(2,1246)	1:20:B:ALA:HB3	1:50:B:PHE:HE1	1	2.74
(2,1245)	1:20:A:ALA:HB3	1:50:A:PHE:HE1	1	2.74
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD12	9	2.74
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	4	2.73
(2,1623)	1:39:A:LEU:HD11	1:17:A:LEU:HA	9	2.73
(2,1224)	1:17:B:LEU:HD22	1:45:B:GLN:HE22	9	2.73
(2,164)	1:19:B:LEU:HD22	1:46:A:ILE:HB	8	2.73
(2,163)	1:19:A:LEU:HD22	1:46:B:ILE:HB	8	2.73
(2,1319)	1:39:A:LEU:HD21	1:9:A:PHE:HD2	5	2.72
(2,252)	1:27:B:LEU:HD13	1:44:B:GLU:HA	7	2.72
(2,1624)	1:39:B:LEU:HD11	1:17:B:LEU:HA	9	2.71
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG23	4	2.71
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG23	4	2.71
(2,1320)	1:39:B:LEU:HD21	1:9:B:PHE:HD2	5	2.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1091)	1:39:A:LEU:HD22	1:27:A:LEU:HD23	6	2.71
(2,104)	1:3:B:LYS:HE3	1:12:A:GLU:HG3	1	2.71
(2,103)	1:3:A:LYS:HE3	1:12:B:GLU:HG3	1	2.71
(2,1320)	1:39:B:LEU:HD22	1:9:B:PHE:HD2	8	2.7
(2,1319)	1:39:A:LEU:HD22	1:9:A:PHE:HD2	8	2.7
(2,1092)	1:39:B:LEU:HD22	1:27:B:LEU:HD23	6	2.7
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE22	2	2.7
(2,251)	1:27:A:LEU:HD13	1:44:A:GLU:HA	7	2.7
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	4	2.69
(2,104)	1:3:B:LYS:HE3	1:12:A:GLU:HG3	2	2.68
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD11	7	2.67
(2,1149)	1:20:A:ALA:HB3	1:35:A:LEU:HD23	3	2.67
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD12	9	2.67
(2,103)	1:3:A:LYS:HE3	1:12:B:GLU:HG3	2	2.67
(3,45)	1:6:A:ARG:HD3	1:8:A:GLU:HG3	6	2.66
(3,46)	1:6:B:ARG:HD3	1:8:B:GLU:HG3	6	2.65
(2,1245)	1:20:A:ALA:HB1	1:50:A:PHE:HE1	7	2.65
(2,1224)	1:17:B:LEU:HD22	1:45:B:GLN:HE22	3	2.64
(2,665)	1:48:A:ARG:HA	1:51:A:ARG:HG3	6	2.64
(2,666)	1:48:B:ARG:HA	1:51:B:ARG:HG3	6	2.63
(2,89)	1:51:A:ARG:HD3	1:59:A:TRP:HD1	2	2.61
(2,1616)	1:27:B:LEU:HD11	1:35:B:LEU:HD11	6	2.6
(2,1615)	1:27:A:LEU:HD11	1:35:A:LEU:HD11	6	2.6
(2,1246)	1:20:B:ALA:HB1	1:50:B:PHE:HE1	7	2.6
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	7	2.59
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	1	2.58
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	7	2.58
(2,1624)	1:39:B:LEU:HD13	1:17:B:LEU:HA	2	2.58
(2,1623)	1:39:A:LEU:HD13	1:17:A:LEU:HA	2	2.58
(2,1319)	1:39:A:LEU:HD23	1:9:A:PHE:HD2	10	2.58
(2,452)	1:39:B:LEU:HD12	1:39:A:LEU:HD12	8	2.58
(2,451)	1:39:A:LEU:HD12	1:39:B:LEU:HD12	8	2.58
(2,438)	1:20:B:ALA:HB1	1:20:A:ALA:H	4	2.58
(2,1223)	1:17:A:LEU:HD22	1:45:A:GLN:HE22	3	2.57
(2,1150)	1:20:B:ALA:HB3	1:35:B:LEU:HD23	3	2.57
(3,2)	1:12:B:GLU:HB2	1:39:A:LEU:HA	4	2.56
(2,452)	1:39:B:LEU:HD12	1:39:A:LEU:HD11	10	2.56
(2,451)	1:39:A:LEU:HD11	1:39:B:LEU:HD12	10	2.56
(2,1223)	1:17:A:LEU:HD21	1:45:A:GLN:HE22	9	2.55
(2,452)	1:39:B:LEU:HD11	1:39:A:LEU:HD11	4	2.55
(2,451)	1:39:A:LEU:HD11	1:39:B:LEU:HD11	4	2.55
(2,252)	1:27:B:LEU:HD13	1:44:B:GLU:HA	5	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG22	5	2.54
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	1	2.53
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG22	5	2.53
(2,1624)	1:39:B:LEU:HD12	1:17:B:LEU:HA	3	2.52
(2,1320)	1:39:B:LEU:HD23	1:9:B:PHE:HD2	10	2.52
(2,1319)	1:39:A:LEU:HD21	1:9:A:PHE:HD2	4	2.52
(2,441)	1:16:A:ALA:HB2	1:20:B:ALA:H	5	2.52
(2,215)	1:27:A:LEU:HD21	1:21:A:PHE:HE1	9	2.52
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	3	2.51
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	3	2.51
(2,1631)	1:39:A:LEU:HD12	1:9:A:PHE:HB2	5	2.51
(2,778)	1:9:B:PHE:HA	1:4:B:ARG:HB2	3	2.51
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD12	6	2.51
(2,1632)	1:39:B:LEU:HD12	1:9:B:PHE:HB2	5	2.5
(2,1623)	1:39:A:LEU:HD11	1:17:A:LEU:HA	10	2.5
(2,1320)	1:39:B:LEU:HD21	1:9:B:PHE:HD2	4	2.5
(2,1092)	1:39:B:LEU:HD21	1:27:B:LEU:HD21	1	2.5
(2,777)	1:9:A:PHE:HA	1:4:A:ARG:HB2	3	2.5
(2,103)	1:3:A:LYS:HE2	1:12:B:GLU:HG3	5	2.5
(2,1091)	1:39:A:LEU:HD22	1:27:A:LEU:HD22	5	2.49
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD12	7	2.49
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD12	7	2.49
(2,442)	1:16:B:ALA:HB2	1:20:A:ALA:H	5	2.49
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD12	6	2.49
(2,104)	1:3:B:LYS:HE2	1:12:A:GLU:HG3	5	2.49
(2,1624)	1:39:B:LEU:HD11	1:17:B:LEU:HA	10	2.48
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	10	2.48
(2,1091)	1:39:A:LEU:HD21	1:27:A:LEU:HD21	1	2.48
(2,90)	1:51:B:ARG:HD3	1:59:B:TRP:HD1	2	2.48
(2,1224)	1:17:B:LEU:HD22	1:45:B:GLN:HE22	5	2.47
(2,437)	1:20:A:ALA:HB2	1:20:B:ALA:H	5	2.47
(2,1623)	1:39:A:LEU:HD12	1:17:A:LEU:HA	3	2.46
(2,1223)	1:17:A:LEU:HD21	1:45:A:GLN:HE22	2	2.46
(3,1)	1:12:A:GLU:HB2	1:39:B:LEU:HA	4	2.45
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE21	1	2.45
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	4	2.44
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	4	2.44
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE21	1	2.44
(2,438)	1:20:B:ALA:HB2	1:20:A:ALA:H	5	2.44
(2,216)	1:27:B:LEU:HD21	1:21:B:PHE:HE1	9	2.44
(3,74)	1:39:B:LEU:HG	1:15:A:LYS:HE3	7	2.43
(2,1223)	1:17:A:LEU:HD22	1:45:A:GLN:HE22	5	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1059)	1:27:A:LEU:HD22	1:50:A:PHE:HB2	4	2.43
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	4	2.42
(2,1092)	1:39:B:LEU:HD22	1:27:B:LEU:HD22	5	2.42
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	10	2.41
(2,1224)	1:17:B:LEU:HD21	1:45:B:GLN:HE22	2	2.41
(2,189)	1:17:A:LEU:HD23	1:13:A:GLN:HG2	7	2.41
(2,1245)	1:20:A:ALA:HB2	1:50:A:PHE:HE1	4	2.4
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	9	2.4
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	5	2.4
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD11	8	2.4
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD11	8	2.4
(2,68)	1:65:B:GLU:HA	1:53:B:LYS:HD2	10	2.4
(2,1446)	1:53:B:LYS:HB2	1:21:B:PHE:HZ	4	2.39
(2,1394)	1:46:B:ILE:HD13	1:36:B:SER:HG	4	2.39
(2,68)	1:25:B:ARG:HA	1:19:A:LEU:HD21	4	2.39
(2,67)	1:65:A:GLU:HA	1:53:A:LYS:HD2	10	2.39
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB1	5	2.39
(2,16)	1:36:B:SER:HB3	1:46:B:ILE:HD11	1	2.39
(2,1624)	1:39:B:LEU:HD12	1:17:B:LEU:HA	8	2.38
(2,1623)	1:39:A:LEU:HD12	1:17:A:LEU:HA	8	2.38
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	5	2.38
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	10	2.38
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	10	2.38
(2,15)	1:36:A:SER:HB3	1:46:A:ILE:HD11	1	2.38
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB3	4	2.38
(2,1067)	1:27:A:LEU:HD21	1:32:A:ARG:HB3	5	2.37
(2,1574)	1:27:B:LEU:HD13	1:46:B:ILE:H	5	2.35
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	9	2.35
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE22	8	2.35
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE22	8	2.35
(2,215)	1:27:A:LEU:HD21	1:21:A:PHE:HD1	1	2.35
(3,73)	1:39:A:LEU:HG	1:15:B:LYS:HE3	7	2.34
(2,1068)	1:27:B:LEU:HD21	1:32:B:ARG:HB3	10	2.34
(2,216)	1:27:B:LEU:HD21	1:21:B:PHE:HD1	1	2.34
(2,190)	1:17:B:LEU:HD23	1:13:B:GLN:HG2	7	2.34
(2,1623)	1:39:A:LEU:HD11	1:17:A:LEU:HA	6	2.33
(2,1067)	1:27:A:LEU:HD21	1:32:A:ARG:HB3	10	2.33
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD13	10	2.33
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	1	2.33
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	1	2.33
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG21	2	2.32
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	9	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1624)	1:39:B:LEU:HD11	1:17:B:LEU:HA	6	2.32
(2,1325)	1:40:A:GLY:HA3	1:4:A:ARG:HD3	4	2.32
(2,647)	1:53:A:LYS:HA	1:63:A:GLN:HG3	1	2.32
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD13	10	2.32
(2,163)	1:19:A:LEU:HD23	1:46:B:ILE:HB	10	2.32
(2,1240)	1:20:B:ALA:HB3	1:39:B:LEU:HD21	3	2.31
(2,648)	1:53:B:LYS:HA	1:63:B:GLN:HG3	1	2.31
(2,164)	1:19:B:LEU:HD23	1:46:A:ILE:HB	10	2.31
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	9	2.3
(2,1627)	1:40:A:GLY:HA3	1:41:A:LEU:HD12	5	2.3
(2,1091)	1:39:A:LEU:HD22	1:27:A:LEU:HD22	10	2.3
(2,817)	1:62:A:PRO:HD2	1:60:A:SER:HG	3	2.3
(2,438)	1:20:B:ALA:HB3	1:20:A:ALA:H	6	2.3
(2,437)	1:20:A:ALA:HB3	1:20:B:ALA:H	6	2.3
(2,215)	1:27:A:LEU:HD23	1:21:A:PHE:HE1	3	2.3
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB1	5	2.3
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	8	2.29
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	8	2.29
(2,1636)	1:41:B:LEU:HD12	1:13:B:GLN:HG2	6	2.29
(2,771)	1:54:A:GLU:HA	1:21:A:PHE:HE1	4	2.29
(2,647)	1:53:A:LYS:HA	1:63:A:GLN:HG3	7	2.29
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD11	4	2.29
(2,818)	1:62:B:PRO:HD2	1:60:B:SER:HG	3	2.28
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG21	8	2.28
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG21	8	2.28
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE22	7	2.28
(2,68)	1:25:B:ARG:HA	1:19:A:LEU:HD21	8	2.28
(2,67)	1:25:A:ARG:HA	1:19:B:LEU:HD21	8	2.28
(2,1635)	1:41:A:LEU:HD12	1:13:A:GLN:HG2	6	2.27
(2,1628)	1:40:B:GLY:HA3	1:41:B:LEU:HD12	5	2.27
(2,1573)	1:27:A:LEU:HD12	1:46:A:ILE:H	5	2.27
(2,1326)	1:40:B:GLY:HA3	1:4:B:ARG:HD3	4	2.27
(2,1092)	1:39:B:LEU:HD22	1:27:B:LEU:HD22	10	2.27
(2,1060)	1:27:B:LEU:HD22	1:50:B:PHE:HB2	4	2.27
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE22	7	2.27
(2,1402)	1:46:B:ILE:HD13	1:43:B:GLU:H	4	2.26
(2,452)	1:39:B:LEU:HD11	1:39:A:LEU:HD11	2	2.26
(2,451)	1:39:A:LEU:HD11	1:39:B:LEU:HD11	2	2.26
(2,1575)	1:27:A:LEU:HD11	1:51:A:ARG:H	10	2.25
(2,1446)	1:53:B:LYS:HB2	1:21:B:PHE:HZ	1	2.25
(2,1246)	1:20:B:ALA:HB2	1:50:B:PHE:HE1	4	2.25
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG21	2	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1445)	1:53:A:LYS:HB2	1:21:A:PHE:HZ	1	2.24
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD13	4	2.24
(2,648)	1:53:B:LYS:HA	1:63:B:GLN:HG3	7	2.24
(2,1576)	1:27:B:LEU:HD11	1:51:B:ARG:H	10	2.23
(2,1239)	1:20:A:ALA:HB3	1:39:A:LEU:HD21	3	2.23
(2,471)	1:19:A:LEU:HD22	1:19:B:LEU:HG	10	2.23
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD11	4	2.23
(2,1320)	1:39:B:LEU:HD22	1:9:B:PHE:HD2	3	2.21
(2,472)	1:19:B:LEU:HD22	1:19:A:LEU:HG	10	2.21
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD22	4	2.21
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD12	1	2.21
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD12	1	2.21
(2,1574)	1:27:B:LEU:HD12	1:46:B:ILE:H	6	2.2
(2,1573)	1:27:A:LEU:HD11	1:46:A:ILE:H	6	2.2
(2,1402)	1:46:B:ILE:HD12	1:43:B:GLU:H	3	2.2
(2,1224)	1:17:B:LEU:HD22	1:45:B:GLN:HE22	7	2.2
(2,216)	1:27:B:LEU:HD22	1:21:B:PHE:HD1	7	2.2
(2,1631)	1:39:A:LEU:HD12	1:9:A:PHE:HB2	10	2.19
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD12	3	2.19
(2,216)	1:27:B:LEU:HD22	1:21:B:PHE:HE1	5	2.19
(2,1319)	1:39:A:LEU:HD22	1:9:A:PHE:HD2	3	2.18
(2,1223)	1:17:A:LEU:HD22	1:45:A:GLN:HE22	7	2.18
(2,1061)	1:27:A:LEU:HD22	1:50:A:PHE:HB3	4	2.18
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD22	8	2.18
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD22	8	2.18
(2,461)	1:49:A:TRP:HD1	1:14:A:LYS:HE3	10	2.18
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD23	9	2.18
(2,1622)	1:39:B:LEU:HD12	1:18:B:ASP:H	8	2.17
(2,1621)	1:39:A:LEU:HD12	1:18:A:ASP:H	8	2.17
(2,215)	1:27:A:LEU:HD22	1:21:A:PHE:HD1	7	2.17
(2,164)	1:19:B:LEU:HD21	1:24:A:ASP:HB2	5	2.17
(2,1901)	1:59:A:TRP:H	1:62:A:PRO:HD2	3	2.16
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD21	4	2.16
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD21	4	2.16
(2,1632)	1:39:B:LEU:HD12	1:9:B:PHE:HB2	10	2.16
(2,1240)	1:20:B:ALA:HB2	1:39:B:LEU:HD23	8	2.16
(2,1239)	1:20:A:ALA:HB2	1:39:A:LEU:HD23	8	2.16
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD21	4	2.16
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD12	3	2.16
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD22	4	2.16
(2,15)	1:36:A:SER:HB3	1:46:A:ILE:HD11	7	2.16
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD13	9	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1152)	1:46:B:ILE:HG21	1:27:B:LEU:HD22	4	2.15
(2,1151)	1:46:A:ILE:HG21	1:27:A:LEU:HD22	4	2.15
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	2	2.15
(2,462)	1:49:B:TRP:HD1	1:14:B:LYS:HE3	10	2.15
(2,260)	1:45:B:GLN:HG3	1:48:B:ARG:HD3	6	2.15
(2,259)	1:45:A:GLN:HG3	1:48:A:ARG:HD3	6	2.15
(2,1401)	1:46:A:ILE:HD13	1:43:A:GLU:H	4	2.14
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD13	4	2.14
(2,192)	1:17:B:LEU:HD22	1:14:B:LYS:HB3	8	2.14
(2,191)	1:17:A:LEU:HD22	1:14:A:LYS:HB3	8	2.14
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	3	2.13
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG23	10	2.13
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG23	10	2.13
(2,1401)	1:46:A:ILE:HD12	1:43:A:GLU:H	3	2.13
(2,20)	1:5:B:PRO:HA	1:4:B:ARG:HG3	1	2.13
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	9	2.12
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD21	8	2.12
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD21	8	2.12
(2,252)	1:27:B:LEU:HD12	1:44:B:GLU:HA	6	2.12
(2,226)	1:46:B:ILE:HD13	1:9:B:PHE:HB2	7	2.12
(2,216)	1:27:B:LEU:HD23	1:21:B:PHE:HE1	3	2.12
(2,19)	1:5:A:PRO:HA	1:4:A:ARG:HG3	1	2.12
(2,1624)	1:39:B:LEU:HD11	1:17:B:LEU:HA	5	2.11
(2,1401)	1:46:A:ILE:HD13	1:43:A:GLU:H	6	2.11
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD11	4	2.11
(2,1150)	1:20:B:ALA:HB3	1:35:B:LEU:HD21	6	2.11
(2,1149)	1:20:A:ALA:HB3	1:35:A:LEU:HD21	6	2.11
(2,437)	1:20:A:ALA:HB1	1:20:B:ALA:H	4	2.11
(2,251)	1:27:A:LEU:HD12	1:44:A:GLU:HA	6	2.11
(2,1402)	1:46:B:ILE:HD13	1:43:B:GLU:H	6	2.1
(2,1393)	1:46:A:ILE:HD13	1:36:A:SER:HG	4	2.1
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG22	1	2.1
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG22	1	2.1
(2,225)	1:46:A:ILE:HD13	1:9:A:PHE:HB2	7	2.1
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	6	2.09
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	6	2.09
(3,1)	1:12:A:GLU:HB2	1:39:B:LEU:HA	10	2.09
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD13	9	2.09
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	2	2.09
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD23	9	2.09
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD12	5	2.09
(2,163)	1:19:A:LEU:HD21	1:24:B:ASP:HB2	5	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,95)	1:59:A:TRP:HB2	1:55:A:GLN:H	6	2.08
(2,1632)	1:39:B:LEU:HD11	1:9:B:PHE:HB2	4	2.08
(2,1623)	1:39:A:LEU:HD11	1:17:A:LEU:HA	5	2.08
(2,1402)	1:46:B:ILE:HD13	1:43:B:GLU:H	8	2.08
(2,1401)	1:46:A:ILE:HD13	1:43:A:GLU:H	8	2.08
(2,848)	1:51:B:ARG:HD2	1:52:B:ARG:HA	10	2.08
(2,847)	1:51:A:ARG:HD2	1:52:A:ARG:HA	10	2.08
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD21	4	2.08
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD23	10	2.08
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD12	5	2.08
(2,317)	1:59:A:TRP:HB2	1:55:A:GLN:H	6	2.08
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB3	9	2.08
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	2	2.08
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	9	2.07
(3,96)	1:59:B:TRP:HB2	1:55:B:GLN:H	6	2.07
(2,1068)	1:27:B:LEU:HD21	1:32:B:ARG:HB3	8	2.07
(2,1067)	1:27:A:LEU:HD21	1:32:A:ARG:HB3	8	2.07
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE21	10	2.07
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD23	10	2.07
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD22	4	2.07
(2,318)	1:59:B:TRP:HB2	1:55:B:GLN:H	6	2.07
(2,260)	1:54:B:GLU:HG3	1:59:B:TRP:HB2	8	2.07
(2,259)	1:54:A:GLU:HG3	1:59:A:TRP:HB2	8	2.07
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD12	7	2.06
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	2	2.06
(2,16)	1:36:B:SER:HB3	1:46:B:ILE:HD11	7	2.06
(2,1678)	1:30:B:GLU:HA	1:33:B:ARG:HD3	3	2.05
(2,1678)	1:30:B:GLU:HA	1:33:B:ARG:HD3	10	2.05
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	4	2.05
(2,452)	1:39:B:LEU:HD13	1:39:A:LEU:HD13	3	2.05
(2,451)	1:39:A:LEU:HD13	1:39:B:LEU:HD13	3	2.05
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD21	3	2.05
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD22	8	2.05
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD21	3	2.05
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD22	8	2.05
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD12	7	2.05
(2,190)	1:17:B:LEU:HD23	1:13:B:GLN:HG2	10	2.05
(2,189)	1:17:A:LEU:HD23	1:13:A:GLN:HG2	10	2.05
(2,68)	1:65:B:GLU:HA	1:53:B:LYS:HD2	2	2.05
(2,67)	1:65:A:GLU:HA	1:53:A:LYS:HD2	2	2.05
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	6	2.05
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	2	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1062)	1:27:B:LEU:HD22	1:50:B:PHE:HB3	4	2.04
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE21	10	2.04
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	6	2.04
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	4	2.03
(2,1067)	1:27:A:LEU:HD21	1:32:A:ARG:HB3	7	2.03
(2,260)	1:45:B:GLN:HG3	1:48:B:ARG:HD3	1	2.03
(2,259)	1:45:A:GLN:HG3	1:48:A:ARG:HD3	1	2.03
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	2	2.02
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	6	2.02
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	1	2.02
(2,462)	1:49:B:TRP:HD1	1:14:B:LYS:HE3	5	2.02
(2,461)	1:49:A:TRP:HD1	1:14:A:LYS:HE3	5	2.02
(2,253)	1:27:A:LEU:HD11	1:32:A:ARG:HB2	1	2.02
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	6	2.01
(2,1622)	1:39:B:LEU:HD12	1:18:B:ASP:H	9	2.01
(2,1574)	1:27:B:LEU:HD13	1:46:B:ILE:H	7	2.01
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	10	2.01
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD13	8	2.01
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD13	8	2.01
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	4	2.01
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG23	4	2.01
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	1	2.01
(2,254)	1:27:B:LEU:HD11	1:32:B:ARG:HB2	1	2.01
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	7	2.01
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	2	2.0
(3,154)	1:11:B:GLU:H	1:13:B:GLN:HG3	2	2.0
(3,153)	1:11:A:GLU:H	1:13:A:GLN:HG3	2	2.0
(2,1690)	1:9:B:PHE:HB3	1:14:B:LYS:HG3	2	2.0
(2,1689)	1:9:A:PHE:HB3	1:14:A:LYS:HG3	2	2.0
(2,1677)	1:30:A:GLU:HA	1:33:A:ARG:HD3	10	2.0
(2,1632)	1:39:B:LEU:HD12	1:9:B:PHE:HB2	9	2.0
(2,1631)	1:39:A:LEU:HD11	1:9:A:PHE:HB2	4	2.0
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	10	2.0
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB2	5	2.0
(2,190)	1:17:B:LEU:HD23	1:13:B:GLN:HG2	9	2.0
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB2	10	2.0
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	2	1.99
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	10	1.99
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	3	1.99
(2,1601)	1:53:A:LYS:HG3	1:21:A:PHE:HZ	4	1.99
(2,1573)	1:27:A:LEU:HD13	1:46:A:ILE:H	7	1.99
(2,1092)	1:39:B:LEU:HD22	1:27:B:LEU:HD23	2	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1091)	1:39:A:LEU:HD22	1:27:A:LEU:HD23	2	1.99
(2,778)	1:9:B:PHE:HA	1:4:B:ARG:HB2	10	1.99
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	7	1.99
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	10	1.98
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	10	1.98
(2,1394)	1:46:B:ILE:HD13	1:36:B:SER:HG	8	1.98
(2,1393)	1:46:A:ILE:HD13	1:36:A:SER:HG	8	1.98
(2,180)	1:16:B:ALA:HB1	1:15:B:LYS:HE3	8	1.98
(2,179)	1:16:A:ALA:HB1	1:15:A:LYS:HE3	8	1.98
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	10	1.97
(2,1068)	1:27:B:LEU:HD21	1:32:B:ARG:HB3	7	1.97
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	9	1.97
(2,777)	1:9:A:PHE:HA	1:4:A:ARG:HB2	10	1.97
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	2	1.97
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	3	1.97
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	6	1.96
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	6	1.96
(2,2187)	1:54:A:GLU:H	1:21:A:PHE:HE1	4	1.96
(2,1616)	1:27:B:LEU:HD11	1:35:B:LEU:HD11	8	1.96
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG23	7	1.96
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG23	7	1.96
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	5	1.96
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	6	1.96
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	6	1.96
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB2	5	1.96
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB2	10	1.96
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD21	5	1.95
(2,1632)	1:39:B:LEU:HD13	1:9:B:PHE:HB2	3	1.95
(2,1615)	1:27:A:LEU:HD11	1:35:A:LEU:HD11	8	1.95
(2,1402)	1:46:B:ILE:HD12	1:43:B:GLU:H	2	1.95
(2,442)	1:16:B:ALA:HB3	1:20:A:ALA:H	8	1.95
(2,441)	1:16:A:ALA:HB3	1:20:B:ALA:H	8	1.95
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	2	1.95
(2,182)	1:16:B:ALA:HB1	1:15:B:LYS:HB3	8	1.95
(2,181)	1:16:A:ALA:HB1	1:15:A:LYS:HB3	8	1.95
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD21	5	1.94
(2,1621)	1:39:A:LEU:HD12	1:18:A:ASP:H	9	1.94
(2,1401)	1:46:A:ILE:HD12	1:43:A:GLU:H	2	1.94
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	4	1.94
(2,453)	1:39:A:LEU:HD11	1:16:B:ALA:HB2	2	1.94
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD22	4	1.94
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	3	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	2	1.93
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	6	1.93
(3,67)	1:63:A:GLN:HG2	1:54:A:GLU:HA	10	1.93
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	3	1.93
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	3	1.93
(2,1631)	1:39:A:LEU:HD13	1:9:A:PHE:HB2	3	1.93
(2,1622)	1:39:B:LEU:HD12	1:18:B:ASP:H	5	1.93
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD13	4	1.93
(2,86)	1:6:B:ARG:HD3	1:4:B:ARG:HA	2	1.93
(2,85)	1:6:A:ARG:HD3	1:4:A:ARG:HA	2	1.93
(3,2)	1:12:B:GLU:HB2	1:39:A:LEU:HA	10	1.92
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	3	1.92
(2,1411)	1:46:A:ILE:HG23	1:50:A:PHE:HD1	7	1.92
(2,944)	1:54:B:GLU:HG2	1:21:B:PHE:HZ	4	1.92
(2,599)	1:50:A:PHE:HA	1:53:A:LYS:HB3	5	1.92
(2,251)	1:27:A:LEU:HD11	1:44:A:GLU:HA	3	1.92
(2,195)	1:18:A:ASP:HA	1:19:B:LEU:HD22	7	1.92
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	1	1.92
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	1	1.92
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	5	1.91
(3,115)	1:3:A:LYS:HG3	1:1:A:MET:HA	9	1.91
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	2	1.91
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD23	2	1.91
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD23	2	1.91
(2,1621)	1:39:A:LEU:HD12	1:18:A:ASP:H	5	1.91
(2,1573)	1:27:A:LEU:HD11	1:46:A:ILE:H	3	1.91
(2,1412)	1:46:B:ILE:HG23	1:50:B:PHE:HD1	7	1.91
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG23	4	1.91
(2,454)	1:39:B:LEU:HD11	1:16:A:ALA:HB2	2	1.91
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD23	1	1.91
(2,180)	1:16:B:ALA:HB3	1:15:A:LYS:HE3	9	1.91
(2,163)	1:19:A:LEU:HD22	1:46:B:ILE:HB	3	1.91
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	6	1.91
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	5	1.9
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	4	1.9
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	4	1.9
(3,116)	1:3:B:LYS:HG3	1:1:B:MET:HA	9	1.9
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	6	1.9
(3,68)	1:63:B:GLN:HG2	1:54:B:GLU:HA	10	1.9
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	3	1.9
(2,817)	1:62:A:PRO:HD2	1:60:A:SER:HG	6	1.9
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD23	1	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1631)	1:39:A:LEU:HD12	1:9:A:PHE:HB2	9	1.89
(2,1311)	1:39:A:LEU:HD22	1:17:A:LEU:HA	2	1.89
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD11	1	1.89
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD11	1	1.89
(2,818)	1:62:B:PRO:HD2	1:60:B:SER:HG	6	1.89
(2,775)	1:27:A:LEU:HA	1:32:A:ARG:HE	9	1.89
(2,600)	1:50:B:PHE:HA	1:53:B:LYS:HB3	5	1.89
(2,189)	1:17:A:LEU:HD23	1:13:A:GLN:HG2	9	1.89
(2,1632)	1:39:B:LEU:HD12	1:9:B:PHE:HB2	8	1.88
(2,1631)	1:39:A:LEU:HD12	1:9:A:PHE:HB2	8	1.88
(2,1312)	1:39:B:LEU:HD22	1:17:B:LEU:HA	2	1.88
(2,1150)	1:20:B:ALA:HB2	1:35:B:LEU:HD22	8	1.88
(2,1149)	1:20:A:ALA:HB2	1:35:A:LEU:HD22	8	1.88
(2,1092)	1:39:B:LEU:HD21	1:27:B:LEU:HD21	9	1.88
(2,1067)	1:27:A:LEU:HD21	1:32:A:ARG:HB3	4	1.88
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	3	1.88
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	6	1.88
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	6	1.87
(2,1901)	1:59:A:TRP:H	1:62:A:PRO:HD2	6	1.87
(2,1574)	1:27:B:LEU:HD11	1:46:B:ILE:H	3	1.87
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	9	1.87
(2,456)	1:39:B:LEU:HD12	1:15:A:LYS:HE3	7	1.87
(2,179)	1:16:A:ALA:HB3	1:15:B:LYS:HE3	9	1.87
(2,164)	1:19:B:LEU:HD21	1:24:A:ASP:HB2	1	1.87
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	7	1.87
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	8	1.86
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	8	1.86
(3,62)	1:27:B:LEU:HB2	1:21:B:PHE:H	3	1.86
(2,1677)	1:30:A:GLU:HA	1:33:A:ARG:HD3	3	1.86
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	5	1.86
(2,776)	1:27:B:LEU:HA	1:32:B:ARG:HE	9	1.86
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD12	1	1.86
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD12	1	1.86
(2,163)	1:19:A:LEU:HD21	1:24:B:ASP:HB2	1	1.86
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	7	1.86
(2,2436)	1:27:B:LEU:HD12	1:47:B:GLU:H	1	1.85
(2,1622)	1:39:B:LEU:HD13	1:18:B:ASP:H	3	1.85
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD13	6	1.85
(2,1091)	1:39:A:LEU:HD21	1:27:A:LEU:HD21	9	1.85
(2,216)	1:27:B:LEU:HD22	1:21:B:PHE:HE1	8	1.85
(2,215)	1:27:A:LEU:HD22	1:21:A:PHE:HE1	8	1.85
(2,196)	1:18:B:ASP:HA	1:19:A:LEU:HD22	7	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2435)	1:27:A:LEU:HD12	1:47:A:GLU:H	1	1.84
(2,1626)	1:41:B:LEU:HD13	1:36:B:SER:HA	5	1.84
(2,1402)	1:46:B:ILE:HD13	1:43:B:GLU:H	9	1.84
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD13	6	1.84
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	10	1.84
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	10	1.84
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD2	2	1.84
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD2	2	1.84
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD23	7	1.84
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD23	7	1.84
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG23	4	1.84
(2,1625)	1:41:A:LEU:HD13	1:36:A:SER:HA	5	1.83
(2,1319)	1:39:A:LEU:HD21	1:9:A:PHE:HD2	6	1.83
(2,1068)	1:27:B:LEU:HD21	1:32:B:ARG:HB3	4	1.83
(2,252)	1:27:B:LEU:HD11	1:44:B:GLU:HA	3	1.83
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG23	4	1.83
(2,226)	1:46:B:ILE:HD12	1:9:B:PHE:HB2	4	1.83
(2,190)	1:17:B:LEU:HD22	1:13:B:GLN:HG2	8	1.83
(2,10)	1:16:B:ALA:HB1	1:39:A:LEU:HB2	8	1.83
(2,9)	1:16:A:ALA:HB1	1:39:B:LEU:HB2	8	1.83
(3,61)	1:27:A:LEU:HB2	1:21:A:PHE:H	4	1.82
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	9	1.82
(2,1576)	1:27:B:LEU:HD12	1:51:B:ARG:H	1	1.82
(2,1575)	1:27:A:LEU:HD12	1:51:A:ARG:H	1	1.82
(2,1400)	1:46:B:ILE:HD12	1:44:B:GLU:H	4	1.82
(2,1311)	1:39:A:LEU:HD22	1:17:A:LEU:HA	10	1.82
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	9	1.82
(2,225)	1:46:A:ILE:HD12	1:9:A:PHE:HB2	4	1.82
(2,189)	1:17:A:LEU:HD22	1:13:A:GLN:HG2	8	1.82
(2,164)	1:19:B:LEU:HD22	1:46:A:ILE:HB	3	1.82
(3,61)	1:27:A:LEU:HB2	1:21:A:PHE:H	3	1.81
(2,1576)	1:27:B:LEU:HD12	1:51:B:ARG:H	8	1.81
(2,1575)	1:27:A:LEU:HD12	1:51:A:ARG:H	8	1.81
(2,1401)	1:46:A:ILE:HD13	1:43:A:GLU:H	9	1.81
(2,1393)	1:46:A:ILE:HD13	1:36:A:SER:HG	10	1.81
(2,1312)	1:39:B:LEU:HD22	1:17:B:LEU:HA	10	1.81
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD12	2	1.81
(2,180)	1:16:B:ALA:HB2	1:15:A:LYS:HE3	2	1.81
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	3	1.81
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	3	1.81
(3,90)	1:26:B:ARG:HA	1:31:B:TRP:HA	9	1.8
(3,89)	1:26:A:ARG:HA	1:31:A:TRP:HA	9	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2437)	1:53:A:LYS:H	1:21:A:PHE:HE1	4	1.8
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD22	9	1.8
(2,1401)	1:46:A:ILE:HD11	1:43:A:GLU:H	7	1.8
(2,1399)	1:46:A:ILE:HD12	1:44:A:GLU:H	4	1.8
(2,1320)	1:39:B:LEU:HD21	1:9:B:PHE:HD2	6	1.8
(2,1320)	1:39:B:LEU:HD22	1:9:B:PHE:HD2	9	1.8
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD12	2	1.8
(2,1149)	1:20:A:ALA:HB1	1:35:A:LEU:HD22	9	1.8
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD22	5	1.8
(2,455)	1:39:A:LEU:HD12	1:15:B:LYS:HE3	7	1.8
(2,298)	1:16:B:ALA:H	1:38:A:ARG:HB3	7	1.8
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG22	1	1.8
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG22	1	1.8
(2,179)	1:16:A:ALA:HB2	1:15:B:LYS:HE3	2	1.8
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB3	9	1.8
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	4	1.79
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD22	9	1.79
(2,1622)	1:39:B:LEU:HD11	1:18:B:ASP:H	2	1.79
(2,1621)	1:39:A:LEU:HD11	1:18:A:ASP:H	2	1.79
(2,1402)	1:46:B:ILE:HD11	1:43:B:GLU:H	1	1.79
(2,1402)	1:46:B:ILE:HD11	1:43:B:GLU:H	7	1.79
(2,1394)	1:46:B:ILE:HD13	1:36:B:SER:HG	10	1.79
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	7	1.79
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	4	1.78
(2,1648)	1:39:B:LEU:HD11	1:13:B:GLN:HG2	4	1.78
(2,1401)	1:46:A:ILE:HD11	1:43:A:GLU:H	1	1.78
(2,1400)	1:46:B:ILE:HD12	1:44:B:GLU:H	6	1.78
(2,1399)	1:46:A:ILE:HD12	1:44:A:GLU:H	6	1.78
(2,1331)	1:27:A:LEU:HD22	1:50:A:PHE:H	9	1.78
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG23	2	1.78
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	10	1.78
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	10	1.78
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	9	1.77
(2,1621)	1:39:A:LEU:HD13	1:18:A:ASP:H	3	1.77
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE1	4	1.77
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD11	8	1.77
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD11	8	1.77
(2,298)	1:16:B:ALA:H	1:39:A:LEU:HB2	5	1.77
(2,297)	1:16:A:ALA:H	1:39:B:LEU:HB2	5	1.77
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG23	2	1.77
(2,225)	1:46:A:ILE:HD13	1:9:A:PHE:HB2	5	1.77
(2,2306)	1:58:B:GLY:H	1:60:B:SER:HG	1	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2305)	1:58:A:GLY:H	1:60:A:SER:HG	1	1.76
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD11	4	1.76
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	3	1.76
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	3	1.76
(2,1616)	1:27:B:LEU:HD11	1:35:B:LEU:HD13	1	1.76
(2,1615)	1:27:A:LEU:HD11	1:35:A:LEU:HD13	1	1.76
(2,1332)	1:27:B:LEU:HD22	1:50:B:PHE:H	9	1.76
(2,1312)	1:39:B:LEU:HD23	1:17:B:LEU:HA	8	1.76
(2,1312)	1:39:B:LEU:HD21	1:17:B:LEU:HA	9	1.76
(2,1311)	1:39:A:LEU:HD23	1:17:A:LEU:HA	8	1.76
(2,1311)	1:39:A:LEU:HD21	1:17:A:LEU:HA	9	1.76
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	4	1.76
(2,947)	1:54:A:GLU:HG2	1:21:A:PHE:HE1	4	1.76
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	9	1.76
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	7	1.75
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	7	1.75
(2,1647)	1:39:A:LEU:HD11	1:13:A:GLN:HG2	4	1.75
(2,1400)	1:46:B:ILE:HD12	1:44:B:GLU:H	8	1.75
(2,1399)	1:46:A:ILE:HD12	1:44:A:GLU:H	8	1.75
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	4	1.75
(2,85)	1:6:A:ARG:HD3	1:4:A:ARG:HA	10	1.75
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	6	1.75
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	6	1.75
(3,153)	1:11:A:GLU:H	1:13:A:GLN:HG3	5	1.74
(2,1607)	1:16:A:ALA:HB2	1:35:A:LEU:HD23	3	1.74
(2,1576)	1:27:B:LEU:HD11	1:51:B:ARG:H	7	1.74
(2,1400)	1:46:B:ILE:HD12	1:44:B:GLU:H	10	1.74
(2,1399)	1:46:A:ILE:HD12	1:44:A:GLU:H	10	1.74
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	4	1.74
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	3	1.74
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	3	1.74
(2,235)	1:46:A:ILE:HG22	1:50:A:PHE:HZ	5	1.74
(2,216)	1:27:B:LEU:HD23	1:21:B:PHE:HE1	6	1.74
(2,91)	1:51:A:ARG:HD2	1:52:A:ARG:H	10	1.74
(3,154)	1:11:B:GLU:H	1:13:B:GLN:HG3	5	1.73
(3,1)	1:12:A:GLU:HB2	1:39:B:LEU:HA	7	1.73
(2,1909)	1:59:A:TRP:H	1:57:A:ILE:HG12	2	1.73
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	2	1.73
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	8	1.73
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	9	1.73
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	8	1.73
(2,1246)	1:20:B:ALA:HB2	1:50:B:PHE:HE1	2	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD13	10	1.73
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD13	10	1.73
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	10	1.73
(2,452)	1:39:B:LEU:HD12	1:39:A:LEU:HD12	9	1.73
(2,451)	1:39:A:LEU:HD12	1:39:B:LEU:HD12	9	1.73
(2,236)	1:46:B:ILE:HG22	1:50:B:PHE:HZ	5	1.73
(2,215)	1:27:A:LEU:HD23	1:21:A:PHE:HE1	6	1.73
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	7	1.73
(2,92)	1:51:B:ARG:HD2	1:52:B:ARG:H	10	1.73
(3,167)	1:59:A:TRP:H	1:61:A:HIS:HB3	3	1.72
(2,1576)	1:27:B:LEU:HD13	1:51:B:ARG:H	5	1.72
(2,1575)	1:27:A:LEU:HD11	1:51:A:ARG:H	7	1.72
(2,1402)	1:46:B:ILE:HD13	1:43:B:GLU:H	10	1.72
(2,1401)	1:46:A:ILE:HD13	1:43:A:GLU:H	10	1.72
(2,1319)	1:39:A:LEU:HD22	1:9:A:PHE:HD2	9	1.72
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	2	1.72
(2,1245)	1:20:A:ALA:HB2	1:50:A:PHE:HE1	2	1.72
(2,1236)	1:20:B:ALA:HB1	1:26:B:ARG:HD3	5	1.72
(2,306)	1:49:B:TRP:H	1:53:B:LYS:HB3	1	1.72
(2,305)	1:49:A:TRP:H	1:53:A:LYS:HB3	1	1.72
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB2	9	1.72
(2,226)	1:46:B:ILE:HD13	1:9:B:PHE:HB2	5	1.72
(2,86)	1:6:B:ARG:HD3	1:4:B:ARG:HA	10	1.72
(3,168)	1:59:B:TRP:H	1:61:B:HIS:HB3	3	1.71
(2,1588)	1:54:B:GLU:HB3	1:59:B:TRP:HB2	7	1.71
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	9	1.71
(2,1108)	1:39:B:LEU:HD22	1:17:B:LEU:HG	2	1.71
(2,1068)	1:27:B:LEU:HD21	1:32:B:ARG:HB3	5	1.71
(2,477)	1:19:A:LEU:HD22	1:19:B:LEU:HA	10	1.71
(2,298)	1:16:B:ALA:H	1:39:B:LEU:HB2	9	1.71
(2,297)	1:16:A:ALA:H	1:39:B:LEU:HB2	3	1.71
(2,297)	1:16:A:ALA:H	1:38:B:ARG:HB3	7	1.71
(2,191)	1:17:A:LEU:HD22	1:14:A:LYS:HB3	5	1.71
(2,180)	1:16:B:ALA:HB3	1:15:A:LYS:HE3	3	1.71
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	4	1.7
(2,1400)	1:46:B:ILE:HD11	1:44:B:GLU:H	2	1.7
(2,1400)	1:46:B:ILE:HD11	1:44:B:GLU:H	3	1.7
(2,1061)	1:27:A:LEU:HD22	1:50:A:PHE:HB3	9	1.7
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	9	1.7
(2,1647)	1:39:A:LEU:HD11	1:13:A:GLN:HG2	7	1.69
(2,1399)	1:46:A:ILE:HD11	1:44:A:GLU:H	2	1.69
(2,1107)	1:39:A:LEU:HD22	1:17:A:LEU:HG	2	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD22	9	1.69
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD23	10	1.69
(2,298)	1:16:B:ALA:H	1:38:A:ARG:HB3	1	1.69
(2,297)	1:16:A:ALA:H	1:39:B:LEU:HB2	1	1.69
(2,236)	1:46:B:ILE:HG22	1:9:B:PHE:HD2	8	1.69
(2,235)	1:46:A:ILE:HG22	1:9:A:PHE:HD2	8	1.69
(2,1910)	1:59:B:TRP:H	1:57:B:ILE:HG12	2	1.68
(2,1648)	1:39:B:LEU:HD11	1:13:B:GLN:HG2	7	1.68
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD21	6	1.68
(2,1401)	1:46:A:ILE:HD11	1:43:A:GLU:H	5	1.68
(2,1150)	1:20:B:ALA:HB3	1:35:B:LEU:HD22	7	1.68
(2,1150)	1:20:B:ALA:HB1	1:35:B:LEU:HD22	9	1.68
(2,1108)	1:39:B:LEU:HD21	1:17:B:LEU:HG	3	1.68
(2,1107)	1:39:A:LEU:HD21	1:17:A:LEU:HG	9	1.68
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD22	9	1.68
(2,478)	1:19:B:LEU:HD22	1:19:A:LEU:HA	10	1.68
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE21	9	1.68
(2,454)	1:39:B:LEU:HD12	1:16:A:ALA:HB1	9	1.68
(2,298)	1:16:B:ALA:H	1:39:A:LEU:HB2	3	1.68
(2,297)	1:16:A:ALA:H	1:39:A:LEU:HB2	2	1.68
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB2	9	1.68
(2,252)	1:27:B:LEU:HD13	1:44:B:GLU:HA	9	1.68
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	4	1.68
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	5	1.67
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	5	1.67
(3,2)	1:12:B:GLU:HB2	1:39:A:LEU:HA	7	1.67
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	8	1.67
(2,1587)	1:54:A:GLU:HB3	1:59:A:TRP:HB2	7	1.67
(2,1402)	1:46:B:ILE:HD11	1:43:B:GLU:H	5	1.67
(2,1399)	1:46:A:ILE:HD11	1:44:A:GLU:H	3	1.67
(2,1398)	1:46:B:ILE:HD12	1:35:B:LEU:H	2	1.67
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD13	5	1.67
(2,1149)	1:20:A:ALA:HB3	1:35:A:LEU:HD22	7	1.67
(2,1108)	1:39:B:LEU:HD23	1:17:B:LEU:HG	8	1.67
(2,1107)	1:39:A:LEU:HD23	1:17:A:LEU:HG	8	1.67
(2,1062)	1:27:B:LEU:HD22	1:50:B:PHE:HB3	9	1.67
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	1	1.67
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	7	1.67
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD23	10	1.67
(2,298)	1:16:B:ALA:H	1:39:A:LEU:HB2	4	1.67
(2,224)	1:45:B:GLN:HG3	1:41:B:LEU:HA	2	1.67
(2,192)	1:17:B:LEU:HD22	1:14:B:LYS:HB3	5	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD22	9	1.66
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD22	9	1.66
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD23	1	1.66
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD23	1	1.66
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	4	1.66
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	8	1.66
(2,1397)	1:46:A:ILE:HD12	1:35:A:LEU:H	2	1.66
(2,1394)	1:46:B:ILE:HD13	1:36:B:SER:HG	9	1.66
(2,1235)	1:20:A:ALA:HB1	1:26:A:ARG:HD3	5	1.66
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	7	1.66
(2,755)	1:43:A:GLU:HA	1:36:A:SER:HB2	1	1.66
(2,298)	1:16:B:ALA:H	1:39:B:LEU:HB2	2	1.66
(2,223)	1:45:A:GLN:HG3	1:41:A:LEU:HA	2	1.66
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD21	6	1.65
(2,1400)	1:46:B:ILE:HD12	1:44:B:GLU:H	9	1.65
(2,1398)	1:46:B:ILE:HD13	1:35:B:LEU:H	4	1.65
(2,1394)	1:46:B:ILE:HD12	1:36:B:SER:HG	3	1.65
(2,1344)	1:41:B:LEU:HD12	1:17:B:LEU:HD23	6	1.65
(2,1312)	1:39:B:LEU:HD22	1:17:B:LEU:HA	5	1.65
(2,1311)	1:39:A:LEU:HD22	1:17:A:LEU:HA	5	1.65
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	6	1.65
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	10	1.65
(2,251)	1:27:A:LEU:HD13	1:44:A:GLU:HA	10	1.65
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG22	5	1.65
(2,179)	1:16:A:ALA:HB2	1:15:B:LYS:HE3	3	1.65
(2,103)	1:3:A:LYS:HE3	1:12:B:GLU:HG3	3	1.65
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD22	3	1.64
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD22	3	1.64
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	1	1.64
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	1	1.64
(2,1399)	1:46:A:ILE:HD12	1:44:A:GLU:H	9	1.64
(2,1240)	1:20:B:ALA:HB3	1:39:B:LEU:HD21	1	1.64
(2,1108)	1:39:B:LEU:HD21	1:17:B:LEU:HG	9	1.64
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	7	1.64
(2,297)	1:16:A:ALA:H	1:39:B:LEU:HB2	4	1.64
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG22	5	1.64
(1,6)	1:20:A:ALA:H	1:16:A:ALA:O	9	1.64
(3,75)	1:57:A:ILE:HG12	1:61:A:HIS:HB2	2	1.63
(2,1616)	1:27:B:LEU:HD13	1:35:B:LEU:HD13	10	1.63
(2,1615)	1:27:A:LEU:HD13	1:35:A:LEU:HD13	10	1.63
(2,1393)	1:46:A:ILE:HD13	1:36:A:SER:HG	9	1.63
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	2	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	2	1.63
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD23	3	1.63
(2,252)	1:27:B:LEU:HD13	1:44:B:GLU:HA	10	1.63
(2,226)	1:46:B:ILE:HD12	1:9:B:PHE:HB2	9	1.63
(2,225)	1:46:A:ILE:HD12	1:9:A:PHE:HB2	9	1.63
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	4	1.62
(2,1239)	1:20:A:ALA:HB3	1:39:A:LEU:HD21	1	1.62
(2,1155)	1:57:A:ILE:HG21	1:58:A:GLY:H	2	1.62
(2,440)	1:20:B:ALA:HB1	1:20:A:ALA:HB1	2	1.62
(2,439)	1:20:A:ALA:HB1	1:20:B:ALA:HB1	2	1.62
(2,251)	1:27:A:LEU:HD13	1:44:A:GLU:HA	9	1.62
(2,89)	1:38:A:ARG:HD3	1:64:B:PHE:HD2	5	1.62
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB2	3	1.62
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB3	7	1.62
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD11	4	1.61
(2,1635)	1:41:A:LEU:HD11	1:13:A:GLN:HG2	4	1.61
(2,1608)	1:16:B:ALA:HB2	1:35:B:LEU:HD23	3	1.61
(2,1400)	1:46:B:ILE:HD13	1:44:B:GLU:H	1	1.61
(2,1400)	1:46:B:ILE:HD13	1:44:B:GLU:H	7	1.61
(2,1399)	1:46:A:ILE:HD13	1:44:A:GLU:H	1	1.61
(2,1399)	1:46:A:ILE:HD13	1:44:A:GLU:H	7	1.61
(2,1343)	1:41:A:LEU:HD12	1:17:A:LEU:HD23	6	1.61
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	6	1.61
(2,1107)	1:39:A:LEU:HD21	1:17:A:LEU:HG	3	1.61
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	1	1.61
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	1	1.61
(2,454)	1:39:B:LEU:HD11	1:16:A:ALA:HB3	5	1.61
(3,135)	1:27:A:LEU:H	1:31:A:TRP:HA	9	1.6
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	4	1.6
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	7	1.6
(3,76)	1:57:B:ILE:HG12	1:61:B:HIS:HB2	2	1.6
(3,4)	1:12:B:GLU:HG3	1:12:A:GLU:HB2	9	1.6
(2,2436)	1:27:B:LEU:HD12	1:47:B:GLU:H	8	1.6
(2,2435)	1:27:A:LEU:HD12	1:47:A:GLU:H	8	1.6
(2,2256)	1:64:B:PHE:H	1:61:B:HIS:HA	1	1.6
(2,2255)	1:64:A:PHE:H	1:61:A:HIS:HA	1	1.6
(2,1605)	1:54:A:GLU:HB3	1:21:A:PHE:HZ	8	1.6
(2,1576)	1:27:B:LEU:HD13	1:51:B:ARG:H	9	1.6
(2,1574)	1:27:B:LEU:HD13	1:46:B:ILE:H	10	1.6
(2,1573)	1:27:A:LEU:HD13	1:46:A:ILE:H	10	1.6
(2,1156)	1:57:B:ILE:HG21	1:58:B:GLY:H	2	1.6
(2,1057)	1:47:A:GLU:HA	1:27:A:LEU:HD22	9	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD23	3	1.6
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD13	8	1.6
(2,453)	1:39:A:LEU:HD11	1:16:B:ALA:HB3	5	1.6
(2,297)	1:16:A:ALA:H	1:39:A:LEU:HB2	9	1.6
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	8	1.6
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	4	1.6
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	8	1.6
(2,104)	1:3:B:LYS:HE3	1:12:A:GLU:HG3	3	1.6
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB3	4	1.6
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	7	1.59
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	4	1.59
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG23	2	1.59
(2,1606)	1:54:B:GLU:HB3	1:21:B:PHE:HZ	8	1.59
(2,1575)	1:27:A:LEU:HD13	1:51:A:ARG:H	9	1.59
(2,1393)	1:46:A:ILE:HD12	1:36:A:SER:HG	3	1.59
(2,1058)	1:47:B:GLU:HA	1:27:B:LEU:HD22	9	1.59
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	10	1.59
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD1	3	1.59
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	7	1.59
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD13	8	1.59
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	2	1.59
(3,3)	1:12:A:GLU:HG3	1:12:B:GLU:HB2	9	1.58
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG23	2	1.58
(2,1636)	1:41:B:LEU:HD11	1:13:B:GLN:HG2	4	1.58
(2,1635)	1:41:A:LEU:HD12	1:13:A:GLN:HG2	7	1.58
(2,1312)	1:39:B:LEU:HD22	1:17:B:LEU:HA	6	1.58
(2,1311)	1:39:A:LEU:HD22	1:17:A:LEU:HA	6	1.58
(2,1068)	1:27:B:LEU:HD22	1:32:B:ARG:HB3	2	1.58
(2,1067)	1:27:A:LEU:HD22	1:32:A:ARG:HB3	2	1.58
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	10	1.58
(2,453)	1:39:A:LEU:HD12	1:16:B:ALA:HB1	9	1.58
(2,442)	1:16:B:ALA:HB3	1:20:A:ALA:H	4	1.58
(2,442)	1:16:B:ALA:HB2	1:20:A:ALA:H	6	1.58
(2,248)	1:63:B:GLN:HG2	1:56:B:GLN:H	4	1.58
(2,76)	1:65:B:GLU:HA	1:15:B:LYS:HA	9	1.58
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB2	3	1.58
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	2	1.58
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	5	1.57
(3,136)	1:27:B:LEU:H	1:31:B:TRP:HA	9	1.57
(2,1399)	1:46:A:ILE:HD13	1:44:A:GLU:H	5	1.57
(2,956)	1:8:B:GLU:HG3	1:9:B:PHE:H	5	1.57
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	9	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	4	1.57
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD12	8	1.57
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD12	8	1.57
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD22	5	1.57
(2,441)	1:16:A:ALA:HB2	1:20:B:ALA:H	6	1.57
(2,374)	1:56:B:GLN:H	1:57:B:ILE:HG13	6	1.57
(2,373)	1:56:A:GLN:H	1:57:A:ILE:HG13	6	1.57
(2,352)	1:4:B:ARG:H	1:12:B:GLU:HG3	8	1.57
(2,351)	1:4:A:ARG:H	1:12:A:GLU:HG3	8	1.57
(2,90)	1:38:B:ARG:HD3	1:64:A:PHE:HD2	5	1.57
(2,90)	1:51:B:ARG:HD3	1:59:B:TRP:HD1	10	1.57
(2,75)	1:65:A:GLU:HA	1:15:A:LYS:HA	9	1.57
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	4	1.57
(2,1636)	1:41:B:LEU:HD12	1:13:B:GLN:HG2	7	1.56
(2,955)	1:8:A:GLU:HG3	1:9:A:PHE:H	5	1.56
(2,140)	1:55:B:GLN:HB3	1:56:B:GLN:H	10	1.56
(2,89)	1:51:A:ARG:HD3	1:59:A:TRP:HD1	10	1.56
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	5	1.55
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	5	1.55
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	5	1.55
(2,1636)	1:41:B:LEU:HD13	1:13:B:GLN:HG2	1	1.55
(2,1624)	1:39:B:LEU:HD13	1:17:B:LEU:HA	1	1.55
(2,1400)	1:46:B:ILE:HD13	1:44:B:GLU:H	5	1.55
(2,1324)	1:39:B:LEU:HD21	1:46:B:ILE:H	4	1.55
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	4	1.55
(2,454)	1:39:B:LEU:HD13	1:16:A:ALA:HB3	1	1.55
(2,453)	1:39:A:LEU:HD13	1:16:B:ALA:HB3	1	1.55
(2,441)	1:16:A:ALA:HB2	1:20:B:ALA:H	3	1.55
(2,264)	1:39:B:LEU:HD11	1:16:A:ALA:H	8	1.55
(2,215)	1:27:A:LEU:HD22	1:21:A:PHE:HE1	5	1.55
(2,193)	1:18:A:ASP:HA	1:53:A:LYS:HE3	7	1.55
(2,139)	1:55:A:GLN:HB3	1:56:A:GLN:H	10	1.55
(3,192)	1:44:B:GLU:H	1:36:B:SER:HB2	1	1.54
(3,191)	1:44:A:GLU:H	1:36:A:SER:HB2	1	1.54
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	7	1.54
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD21	7	1.54
(2,1603)	1:53:A:LYS:HB3	1:21:A:PHE:HZ	4	1.54
(2,1312)	1:39:B:LEU:HD21	1:17:B:LEU:HA	3	1.54
(2,817)	1:62:A:PRO:HD2	1:60:A:SER:HG	9	1.54
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	1	1.54
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	1	1.54
(2,263)	1:39:A:LEU:HD11	1:16:B:ALA:H	8	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,253)	1:27:A:LEU:HD13	1:32:A:ARG:HB2	7	1.54
(2,247)	1:63:A:GLN:HG2	1:56:A:GLN:H	4	1.54
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	5	1.54
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	5	1.54
(2,1623)	1:39:A:LEU:HD13	1:17:A:LEU:HA	1	1.53
(2,1108)	1:39:B:LEU:HD22	1:17:B:LEU:HG	5	1.53
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	7	1.53
(2,454)	1:39:B:LEU:HD11	1:16:A:ALA:HB1	10	1.53
(2,194)	1:18:B:ASP:HA	1:53:B:LYS:HE3	7	1.53
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD21	7	1.52
(2,1622)	1:39:B:LEU:HD11	1:18:B:ASP:H	1	1.52
(2,1323)	1:39:A:LEU:HD21	1:46:A:ILE:H	4	1.52
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD12	6	1.52
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD12	6	1.52
(2,1107)	1:39:A:LEU:HD22	1:17:A:LEU:HG	5	1.52
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	8	1.52
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	8	1.52
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	9	1.52
(2,254)	1:27:B:LEU:HD13	1:32:B:ARG:HB2	7	1.52
(2,251)	1:27:A:LEU:HD13	1:44:A:GLU:HA	2	1.52
(2,190)	1:17:B:LEU:HD21	1:53:B:LYS:HE3	1	1.52
(2,189)	1:17:A:LEU:HD21	1:53:A:LYS:HE3	1	1.52
(2,67)	1:25:A:ARG:HA	1:19:B:LEU:HD22	7	1.52
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB3	3	1.52
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB3	7	1.52
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	4	1.51
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	8	1.51
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	8	1.51
(2,1244)	1:20:B:ALA:HB2	1:35:B:LEU:HD11	10	1.51
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	2	1.51
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	2	1.51
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	6	1.51
(2,665)	1:48:A:ARG:HA	1:51:A:ARG:HG2	10	1.51
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE21	6	1.51
(2,252)	1:27:B:LEU:HD13	1:44:B:GLU:HA	2	1.51
(2,219)	1:43:A:GLU:HA	1:47:A:GLU:HG2	5	1.51
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB1	10	1.51
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB1	10	1.51
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD21	6	1.5
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	4	1.5
(2,1635)	1:41:A:LEU:HD13	1:13:A:GLN:HG2	1	1.5
(2,1574)	1:27:B:LEU:HD13	1:46:B:ILE:H	2	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1573)	1:27:A:LEU:HD13	1:46:A:ILE:H	2	1.5
(2,1397)	1:46:A:ILE:HD13	1:35:A:LEU:H	4	1.5
(2,1312)	1:39:B:LEU:HD21	1:17:B:LEU:HA	1	1.5
(2,1311)	1:39:A:LEU:HD21	1:17:A:LEU:HA	1	1.5
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	6	1.5
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	8	1.5
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	8	1.5
(2,1068)	1:27:B:LEU:HD23	1:32:B:ARG:HB3	1	1.5
(2,1067)	1:27:A:LEU:HD23	1:32:A:ARG:HB3	1	1.5
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	7	1.5
(2,666)	1:48:B:ARG:HA	1:51:B:ARG:HG2	10	1.5
(2,462)	1:49:B:TRP:HD1	1:14:B:LYS:HE3	4	1.5
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	6	1.5
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	10	1.5
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	2	1.5
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB3	9	1.5
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	7	1.49
(2,1696)	1:7:B:THR:HB	1:45:B:GLN:HB2	2	1.49
(2,1621)	1:39:A:LEU:HD11	1:18:A:ASP:H	1	1.49
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	9	1.49
(2,818)	1:62:B:PRO:HD2	1:60:B:SER:HG	9	1.49
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE21	6	1.49
(2,454)	1:39:B:LEU:HD13	1:16:A:ALA:HB2	7	1.49
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD22	8	1.49
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD22	8	1.49
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG23	10	1.49
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG23	10	1.49
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	10	1.49
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	5	1.48
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	5	1.48
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD21	6	1.48
(2,1232)	1:18:B:ASP:HA	1:49:B:TRP:HE1	7	1.48
(2,442)	1:16:B:ALA:HB2	1:20:A:ALA:H	3	1.48
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	6	1.48
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	10	1.48
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB3	6	1.48
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB3	6	1.48
(2,220)	1:43:B:GLU:HA	1:47:B:GLU:HG2	3	1.48
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD22	4	1.47
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD22	6	1.47
(2,1695)	1:7:A:THR:HB	1:45:A:GLN:HB2	2	1.47
(2,1412)	1:46:B:ILE:HG23	1:50:B:PHE:HD1	1	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1411)	1:46:A:ILE:HG23	1:50:A:PHE:HD1	1	1.47
(2,1324)	1:39:B:LEU:HD22	1:46:B:ILE:H	9	1.47
(2,1243)	1:20:A:ALA:HB2	1:35:A:LEU:HD11	10	1.47
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	3	1.47
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	3	1.47
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD1	3	1.47
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG22	5	1.47
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG22	5	1.47
(2,453)	1:39:A:LEU:HD13	1:16:B:ALA:HB2	7	1.47
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	6	1.47
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	6	1.47
(2,236)	1:46:B:ILE:HG21	1:9:B:PHE:HD2	7	1.47
(2,219)	1:43:A:GLU:HA	1:47:A:GLU:HG2	3	1.47
(2,215)	1:27:A:LEU:HD22	1:21:A:PHE:HD1	10	1.47
(2,190)	1:17:B:LEU:HD22	1:53:B:LYS:HE3	2	1.47
(2,189)	1:17:A:LEU:HD22	1:53:A:LYS:HE3	2	1.47
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	4	1.47
(2,107)	1:9:A:PHE:HB2	1:8:A:GLU:HB3	10	1.47
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB2	7	1.47
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB2	7	1.47
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	1	1.47
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	9	1.46
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD22	6	1.46
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD22	10	1.46
(2,1678)	1:30:B:GLU:HA	1:33:B:ARG:HD3	2	1.46
(2,1666)	1:57:B:ILE:HG12	1:60:B:SER:H	8	1.46
(2,1665)	1:57:A:ILE:HG12	1:60:A:SER:H	8	1.46
(2,1311)	1:39:A:LEU:HD21	1:17:A:LEU:HA	3	1.46
(2,495)	1:28:A:THR:HB	1:29:A:PRO:HD3	6	1.46
(2,453)	1:39:A:LEU:HD11	1:16:B:ALA:HB1	10	1.46
(2,216)	1:27:B:LEU:HD22	1:21:B:PHE:HD1	10	1.46
(2,191)	1:17:A:LEU:HD23	1:14:A:LYS:HB3	10	1.46
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	4	1.46
(2,108)	1:9:B:PHE:HB2	1:8:B:GLU:HB3	10	1.46
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	1	1.46
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB3	9	1.46
(3,92)	1:27:B:LEU:HA	1:50:B:PHE:HB3	9	1.45
(2,2293)	1:60:A:SER:H	1:57:A:ILE:HG21	2	1.45
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD22	4	1.45
(2,1677)	1:30:A:GLU:HA	1:33:A:ARG:HD3	2	1.45
(2,1498)	1:63:B:GLN:HG2	1:64:B:PHE:HD2	6	1.45
(2,1497)	1:63:A:GLN:HG2	1:64:A:PHE:HD2	6	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1323)	1:39:A:LEU:HD22	1:46:A:ILE:H	9	1.45
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD11	5	1.45
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG23	10	1.45
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD22	6	1.45
(2,350)	1:27:B:LEU:H	1:32:B:ARG:HB2	6	1.45
(2,349)	1:27:A:LEU:H	1:32:A:ARG:HB2	6	1.45
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	9	1.44
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	2	1.44
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	2	1.44
(2,1588)	1:54:B:GLU:HB3	1:59:B:TRP:HB2	2	1.44
(2,1398)	1:46:B:ILE:HD12	1:35:B:LEU:H	5	1.44
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD13	7	1.44
(2,1223)	1:17:A:LEU:HD23	1:45:A:GLN:HE22	4	1.44
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	8	1.44
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	8	1.44
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG23	10	1.44
(2,496)	1:28:B:THR:HB	1:29:B:PRO:HD3	6	1.44
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD22	6	1.44
(2,352)	1:4:B:ARG:H	1:12:B:GLU:HG3	1	1.44
(2,351)	1:4:A:ARG:H	1:12:A:GLU:HG3	1	1.44
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	7	1.44
(2,254)	1:27:B:LEU:HD11	1:32:B:ARG:HB2	6	1.44
(2,253)	1:27:A:LEU:HD11	1:32:A:ARG:HB2	6	1.44
(2,90)	1:51:B:ARG:HD3	1:59:B:TRP:HD1	1	1.44
(2,2)	1:34:B:TYR:HD1	1:20:B:ALA:HB1	2	1.44
(2,1)	1:34:A:TYR:HD1	1:20:A:ALA:HB1	2	1.44
(2,1231)	1:18:A:ASP:HA	1:49:A:TRP:HE1	7	1.43
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	3	1.43
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	3	1.43
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB2	3	1.43
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB2	3	1.43
(2,89)	1:51:A:ARG:HD3	1:59:A:TRP:HD1	1	1.43
(3,91)	1:27:A:LEU:HA	1:50:A:PHE:HB3	9	1.42
(2,2078)	1:48:B:ARG:H	1:51:B:ARG:HG3	6	1.42
(2,2077)	1:48:A:ARG:H	1:51:A:ARG:HG3	6	1.42
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	1	1.42
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	1	1.42
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	7	1.42
(2,1156)	1:57:B:ILE:HG22	1:58:B:GLY:H	1	1.42
(2,1155)	1:57:A:ILE:HG22	1:58:A:GLY:H	1	1.42
(2,453)	1:39:A:LEU:HD13	1:16:B:ALA:HB3	3	1.42
(2,406)	1:9:B:PHE:HD1	1:41:B:LEU:HD13	2	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,405)	1:9:A:PHE:HD1	1:41:A:LEU:HD13	2	1.42
(2,264)	1:39:B:LEU:HD12	1:16:B:ALA:H	5	1.42
(2,235)	1:46:A:ILE:HG21	1:9:A:PHE:HD2	7	1.42
(2,140)	1:55:B:GLN:HB3	1:56:B:GLN:H	2	1.42
(2,122)	1:47:B:GLU:HG2	1:27:B:LEU:HA	9	1.42
(2,121)	1:47:A:GLU:HG2	1:27:A:LEU:HA	9	1.42
(2,68)	1:25:B:ARG:HA	1:19:A:LEU:HD22	7	1.42
(2,1587)	1:54:A:GLU:HB3	1:59:A:TRP:HB2	2	1.41
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD13	7	1.41
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	7	1.41
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	10	1.41
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	10	1.41
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE21	9	1.41
(2,352)	1:4:B:ARG:H	1:12:B:GLU:HG3	9	1.41
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB3	1	1.41
(2,263)	1:39:A:LEU:HD12	1:16:A:ALA:H	5	1.41
(2,100)	1:51:B:ARG:HD3	1:55:B:GLN:HG3	8	1.41
(2,99)	1:51:A:ARG:HD3	1:55:A:GLN:HG3	8	1.41
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	10	1.41
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	9	1.4
(2,2294)	1:60:B:SER:H	1:57:B:ILE:HG21	2	1.4
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD22	10	1.4
(2,1632)	1:39:B:LEU:HD11	1:9:B:PHE:HB2	2	1.4
(2,1631)	1:39:A:LEU:HD11	1:9:A:PHE:HB2	2	1.4
(2,1150)	1:20:B:ALA:HB2	1:35:B:LEU:HD22	1	1.4
(2,1108)	1:39:B:LEU:HD22	1:17:B:LEU:HG	6	1.4
(2,1107)	1:39:A:LEU:HD22	1:17:A:LEU:HG	6	1.4
(2,1068)	1:27:B:LEU:HD22	1:32:B:ARG:HB3	3	1.4
(2,454)	1:39:B:LEU:HD11	1:16:A:ALA:HB1	4	1.4
(2,264)	1:39:B:LEU:HD11	1:16:B:ALA:H	1	1.4
(2,108)	1:9:B:PHE:HB2	1:8:B:GLU:HB3	3	1.4
(2,107)	1:9:A:PHE:HB2	1:8:A:GLU:HB3	3	1.4
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	3	1.39
(2,1885)	1:49:A:TRP:H	1:39:A:LEU:HD23	10	1.39
(2,1397)	1:46:A:ILE:HD12	1:35:A:LEU:H	5	1.39
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	7	1.39
(2,352)	1:4:B:ARG:H	1:12:B:GLU:HG3	7	1.39
(2,351)	1:4:A:ARG:H	1:12:A:GLU:HG3	9	1.39
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB3	1	1.39
(2,263)	1:39:A:LEU:HD11	1:16:A:ALA:H	1	1.39
(2,253)	1:27:A:LEU:HD12	1:32:A:ARG:HB2	2	1.39
(2,119)	1:47:A:GLU:HG2	1:27:A:LEU:HD22	9	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1447)	1:53:A:LYS:HB2	1:21:A:PHE:HE1	4	1.38
(2,1397)	1:46:A:ILE:HD12	1:35:A:LEU:H	3	1.38
(2,1324)	1:39:B:LEU:HD21	1:46:B:ILE:H	8	1.38
(2,1323)	1:39:A:LEU:HD21	1:46:A:ILE:H	8	1.38
(2,1149)	1:20:A:ALA:HB2	1:35:A:LEU:HD22	1	1.38
(2,1107)	1:39:A:LEU:HD22	1:17:A:LEU:HG	10	1.38
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	3	1.38
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	8	1.38
(2,453)	1:39:A:LEU:HD11	1:16:B:ALA:HB1	4	1.38
(2,254)	1:27:B:LEU:HD12	1:32:B:ARG:HB2	2	1.38
(2,220)	1:43:B:GLU:HA	1:47:B:GLU:HG2	8	1.38
(2,219)	1:43:A:GLU:HA	1:47:A:GLU:HG2	8	1.38
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	4	1.38
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	4	1.38
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	3	1.37
(2,2306)	1:58:B:GLY:H	1:60:B:SER:HG	2	1.37
(2,2104)	1:9:B:PHE:H	1:13:B:GLN:HG2	8	1.37
(2,2103)	1:9:A:PHE:H	1:13:A:GLN:HG2	8	1.37
(2,1398)	1:46:B:ILE:HD12	1:35:B:LEU:H	3	1.37
(2,1240)	1:20:B:ALA:HB3	1:39:B:LEU:HD22	10	1.37
(2,1239)	1:20:A:ALA:HB3	1:39:A:LEU:HD22	10	1.37
(2,1236)	1:20:B:ALA:HB3	1:26:B:ARG:HD3	2	1.37
(2,1150)	1:20:B:ALA:HB1	1:35:B:LEU:HD23	4	1.37
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	3	1.37
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	8	1.37
(2,351)	1:4:A:ARG:H	1:12:A:GLU:HG3	7	1.37
(2,298)	1:16:B:ALA:H	1:39:A:LEU:HB2	8	1.37
(2,297)	1:16:A:ALA:H	1:39:B:LEU:HB2	8	1.37
(2,253)	1:27:A:LEU:HD13	1:32:A:ARG:HB2	3	1.37
(2,196)	1:18:B:ASP:HA	1:19:A:LEU:HD21	8	1.37
(2,195)	1:18:A:ASP:HA	1:19:B:LEU:HD21	8	1.37
(2,189)	1:17:A:LEU:HD22	1:53:A:LYS:HE3	6	1.37
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	8	1.37
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	8	1.37
(2,120)	1:47:B:GLU:HG2	1:27:B:LEU:HD22	9	1.37
(2,86)	1:6:B:ARG:HD3	1:4:B:ARG:HA	5	1.37
(2,85)	1:6:A:ARG:HD3	1:4:A:ARG:HA	5	1.37
(2,76)	1:3:B:LYS:HA	1:11:B:GLU:HA	10	1.37
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	9	1.36
(2,2306)	1:58:B:GLY:H	1:60:B:SER:HG	10	1.36
(2,2305)	1:58:A:GLY:H	1:60:A:SER:HG	10	1.36
(2,1935)	1:61:A:HIS:H	1:57:A:ILE:HG21	2	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1886)	1:49:B:TRP:H	1:39:B:LEU:HD23	10	1.36
(2,1416)	1:46:B:ILE:HG22	1:32:B:ARG:H	10	1.36
(2,1323)	1:39:A:LEU:HD23	1:46:A:ILE:H	7	1.36
(2,1235)	1:20:A:ALA:HB3	1:26:A:ARG:HD3	2	1.36
(2,1095)	1:41:A:LEU:HD13	1:41:A:LEU:H	5	1.36
(2,1067)	1:27:A:LEU:HD22	1:32:A:ARG:HB3	3	1.36
(2,441)	1:16:A:ALA:HB3	1:20:B:ALA:H	4	1.36
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD13	10	1.36
(3,62)	1:27:B:LEU:HB2	1:21:B:PHE:H	4	1.35
(2,1648)	1:39:B:LEU:HD12	1:13:B:GLN:HG2	9	1.35
(2,1324)	1:39:B:LEU:HD22	1:46:B:ILE:H	3	1.35
(2,1323)	1:39:A:LEU:HD22	1:46:A:ILE:H	3	1.35
(2,1108)	1:39:B:LEU:HD22	1:17:B:LEU:HG	10	1.35
(2,1096)	1:41:B:LEU:HD13	1:41:B:LEU:H	5	1.35
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD1	5	1.35
(2,192)	1:17:B:LEU:HD23	1:14:B:LYS:HB3	10	1.35
(2,190)	1:17:B:LEU:HD22	1:53:B:LYS:HE3	6	1.35
(2,179)	1:16:A:ALA:HB1	1:15:B:LYS:HE3	4	1.35
(3,1)	1:12:A:GLU:HB2	1:39:B:LEU:HA	3	1.34
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	1	1.34
(2,1601)	1:53:A:LYS:HG3	1:21:A:PHE:HZ	2	1.34
(2,1325)	1:40:A:GLY:HA3	1:4:A:ARG:HD3	7	1.34
(2,1324)	1:39:B:LEU:HD23	1:46:B:ILE:H	7	1.34
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD11	5	1.34
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD1	5	1.34
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	7	1.34
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD21	2	1.34
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD21	2	1.34
(1,48)	1:20:B:ALA:H	1:16:B:ALA:O	9	1.34
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	6	1.34
(1,1)	1:15:A:LYS:H	1:11:A:GLU:O	4	1.34
(2,2256)	1:64:B:PHE:H	1:61:B:HIS:HA	3	1.33
(2,2255)	1:64:A:PHE:H	1:61:A:HIS:HA	3	1.33
(2,1602)	1:53:B:LYS:HG3	1:21:B:PHE:HZ	7	1.33
(2,1324)	1:39:B:LEU:HD22	1:46:B:ILE:H	1	1.33
(2,1323)	1:39:A:LEU:HD22	1:46:A:ILE:H	1	1.33
(2,1158)	1:57:B:ILE:HG22	1:57:B:ILE:H	8	1.33
(2,1157)	1:57:A:ILE:HG22	1:57:A:ILE:H	8	1.33
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD21	7	1.33
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD23	6	1.33
(2,391)	1:34:A:TYR:HD2	1:35:A:LEU:HD23	10	1.33
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	7	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,240)	1:49:B:TRP:HB3	1:52:B:ARG:HG2	9	1.33
(3,123)	1:7:A:THR:HB	1:44:A:GLU:HG2	7	1.32
(3,92)	1:27:B:LEU:HA	1:50:B:PHE:HB3	10	1.32
(3,91)	1:27:A:LEU:HA	1:50:A:PHE:HB3	10	1.32
(3,2)	1:12:B:GLU:HB2	1:39:A:LEU:HA	3	1.32
(2,2305)	1:58:A:GLY:H	1:60:A:SER:HG	2	1.32
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	6	1.32
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	1	1.32
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	6	1.32
(2,1602)	1:53:B:LYS:HG3	1:21:B:PHE:HZ	2	1.32
(2,1415)	1:46:A:ILE:HG22	1:32:A:ARG:H	10	1.32
(2,1338)	1:27:B:LEU:HD23	1:50:B:PHE:HD2	4	1.32
(2,1337)	1:27:A:LEU:HD23	1:50:A:PHE:HD2	4	1.32
(2,1326)	1:40:B:GLY:HA3	1:4:B:ARG:HD3	7	1.32
(2,1068)	1:27:B:LEU:HD22	1:32:B:ARG:HB3	6	1.32
(2,1067)	1:27:A:LEU:HD22	1:32:A:ARG:HB3	6	1.32
(2,818)	1:62:B:PRO:HD2	1:60:B:SER:HG	5	1.32
(2,817)	1:62:A:PRO:HD2	1:60:A:SER:HG	5	1.32
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD23	6	1.32
(2,461)	1:49:A:TRP:HD1	1:14:A:LYS:HE3	4	1.32
(2,392)	1:34:B:TYR:HD2	1:35:B:LEU:HD23	10	1.32
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD22	9	1.32
(2,260)	1:54:B:GLU:HG3	1:51:B:ARG:HD2	5	1.32
(2,254)	1:27:B:LEU:HD11	1:51:B:ARG:HB3	3	1.32
(2,239)	1:49:A:TRP:HB3	1:52:A:ARG:HG2	9	1.32
(2,220)	1:43:B:GLU:HA	1:47:B:GLU:HG2	7	1.32
(2,219)	1:43:A:GLU:HA	1:47:A:GLU:HG2	7	1.32
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	7	1.32
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	6	1.32
(2,1948)	1:61:B:HIS:H	1:60:B:SER:HG	2	1.31
(2,1939)	1:61:A:HIS:H	1:54:A:GLU:HB2	6	1.31
(2,1647)	1:39:A:LEU:HD11	1:13:A:GLN:HG2	1	1.31
(2,1601)	1:53:A:LYS:HG3	1:21:A:PHE:HZ	7	1.31
(2,1323)	1:39:A:LEU:HD23	1:46:A:ILE:H	10	1.31
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	3	1.31
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	2	1.31
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD21	6	1.31
(2,259)	1:54:A:GLU:HG3	1:51:A:ARG:HD2	5	1.31
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	7	1.31
(3,124)	1:7:B:THR:HB	1:44:B:GLU:HG2	7	1.3
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	7	1.3
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	7	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD22	5	1.3
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD22	5	1.3
(2,1940)	1:61:B:HIS:H	1:54:B:GLU:HB2	6	1.3
(2,1648)	1:39:B:LEU:HD11	1:13:B:GLN:HG2	1	1.3
(2,1647)	1:39:A:LEU:HD12	1:13:A:GLN:HG2	9	1.3
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	3	1.3
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	6	1.3
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	6	1.3
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD11	10	1.3
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD13	10	1.3
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD22	9	1.3
(2,254)	1:27:B:LEU:HD12	1:51:B:ARG:HB3	8	1.3
(2,253)	1:27:A:LEU:HD12	1:51:A:ARG:HB3	8	1.3
(2,235)	1:46:A:ILE:HG22	1:9:A:PHE:HD2	4	1.3
(2,87)	1:48:A:ARG:HD3	1:45:A:GLN:HE21	2	1.3
(3,168)	1:59:B:TRP:H	1:61:B:HIS:HB3	4	1.29
(2,1948)	1:61:B:HIS:H	1:60:B:SER:HG	1	1.29
(2,1948)	1:61:B:HIS:H	1:60:B:SER:HG	10	1.29
(2,1947)	1:61:A:HIS:H	1:60:A:SER:HG	1	1.29
(2,1947)	1:61:A:HIS:H	1:60:A:SER:HG	2	1.29
(2,1947)	1:61:A:HIS:H	1:60:A:SER:HG	10	1.29
(2,1936)	1:61:B:HIS:H	1:57:B:ILE:HG21	2	1.29
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	2	1.29
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	5	1.29
(2,1397)	1:46:A:ILE:HD13	1:35:A:LEU:H	6	1.29
(2,1239)	1:20:A:ALA:HB1	1:39:A:LEU:HD21	9	1.29
(2,1149)	1:20:A:ALA:HB2	1:35:A:LEU:HD23	5	1.29
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	3	1.29
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD21	7	1.29
(2,454)	1:39:B:LEU:HD13	1:16:A:ALA:HB3	3	1.29
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD13	5	1.29
(2,236)	1:46:B:ILE:HG22	1:9:B:PHE:HD2	4	1.29
(2,226)	1:46:B:ILE:HD12	1:9:B:PHE:HB2	8	1.29
(2,225)	1:46:A:ILE:HD12	1:9:A:PHE:HB2	8	1.29
(2,216)	1:27:B:LEU:HD23	1:21:B:PHE:HD1	2	1.29
(2,215)	1:27:A:LEU:HD23	1:21:A:PHE:HD1	2	1.29
(2,182)	1:16:B:ALA:HB1	1:15:A:LYS:HB3	7	1.29
(2,181)	1:16:A:ALA:HB1	1:15:B:LYS:HB3	7	1.29
(2,1587)	1:54:A:GLU:HB3	1:59:A:TRP:HB2	9	1.28
(2,1150)	1:20:B:ALA:HB2	1:35:B:LEU:HD23	5	1.28
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	5	1.28
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	5	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD11	10	1.28
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD21	6	1.28
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	4	1.28
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	5	1.27
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	5	1.27
(2,1588)	1:54:B:GLU:HB3	1:59:B:TRP:HB2	9	1.27
(2,1575)	1:27:A:LEU:HD11	1:51:A:ARG:H	3	1.27
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	5	1.27
(2,1412)	1:46:B:ILE:HG21	1:50:B:PHE:HD1	8	1.27
(2,1411)	1:46:A:ILE:HG21	1:50:A:PHE:HD1	8	1.27
(2,1398)	1:46:B:ILE:HD13	1:35:B:LEU:H	6	1.27
(2,1324)	1:39:B:LEU:HD23	1:46:B:ILE:H	10	1.27
(2,1224)	1:17:B:LEU:HD23	1:45:B:GLN:HE22	4	1.27
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	4	1.27
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	3	1.27
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	7	1.27
(3,182)	1:64:B:PHE:H	1:62:B:PRO:HB3	1	1.26
(3,181)	1:64:A:PHE:H	1:62:A:PRO:HB3	1	1.26
(3,167)	1:59:A:TRP:H	1:61:A:HIS:HB3	4	1.26
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	10	1.26
(3,50)	1:39:B:LEU:HB2	1:15:A:LYS:HE3	7	1.26
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	10	1.26
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	10	1.26
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	2	1.26
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	7	1.26
(2,471)	1:19:A:LEU:HD22	1:19:B:LEU:HG	7	1.26
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD13	5	1.26
(2,189)	1:17:A:LEU:HD21	1:53:A:LYS:HE3	3	1.26
(2,20)	1:5:B:PRO:HA	1:6:B:ARG:HG3	2	1.26
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB3	3	1.26
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	10	1.25
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	3	1.25
(2,2084)	1:14:B:LYS:H	1:9:B:PHE:HB3	6	1.25
(2,1622)	1:39:B:LEU:HD12	1:18:B:ASP:H	10	1.25
(2,1621)	1:39:A:LEU:HD12	1:18:A:ASP:H	10	1.25
(2,1323)	1:39:A:LEU:HD23	1:46:A:ILE:H	5	1.25
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	3	1.25
(2,1038)	1:51:B:ARG:HG2	1:52:B:ARG:HA	6	1.25
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	8	1.25
(2,1037)	1:51:A:ARG:HG2	1:52:A:ARG:HA	6	1.25
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	8	1.25
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	7	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:39:B:LEU:HG	1:13:B:GLN:H	4	1.25
(2,88)	1:48:B:ARG:HD3	1:45:B:GLN:HE21	2	1.25
(2,19)	1:5:A:PRO:HA	1:6:A:ARG:HG3	2	1.25
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	10	1.24
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	10	1.24
(2,2103)	1:9:A:PHE:H	1:13:A:GLN:HG2	6	1.24
(2,1394)	1:46:B:ILE:HD12	1:36:B:SER:HG	2	1.24
(2,1393)	1:46:A:ILE:HD12	1:36:A:SER:HG	2	1.24
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD12	8	1.24
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD12	8	1.24
(2,472)	1:19:B:LEU:HD22	1:19:A:LEU:HG	7	1.24
(2,220)	1:43:B:GLU:HA	1:47:B:GLU:HG2	5	1.24
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB2	5	1.24
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB2	5	1.24
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	3	1.23
(2,2104)	1:9:B:PHE:H	1:13:B:GLN:HG2	6	1.23
(2,2083)	1:14:A:LYS:H	1:9:A:PHE:HB3	6	1.23
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	7	1.23
(2,1624)	1:39:B:LEU:HD11	1:17:B:LEU:HA	4	1.23
(2,1622)	1:39:B:LEU:HD12	1:18:B:ASP:H	6	1.23
(2,1621)	1:39:A:LEU:HD12	1:18:A:ASP:H	6	1.23
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD12	5	1.23
(2,1155)	1:57:A:ILE:HG23	1:58:A:GLY:H	4	1.23
(2,1150)	1:20:B:ALA:HB3	1:35:B:LEU:HD22	10	1.23
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	2	1.23
(2,637)	1:53:A:LYS:HA	1:53:A:LYS:HD2	3	1.23
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB3	7	1.23
(2,236)	1:46:B:ILE:HG23	1:9:B:PHE:HD2	3	1.23
(2,235)	1:46:A:ILE:HG23	1:9:A:PHE:HD2	3	1.23
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	3	1.23
(3,168)	1:59:B:TRP:H	1:61:B:HIS:HB3	1	1.22
(3,167)	1:59:A:TRP:H	1:61:A:HIS:HB3	1	1.22
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	3	1.22
(2,2149)	1:52:A:ARG:HB3	1:56:A:GLN:H	6	1.22
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG22	5	1.22
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG22	5	1.22
(2,1606)	1:54:B:GLU:HB3	1:21:B:PHE:HZ	5	1.22
(2,1605)	1:54:A:GLU:HB3	1:21:A:PHE:HZ	5	1.22
(2,1412)	1:46:B:ILE:HG23	1:50:B:PHE:HD1	2	1.22
(2,1397)	1:46:A:ILE:HD11	1:35:A:LEU:H	1	1.22
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	4	1.22
(2,1344)	1:41:B:LEU:HD13	1:17:B:LEU:HD21	8	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1343)	1:41:A:LEU:HD13	1:17:A:LEU:HD21	8	1.22
(2,1324)	1:39:B:LEU:HD23	1:46:B:ILE:H	2	1.22
(2,1323)	1:39:A:LEU:HD23	1:46:A:ILE:H	2	1.22
(2,1320)	1:39:B:LEU:HD21	1:9:B:PHE:HD2	7	1.22
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD11	7	1.22
(2,1002)	1:44:B:GLU:HB3	1:45:B:GLN:H	2	1.22
(2,1002)	1:44:B:GLU:HB3	1:45:B:GLN:H	10	1.22
(2,1001)	1:44:A:GLU:HB3	1:45:A:GLN:H	2	1.22
(2,1001)	1:44:A:GLU:HB3	1:45:A:GLN:H	10	1.22
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	4	1.22
(2,638)	1:53:B:LYS:HA	1:53:B:LYS:HD2	3	1.22
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE21	3	1.22
(2,435)	1:16:A:ALA:HB3	1:39:B:LEU:HD11	6	1.22
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB2	1	1.22
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	7	1.22
(3,122)	1:14:B:LYS:HE3	1:49:B:TRP:HB2	1	1.21
(3,121)	1:14:A:LYS:HE3	1:49:A:TRP:HB2	1	1.21
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	2	1.21
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	4	1.21
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD21	3	1.21
(2,1847)	1:53:A:LYS:H	1:55:A:GLN:HB3	7	1.21
(2,1576)	1:27:B:LEU:HD11	1:51:B:ARG:H	3	1.21
(2,1398)	1:46:B:ILE:HD11	1:35:B:LEU:H	1	1.21
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	4	1.21
(2,1324)	1:39:B:LEU:HD23	1:46:B:ILE:H	5	1.21
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD11	7	1.21
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	10	1.21
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	10	1.21
(2,1156)	1:57:B:ILE:HG23	1:58:B:GLY:H	4	1.21
(2,1149)	1:20:A:ALA:HB3	1:35:A:LEU:HD22	10	1.21
(2,896)	1:42:B:ASN:HB3	1:44:B:GLU:HB3	4	1.21
(2,895)	1:42:A:ASN:HB3	1:44:A:GLU:HB3	4	1.21
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE21	3	1.21
(2,436)	1:16:B:ALA:HB3	1:39:A:LEU:HD11	6	1.21
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB3	7	1.21
(2,239)	1:49:A:TRP:HB3	1:46:A:ILE:HG12	3	1.21
(2,236)	1:46:B:ILE:HG22	1:50:B:PHE:HZ	6	1.21
(2,235)	1:46:A:ILE:HG22	1:50:A:PHE:HZ	6	1.21
(2,196)	1:18:B:ASP:HA	1:19:A:LEU:HD21	1	1.21
(2,195)	1:18:A:ASP:HA	1:19:B:LEU:HD21	1	1.21
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB2	1	1.21
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	1:12:A:GLU:HB2	1:39:B:LEU:HA	1	1.2
(2,2150)	1:52:B:ARG:HB3	1:56:B:GLN:H	6	1.2
(2,1411)	1:46:A:ILE:HG23	1:50:A:PHE:HD1	2	1.2
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD12	2	1.2
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD11	1	1.2
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	9	1.2
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	9	1.2
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	4	1.2
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB2	2	1.2
(2,220)	1:43:B:GLU:HA	1:47:B:GLU:HG2	6	1.2
(2,219)	1:43:A:GLU:HA	1:47:A:GLU:HG2	6	1.2
(2,182)	1:16:B:ALA:HB3	1:15:B:LYS:HB3	5	1.2
(2,181)	1:16:A:ALA:HB3	1:15:A:LYS:HB3	5	1.2
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB2	2	1.2
(1,43)	1:15:B:LYS:H	1:11:B:GLU:O	4	1.2
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	6	1.19
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	7	1.19
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	7	1.19
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	3	1.19
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG23	4	1.19
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	10	1.19
(2,1700)	1:12:B:GLU:HB3	1:13:B:GLN:H	6	1.19
(2,1699)	1:12:A:GLU:HB3	1:13:A:GLN:H	6	1.19
(2,1616)	1:27:B:LEU:HD13	1:35:B:LEU:HD12	7	1.19
(2,1613)	1:16:A:ALA:HB1	1:35:A:LEU:HD13	7	1.19
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	10	1.19
(2,1319)	1:39:A:LEU:HD21	1:9:A:PHE:HD2	7	1.19
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD12	2	1.19
(2,1239)	1:20:A:ALA:HB1	1:39:A:LEU:HD22	2	1.19
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD11	1	1.19
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	4	1.19
(2,662)	1:52:B:ARG:HA	1:55:B:GLN:HG2	9	1.19
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	4	1.19
(2,657)	1:52:A:ARG:HA	1:55:A:GLN:HB3	6	1.19
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD13	5	1.19
(2,305)	1:49:A:TRP:H	1:53:A:LYS:HB3	7	1.19
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB2	2	1.19
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG23	7	1.19
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	6	1.18
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	3	1.18
(2,1948)	1:61:B:HIS:H	1:60:B:SER:HG	4	1.18
(2,1623)	1:39:A:LEU:HD11	1:17:A:LEU:HA	4	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1614)	1:16:B:ALA:HB1	1:35:B:LEU:HD13	7	1.18
(2,1575)	1:27:A:LEU:HD13	1:51:A:ARG:H	5	1.18
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	10	1.18
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD11	6	1.18
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD11	6	1.18
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	1	1.18
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	6	1.18
(2,345)	1:36:A:SER:H	1:41:A:LEU:HD13	10	1.18
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB2	10	1.18
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD23	3	1.18
(2,226)	1:46:B:ILE:HD13	1:9:B:PHE:HB2	1	1.18
(2,225)	1:46:A:ILE:HD13	1:9:A:PHE:HB2	1	1.18
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	10	1.18
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	1	1.17
(3,68)	1:63:B:GLN:HG2	1:54:B:GLU:HA	4	1.17
(3,2)	1:12:B:GLU:HB2	1:39:A:LEU:HA	1	1.17
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	9	1.17
(2,2104)	1:9:B:PHE:H	1:13:B:GLN:HG2	3	1.17
(2,2103)	1:9:A:PHE:H	1:13:A:GLN:HG2	3	1.17
(2,2006)	1:64:B:PHE:H	1:63:B:GLN:H	1	1.17
(2,2005)	1:64:A:PHE:H	1:63:A:GLN:H	1	1.17
(2,1948)	1:61:B:HIS:H	1:60:B:SER:HG	5	1.17
(2,1947)	1:61:A:HIS:H	1:60:A:SER:HG	4	1.17
(2,1947)	1:61:A:HIS:H	1:60:A:SER:HG	5	1.17
(2,1651)	1:28:A:THR:HB	1:31:A:TRP:HB3	10	1.17
(2,1615)	1:27:A:LEU:HD13	1:35:A:LEU:HD12	7	1.17
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE1	10	1.17
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD23	9	1.17
(2,1496)	1:61:B:HIS:HA	1:54:B:GLU:HB2	4	1.17
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	1	1.17
(2,1240)	1:20:B:ALA:HB1	1:39:B:LEU:HD22	2	1.17
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	4	1.17
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	5	1.17
(2,294)	1:53:B:LYS:H	1:55:B:GLN:HG3	6	1.17
(2,293)	1:53:A:LYS:H	1:55:A:GLN:HG3	6	1.17
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG23	7	1.17
(2,240)	1:49:B:TRP:HB3	1:46:B:ILE:HG12	3	1.17
(2,191)	1:17:A:LEU:HD21	1:14:A:LYS:HB3	1	1.17
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	8	1.16
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	8	1.16
(3,53)	1:9:A:PHE:HB2	1:39:A:LEU:HG	5	1.16
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	9	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	8	1.16
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	8	1.16
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD11	1	1.16
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD11	1	1.16
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG22	1	1.16
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG22	1	1.16
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	6	1.16
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	6	1.16
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD23	2	1.16
(2,1339)	1:27:A:LEU:HD22	1:46:A:ILE:H	4	1.16
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD13	5	1.16
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD11	7	1.16
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD11	7	1.16
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD21	8	1.16
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD21	8	1.16
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB2	10	1.16
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD23	3	1.16
(2,192)	1:17:B:LEU:HD21	1:14:B:LYS:HB3	6	1.16
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	6	1.15
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	6	1.15
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	7	1.15
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	7	1.15
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	7	1.15
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	4	1.15
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	4	1.15
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	9	1.15
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	6	1.15
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	6	1.15
(2,2103)	1:9:A:PHE:H	1:13:A:GLN:HG2	7	1.15
(2,1848)	1:53:B:LYS:H	1:55:B:GLN:HB3	2	1.15
(2,1624)	1:39:B:LEU:HD11	1:17:B:LEU:HA	7	1.15
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD23	2	1.15
(2,1411)	1:46:A:ILE:HG22	1:50:A:PHE:HD1	3	1.15
(2,1239)	1:20:A:ALA:HB1	1:39:A:LEU:HD22	7	1.15
(2,1202)	1:17:B:LEU:HD22	1:46:B:ILE:HG12	7	1.15
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	4	1.15
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	5	1.15
(2,686)	1:6:B:ARG:HA	1:6:B:ARG:HG3	1	1.15
(2,661)	1:52:A:ARG:HA	1:55:A:GLN:HG2	9	1.15
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD13	5	1.15
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB2	8	1.15
(2,219)	1:43:A:GLU:HA	1:47:A:GLU:HG2	1	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	4	1.15
(2,15)	1:36:A:SER:HB3	1:46:A:ILE:HD13	6	1.15
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB3	6	1.15
(3,54)	1:9:B:PHE:HB2	1:39:B:LEU:HG	5	1.14
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	9	1.14
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	4	1.14
(2,2104)	1:9:B:PHE:H	1:13:B:GLN:HG2	7	1.14
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG23	4	1.14
(2,1665)	1:57:A:ILE:HG12	1:60:A:SER:H	2	1.14
(2,1652)	1:28:B:THR:HB	1:31:B:TRP:HB3	10	1.14
(2,1623)	1:39:A:LEU:HD11	1:17:A:LEU:HA	7	1.14
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE1	10	1.14
(2,1162)	1:36:B:SER:HB2	1:46:B:ILE:HD12	3	1.14
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD1	10	1.14
(2,685)	1:6:A:ARG:HA	1:6:A:ARG:HG3	1	1.14
(2,306)	1:49:B:TRP:H	1:53:B:LYS:HB3	7	1.14
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB2	8	1.14
(2,220)	1:43:B:GLU:HA	1:47:B:GLU:HG2	1	1.14
(2,192)	1:17:B:LEU:HD21	1:14:B:LYS:HB3	1	1.14
(2,179)	1:16:A:ALA:HB2	1:15:B:LYS:HE3	5	1.14
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	8	1.14
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	8	1.14
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB2	2	1.14
(2,16)	1:36:B:SER:HB3	1:46:B:ILE:HD13	6	1.14
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB3	6	1.14
(3,49)	1:39:A:LEU:HB2	1:15:B:LYS:HE3	7	1.13
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	8	1.13
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	7	1.13
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	8	1.13
(2,2305)	1:58:A:GLY:H	1:60:A:SER:HG	4	1.13
(2,2256)	1:64:B:PHE:H	1:61:B:HIS:HA	10	1.13
(2,2255)	1:64:A:PHE:H	1:61:A:HIS:HA	10	1.13
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD22	2	1.13
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD21	3	1.13
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD22	2	1.13
(2,1909)	1:59:A:TRP:H	1:57:A:ILE:HG12	6	1.13
(2,1631)	1:39:A:LEU:HD12	1:9:A:PHE:HB2	6	1.13
(2,1599)	1:53:A:LYS:HG2	1:21:A:PHE:HZ	2	1.13
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	1	1.13
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	1	1.13
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD23	9	1.13
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD13	3	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1240)	1:20:B:ALA:HB1	1:39:B:LEU:HD22	7	1.13
(2,1146)	1:39:B:LEU:HD12	1:16:B:ALA:HB2	8	1.13
(2,1145)	1:39:A:LEU:HD12	1:16:A:ALA:HB2	8	1.13
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	2	1.13
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD1	10	1.13
(2,190)	1:17:B:LEU:HD22	1:53:B:LYS:HE3	4	1.13
(3,76)	1:57:B:ILE:HG12	1:61:B:HIS:HB2	5	1.12
(3,75)	1:57:A:ILE:HG12	1:61:A:HIS:HB2	5	1.12
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	2	1.12
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	6	1.12
(2,2083)	1:14:A:LYS:H	1:9:A:PHE:HB3	10	1.12
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	4	1.12
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	10	1.12
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	1	1.12
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	8	1.12
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	1	1.12
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	4	1.12
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	8	1.12
(2,1600)	1:53:B:LYS:HG2	1:21:B:PHE:HZ	2	1.12
(2,1201)	1:17:A:LEU:HD22	1:46:A:ILE:HG12	7	1.12
(2,1166)	1:46:B:ILE:HD13	1:36:B:SER:H	4	1.12
(2,1068)	1:27:B:LEU:HD22	1:32:B:ARG:HB3	9	1.12
(2,1067)	1:27:A:LEU:HD22	1:32:A:ARG:HB3	9	1.12
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD21	1	1.12
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD21	1	1.12
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD13	4	1.12
(2,327)	1:35:A:LEU:H	1:27:A:LEU:HD23	9	1.12
(2,226)	1:46:B:ILE:HD12	1:9:B:PHE:HB2	6	1.12
(2,191)	1:17:A:LEU:HD21	1:14:A:LYS:HB3	6	1.12
(2,180)	1:16:B:ALA:HB1	1:15:A:LYS:HE3	4	1.12
(2,180)	1:16:B:ALA:HB2	1:15:A:LYS:HE3	5	1.12
(3,191)	1:44:A:GLU:H	1:36:A:SER:HB2	7	1.11
(3,68)	1:63:B:GLN:HG2	1:54:B:GLU:HA	1	1.11
(3,67)	1:63:A:GLN:HG2	1:54:A:GLU:HA	1	1.11
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	6	1.11
(2,2306)	1:58:B:GLY:H	1:60:B:SER:HG	4	1.11
(2,2103)	1:9:A:PHE:H	1:13:A:GLN:HG2	4	1.11
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	10	1.11
(2,1910)	1:59:B:TRP:H	1:57:B:ILE:HG12	6	1.11
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	4	1.11
(2,1340)	1:27:B:LEU:HD22	1:46:B:ILE:H	4	1.11
(2,1335)	1:27:A:LEU:HD22	1:47:A:GLU:H	4	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1323)	1:39:A:LEU:HD23	1:46:A:ILE:H	6	1.11
(2,1057)	1:47:A:GLU:HA	1:27:A:LEU:HD22	4	1.11
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	3	1.11
(2,467)	1:19:A:LEU:HD21	1:35:B:LEU:HB2	2	1.11
(2,382)	1:34:B:TYR:HD2	1:64:A:PHE:HD1	2	1.11
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB2	6	1.11
(2,20)	1:5:B:PRO:HA	1:6:B:ARG:HG3	9	1.11
(2,19)	1:5:A:PRO:HA	1:6:A:ARG:HG3	9	1.11
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	6	1.1
(3,100)	1:59:B:TRP:HB3	1:54:B:GLU:HA	7	1.1
(2,2322)	1:6:B:ARG:H	1:5:B:PRO:HB3	7	1.1
(2,2321)	1:6:A:ARG:H	1:5:A:PRO:HB3	7	1.1
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	1	1.1
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	1	1.1
(2,1929)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	1.1
(2,1666)	1:57:B:ILE:HG12	1:60:B:SER:H	2	1.1
(2,1632)	1:39:B:LEU:HD12	1:9:B:PHE:HB2	6	1.1
(2,1324)	1:39:B:LEU:HD23	1:46:B:ILE:H	6	1.1
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD13	3	1.1
(2,1244)	1:20:B:ALA:HB3	1:35:B:LEU:HD11	3	1.1
(2,1243)	1:20:A:ALA:HB3	1:35:A:LEU:HD11	3	1.1
(2,1063)	1:27:A:LEU:HD21	1:43:A:GLU:HB3	5	1.1
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	3	1.1
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD1	7	1.1
(2,658)	1:52:B:ARG:HA	1:55:B:GLN:HB3	2	1.1
(2,468)	1:19:B:LEU:HD21	1:35:A:LEU:HB2	2	1.1
(2,372)	1:51:B:ARG:H	1:47:B:GLU:HG2	8	1.1
(2,371)	1:51:A:ARG:H	1:47:A:GLU:HG2	8	1.1
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD12	8	1.1
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD12	8	1.1
(2,225)	1:46:A:ILE:HD12	1:9:A:PHE:HB2	6	1.1
(2,180)	1:16:B:ALA:HB2	1:15:A:LYS:HE3	1	1.1
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	8	1.1
(2,10)	1:16:B:ALA:HB2	1:15:A:LYS:HD3	7	1.1
(1,48)	1:20:B:ALA:H	1:16:B:ALA:O	8	1.1
(1,6)	1:20:A:ALA:H	1:16:A:ALA:O	8	1.1
(3,160)	1:43:B:GLU:H	1:44:B:GLU:HG2	7	1.09
(3,159)	1:43:A:GLU:H	1:44:A:GLU:HG2	7	1.09
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	6	1.09
(2,2262)	1:45:B:GLN:HG3	1:44:B:GLU:H	5	1.09
(2,2167)	1:14:A:LYS:H	1:14:A:LYS:HD3	3	1.09
(2,1930)	1:6:B:ARG:H	1:6:B:ARG:HB2	1	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD21	9	1.09
(2,1412)	1:46:B:ILE:HG22	1:50:B:PHE:HD1	3	1.09
(2,1398)	1:46:B:ILE:HD11	1:35:B:LEU:H	7	1.09
(2,1397)	1:46:A:ILE:HD11	1:35:A:LEU:H	7	1.09
(2,1397)	1:46:A:ILE:HD13	1:35:A:LEU:H	10	1.09
(2,1343)	1:41:A:LEU:HD12	1:17:A:LEU:HD21	2	1.09
(2,1336)	1:27:B:LEU:HD22	1:47:B:GLU:H	4	1.09
(2,1336)	1:27:B:LEU:HD22	1:47:B:GLU:H	9	1.09
(2,1244)	1:20:B:ALA:HB1	1:35:B:LEU:HD11	7	1.09
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	1	1.09
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	1	1.09
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	9	1.09
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD1	1	1.09
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD1	1	1.09
(2,468)	1:19:B:LEU:HD22	1:35:A:LEU:HB2	5	1.09
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD21	1	1.09
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD21	1	1.09
(2,346)	1:36:B:SER:H	1:41:B:LEU:HD13	10	1.09
(2,328)	1:35:B:LEU:H	1:27:B:LEU:HD23	9	1.09
(2,298)	1:16:B:ALA:H	1:39:B:LEU:HB2	10	1.09
(2,204)	1:28:B:THR:HB	1:32:B:ARG:HB2	7	1.09
(2,190)	1:17:B:LEU:HD21	1:53:B:LYS:HE3	3	1.09
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	8	1.09
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	5	1.09
(3,159)	1:43:A:GLU:H	1:44:A:GLU:HG2	1	1.08
(2,2168)	1:14:B:LYS:H	1:14:B:LYS:HD3	3	1.08
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD11	8	1.08
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD11	8	1.08
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	1	1.08
(2,1335)	1:27:A:LEU:HD22	1:47:A:GLU:H	9	1.08
(2,1161)	1:36:A:SER:HB2	1:46:A:ILE:HD12	3	1.08
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD13	4	1.08
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	2	1.08
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	7	1.08
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	5	1.08
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	5	1.08
(2,618)	1:12:B:GLU:HA	1:15:B:LYS:HE3	10	1.08
(2,467)	1:19:A:LEU:HD22	1:35:B:LEU:HB2	5	1.08
(2,336)	1:15:B:LYS:H	1:15:B:LYS:HD3	5	1.08
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	1	1.08
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	1	1.08
(2,203)	1:28:A:THR:HB	1:32:A:ARG:HB2	7	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	1:16:A:ALA:HB2	1:15:B:LYS:HE3	1	1.08
(2,75)	1:3:A:LYS:HA	1:11:A:GLU:HA	10	1.08
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB2	4	1.08
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB2	6	1.08
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	10	1.08
(3,192)	1:44:B:GLU:H	1:36:B:SER:HB2	7	1.07
(3,160)	1:43:B:GLU:H	1:44:B:GLU:HG2	1	1.07
(3,92)	1:27:B:LEU:HA	1:50:B:PHE:HB3	4	1.07
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	4	1.07
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	6	1.07
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	4	1.07
(2,2261)	1:45:A:GLN:HG3	1:44:A:GLU:H	5	1.07
(2,2077)	1:48:A:ARG:H	1:51:A:ARG:HG2	10	1.07
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	1	1.07
(2,1636)	1:41:B:LEU:HD12	1:13:B:GLN:HG2	9	1.07
(2,1344)	1:41:B:LEU:HD12	1:17:B:LEU:HD21	2	1.07
(2,1243)	1:20:A:ALA:HB1	1:35:A:LEU:HD11	7	1.07
(2,468)	1:19:B:LEU:HD23	1:35:A:LEU:HB2	7	1.07
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD13	4	1.07
(2,335)	1:15:A:LYS:H	1:15:A:LYS:HD3	5	1.07
(2,239)	1:49:A:TRP:HB3	1:46:A:ILE:HG12	6	1.07
(2,236)	1:46:B:ILE:HG21	1:9:B:PHE:HD2	9	1.07
(2,18)	1:60:B:SER:HB3	1:57:B:ILE:HA	4	1.07
(3,65)	1:55:A:GLN:HG2	1:54:A:GLU:HA	10	1.06
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	6	1.06
(2,2084)	1:14:B:LYS:H	1:9:B:PHE:HB3	3	1.06
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	2	1.06
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	6	1.06
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	5	1.06
(2,1635)	1:41:A:LEU:HD12	1:13:A:GLN:HG2	9	1.06
(2,1580)	1:27:B:LEU:HD12	1:47:B:GLU:HG3	1	1.06
(2,1579)	1:27:A:LEU:HD12	1:47:A:GLU:HG3	1	1.06
(2,1319)	1:39:A:LEU:HD23	1:9:A:PHE:HD2	1	1.06
(2,755)	1:43:A:GLU:HA	1:36:A:SER:HB2	7	1.06
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD11	5	1.06
(2,240)	1:49:B:TRP:HB3	1:46:B:ILE:HG12	6	1.06
(2,100)	1:51:B:ARG:HD3	1:55:B:GLN:HG3	9	1.06
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	4	1.06
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	5	1.06
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	7	1.05
(3,66)	1:55:B:GLN:HG2	1:54:B:GLU:HA	10	1.05
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	9	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	10	1.05
(2,2104)	1:9:B:PHE:H	1:13:B:GLN:HG2	4	1.05
(2,2078)	1:48:B:ARG:H	1:51:B:ARG:HG2	10	1.05
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	2	1.05
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	6	1.05
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	10	1.05
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	5	1.05
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD21	4	1.05
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD21	4	1.05
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD23	5	1.05
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	7	1.05
(2,1336)	1:27:B:LEU:HD23	1:47:B:GLU:H	8	1.05
(2,1335)	1:27:A:LEU:HD23	1:47:A:GLU:H	8	1.05
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	7	1.05
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	4	1.05
(2,617)	1:12:A:GLU:HA	1:15:A:LYS:HE3	10	1.05
(2,381)	1:34:A:TYR:HD2	1:64:B:PHE:HD1	2	1.05
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD11	5	1.05
(2,297)	1:16:A:ALA:H	1:39:A:LEU:HB2	10	1.05
(2,263)	1:39:A:LEU:HD13	1:16:A:ALA:H	3	1.05
(2,235)	1:46:A:ILE:HG21	1:9:A:PHE:HD2	9	1.05
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	4	1.05
(2,9)	1:16:A:ALA:HB2	1:15:B:LYS:HD3	7	1.05
(3,183)	1:13:A:GLN:H	1:4:A:ARG:HA	4	1.04
(3,172)	1:17:B:LEU:H	1:14:B:LYS:HG3	2	1.04
(3,171)	1:17:A:LEU:H	1:14:A:LYS:HG3	2	1.04
(3,136)	1:27:B:LEU:H	1:31:B:TRP:HA	2	1.04
(3,135)	1:27:A:LEU:H	1:31:A:TRP:HA	2	1.04
(3,76)	1:57:B:ILE:HG12	1:61:B:HIS:HB2	1	1.04
(3,75)	1:57:A:ILE:HG12	1:61:A:HIS:HB2	1	1.04
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	9	1.04
(2,1792)	1:8:B:GLU:H	1:9:B:PHE:H	2	1.04
(2,1791)	1:8:A:GLU:H	1:9:A:PHE:H	2	1.04
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	10	1.04
(2,1605)	1:54:A:GLU:HB3	1:21:A:PHE:HZ	4	1.04
(2,1575)	1:27:A:LEU:HD13	1:51:A:ARG:H	2	1.04
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD23	5	1.04
(2,1320)	1:39:B:LEU:HD23	1:9:B:PHE:HD2	1	1.04
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	4	1.04
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD11	10	1.04
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD22	10	1.04
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD22	10	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD21	10	1.04
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	8	1.03
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	7	1.03
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	8	1.03
(3,99)	1:59:A:TRP:HB3	1:54:A:GLU:HA	7	1.03
(2,2256)	1:64:B:PHE:H	1:61:B:HIS:HA	2	1.03
(2,2083)	1:14:A:LYS:H	1:9:A:PHE:HB3	3	1.03
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	3	1.03
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	3	1.03
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	2	1.03
(2,1580)	1:27:B:LEU:HD12	1:47:B:GLU:HG3	8	1.03
(2,1579)	1:27:A:LEU:HD12	1:47:A:GLU:HG3	8	1.03
(2,1576)	1:27:B:LEU:HD13	1:51:B:ARG:H	2	1.03
(2,1574)	1:27:B:LEU:HD13	1:46:B:ILE:H	9	1.03
(2,1554)	1:27:B:LEU:HB3	1:50:B:PHE:HB2	5	1.03
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD22	4	1.03
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	5	1.03
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	5	1.03
(2,1240)	1:20:B:ALA:HB1	1:39:B:LEU:HD21	9	1.03
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD11	10	1.03
(2,1182)	1:6:B:ARG:HD3	1:6:B:ARG:HB2	1	1.03
(2,1181)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	1	1.03
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	4	1.03
(2,528)	1:57:B:ILE:HA	1:57:B:ILE:HG21	6	1.03
(2,527)	1:57:A:ILE:HA	1:57:A:ILE:HG21	6	1.03
(2,454)	1:39:B:LEU:HD12	1:16:A:ALA:HB1	8	1.03
(2,192)	1:17:B:LEU:HD21	1:14:B:LYS:HB3	4	1.03
(2,154)	1:52:B:ARG:HB2	1:51:B:ARG:HD2	10	1.03
(2,153)	1:52:A:ARG:HB2	1:51:A:ARG:HD2	10	1.03
(2,89)	1:38:A:ARG:HD3	1:64:B:PHE:HD1	6	1.03
(3,168)	1:59:B:TRP:H	1:61:B:HIS:HB3	2	1.02
(3,167)	1:59:A:TRP:H	1:61:A:HIS:HB3	2	1.02
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	10	1.02
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	1	1.02
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	1	1.02
(2,2420)	1:51:B:ARG:H	1:54:B:GLU:HG3	4	1.02
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	10	1.02
(2,2255)	1:64:A:PHE:H	1:61:A:HIS:HA	7	1.02
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	9	1.02
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	4	1.02
(2,1648)	1:39:B:LEU:HD12	1:13:B:GLN:HG2	6	1.02
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	3	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1398)	1:46:B:ILE:HD13	1:35:B:LEU:H	10	1.02
(2,1058)	1:47:B:GLU:HA	1:27:B:LEU:HD22	4	1.02
(2,453)	1:39:A:LEU:HD12	1:16:B:ALA:HB1	8	1.02
(2,442)	1:16:B:ALA:HB1	1:20:A:ALA:H	2	1.02
(2,321)	1:54:A:GLU:H	1:52:A:ARG:HB2	7	1.02
(2,240)	1:49:B:TRP:HB3	1:46:B:ILE:HG12	8	1.02
(2,239)	1:49:A:TRP:HB3	1:46:A:ILE:HG12	8	1.02
(2,236)	1:46:B:ILE:HG21	1:9:B:PHE:HD2	1	1.02
(2,235)	1:46:A:ILE:HG21	1:9:A:PHE:HD2	1	1.02
(2,191)	1:17:A:LEU:HD23	1:14:A:LYS:HB3	3	1.02
(3,160)	1:43:B:GLU:H	1:44:B:GLU:HG2	8	1.01
(3,159)	1:43:A:GLU:H	1:44:A:GLU:HG2	8	1.01
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	7	1.01
(2,2255)	1:64:A:PHE:H	1:61:A:HIS:HA	2	1.01
(2,2167)	1:14:A:LYS:H	1:14:A:LYS:HD3	10	1.01
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	2	1.01
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	4	1.01
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	9	1.01
(2,1690)	1:9:B:PHE:HB3	1:14:B:LYS:HG3	6	1.01
(2,1647)	1:39:A:LEU:HD12	1:13:A:GLN:HG2	6	1.01
(2,1632)	1:39:B:LEU:HD11	1:9:B:PHE:HB2	7	1.01
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD22	4	1.01
(2,1475)	1:58:A:GLY:HA2	1:59:A:TRP:HB3	6	1.01
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	7	1.01
(2,1320)	1:39:B:LEU:HD21	1:9:B:PHE:HD2	2	1.01
(2,1319)	1:39:A:LEU:HD21	1:9:A:PHE:HD2	2	1.01
(2,1236)	1:20:B:ALA:HB2	1:26:B:ARG:HD3	6	1.01
(2,1235)	1:20:A:ALA:HB2	1:26:A:ARG:HD3	6	1.01
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB3	6	1.01
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	9	1.01
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD1	7	1.01
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	9	1.01
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD23	1	1.01
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD23	1	1.01
(2,374)	1:56:B:GLN:H	1:57:B:ILE:HG13	4	1.01
(2,294)	1:53:B:LYS:H	1:54:B:GLU:HB3	1	1.01
(2,293)	1:53:A:LYS:H	1:54:A:GLU:HB3	1	1.01
(2,264)	1:39:B:LEU:HD13	1:16:B:ALA:H	3	1.01
(2,181)	1:16:A:ALA:HB2	1:15:B:LYS:HB3	1	1.01
(2,90)	1:38:B:ARG:HD3	1:64:A:PHE:HD1	6	1.01
(2,17)	1:60:A:SER:HB3	1:57:A:ILE:HA	4	1.01
(3,184)	1:13:B:GLN:H	1:4:B:ARG:HA	4	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,160)	1:43:B:GLU:H	1:44:B:GLU:HG2	5	1.0
(3,159)	1:43:A:GLU:H	1:44:A:GLU:HG2	5	1.0
(2,2436)	1:27:B:LEU:HD13	1:47:B:GLU:H	5	1.0
(2,2321)	1:6:A:ARG:H	1:5:A:PRO:HB3	4	1.0
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	6	1.0
(2,1729)	1:28:A:THR:H	1:27:A:LEU:HD11	4	1.0
(2,1553)	1:27:A:LEU:HB3	1:50:A:PHE:HB2	5	1.0
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD22	6	1.0
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD21	10	1.0
(2,1476)	1:58:B:GLY:HA2	1:59:B:TRP:HB3	6	1.0
(2,1385)	1:46:A:ILE:HD11	1:35:A:LEU:HD13	10	1.0
(2,1340)	1:27:B:LEU:HD21	1:46:B:ILE:H	8	1.0
(2,1339)	1:27:A:LEU:HD21	1:46:A:ILE:H	8	1.0
(2,1332)	1:27:B:LEU:HD23	1:50:B:PHE:H	5	1.0
(2,1146)	1:39:B:LEU:HD11	1:16:B:ALA:HB1	1	1.0
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	7	1.0
(2,874)	1:14:B:LYS:HE3	1:14:B:LYS:HG3	4	1.0
(2,873)	1:14:A:LYS:HE3	1:14:A:LYS:HG3	4	1.0
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	7	1.0
(2,511)	1:46:A:ILE:HA	1:27:A:LEU:HD22	7	1.0
(2,480)	1:19:B:LEU:HD22	1:17:A:LEU:HD13	9	1.0
(2,441)	1:16:A:ALA:HB1	1:20:B:ALA:H	2	1.0
(2,373)	1:56:A:GLN:H	1:57:A:ILE:HG13	4	1.0
(2,182)	1:16:B:ALA:HB2	1:15:A:LYS:HB3	1	1.0
(2,2)	1:34:B:TYR:HD2	1:20:B:ALA:HB2	8	1.0
(2,1)	1:34:A:TYR:HD2	1:20:A:ALA:HB2	8	1.0
(2,2168)	1:14:B:LYS:H	1:14:B:LYS:HD3	10	0.99
(2,2167)	1:14:A:LYS:H	1:14:A:LYS:HD3	6	0.99
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	6	0.99
(2,1730)	1:28:B:THR:H	1:27:B:LEU:HD11	4	0.99
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	9	0.99
(2,1631)	1:39:A:LEU:HD11	1:9:A:PHE:HB2	7	0.99
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD22	6	0.99
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD21	10	0.99
(2,1495)	1:61:A:HIS:HA	1:54:A:GLU:HB2	4	0.99
(2,1416)	1:46:B:ILE:HG21	1:32:B:ARG:H	5	0.99
(2,1411)	1:46:A:ILE:HG21	1:50:A:PHE:HD1	4	0.99
(2,1311)	1:39:A:LEU:HD22	1:17:A:LEU:HA	7	0.99
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB3	6	0.99
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD1	6	0.99
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD1	6	0.99
(2,618)	1:12:B:GLU:HA	1:15:B:LYS:HE3	1	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,512)	1:46:B:ILE:HA	1:27:B:LEU:HD22	7	0.99
(2,480)	1:19:B:LEU:HD23	1:17:A:LEU:HD13	4	0.99
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD22	5	0.99
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD22	5	0.99
(2,191)	1:17:A:LEU:HD22	1:14:A:LYS:HB3	2	0.99
(2,99)	1:51:A:ARG:HD3	1:55:A:GLN:HG3	9	0.99
(3,91)	1:27:A:LEU:HA	1:50:A:PHE:HB3	4	0.98
(2,2419)	1:51:A:ARG:H	1:54:A:GLU:HG3	4	0.98
(2,2168)	1:14:B:LYS:H	1:14:B:LYS:HD3	6	0.98
(2,1689)	1:9:A:PHE:HB3	1:14:A:LYS:HG3	6	0.98
(2,1573)	1:27:A:LEU:HD13	1:46:A:ILE:H	9	0.98
(2,1312)	1:39:B:LEU:HD22	1:17:B:LEU:HA	7	0.98
(2,1048)	1:57:B:ILE:HG13	1:57:B:ILE:H	6	0.98
(2,1047)	1:57:A:ILE:HG13	1:57:A:ILE:H	6	0.98
(2,896)	1:42:B:ASN:HB3	1:44:B:GLU:HB3	10	0.98
(2,895)	1:42:A:ASN:HB3	1:44:A:GLU:HB3	10	0.98
(2,473)	1:19:A:LEU:HD22	1:19:B:LEU:HB3	10	0.98
(2,467)	1:19:A:LEU:HD23	1:35:B:LEU:HB2	7	0.98
(2,372)	1:51:B:ARG:H	1:47:B:GLU:HG2	2	0.98
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	2	0.98
(2,298)	1:16:B:ALA:H	1:39:B:LEU:HB2	6	0.98
(2,253)	1:27:A:LEU:HD11	1:32:A:ARG:HB2	4	0.98
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	10	0.98
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	10	0.98
(2,188)	1:17:B:LEU:HD23	1:45:B:GLN:HB3	6	0.98
(2,162)	1:39:B:LEU:HG	1:13:B:GLN:H	1	0.98
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	2	0.98
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	2	0.98
(2,67)	1:65:A:GLU:HA	1:53:A:LYS:HD2	1	0.98
(1,50)	1:34:B:TYR:H	1:30:B:GLU:O	10	0.98
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	6	0.97
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	6	0.97
(2,2322)	1:6:B:ARG:H	1:5:B:PRO:HB3	4	0.97
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	4	0.97
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	7	0.97
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	7	0.97
(2,1824)	1:8:B:GLU:H	1:9:B:PHE:HB3	2	0.97
(2,1823)	1:8:A:GLU:H	1:9:A:PHE:HB3	2	0.97
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	3	0.97
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	3	0.97
(2,1699)	1:12:A:GLU:HB3	1:13:A:GLN:H	4	0.97
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	4	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1386)	1:46:B:ILE:HD11	1:35:B:LEU:HD13	10	0.97
(2,1145)	1:39:A:LEU:HD11	1:16:A:ALA:HB1	1	0.97
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB2	10	0.97
(2,1020)	1:57:B:ILE:HG12	1:57:B:ILE:HG23	8	0.97
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	7	0.97
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	6	0.97
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	7	0.97
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD12	2	0.97
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD21	10	0.97
(2,192)	1:17:B:LEU:HD22	1:14:B:LYS:HB3	2	0.97
(2,94)	1:32:B:ARG:HD2	1:34:B:TYR:H	7	0.97
(2,68)	1:65:B:GLU:HA	1:53:B:LYS:HD2	1	0.97
(3,66)	1:55:B:GLN:HG2	1:54:B:GLU:HA	5	0.96
(3,65)	1:55:A:GLN:HG2	1:54:A:GLU:HA	5	0.96
(2,2435)	1:27:A:LEU:HD13	1:47:A:GLU:H	5	0.96
(2,2393)	1:7:A:THR:H	1:4:A:ARG:HG3	9	0.96
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	4	0.96
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	9	0.96
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	9	0.96
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD23	4	0.96
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD13	3	0.96
(2,1947)	1:61:A:HIS:H	1:60:A:SER:HG	9	0.96
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	9	0.96
(2,1652)	1:28:B:THR:HB	1:31:B:TRP:HB3	8	0.96
(2,1651)	1:28:A:THR:HB	1:31:A:TRP:HB3	8	0.96
(2,1622)	1:39:B:LEU:HD11	1:18:B:ASP:H	7	0.96
(2,1495)	1:61:A:HIS:HA	1:54:A:GLU:HB2	3	0.96
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD13	10	0.96
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD13	5	0.96
(2,1149)	1:20:A:ALA:HB1	1:35:A:LEU:HD23	4	0.96
(2,1034)	1:41:B:LEU:HB2	1:41:B:LEU:HD23	5	0.96
(2,1033)	1:41:A:LEU:HB2	1:41:A:LEU:HD23	5	0.96
(2,1019)	1:57:A:ILE:HG12	1:57:A:ILE:HG23	8	0.96
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	9	0.96
(2,617)	1:12:A:GLU:HA	1:15:A:LYS:HE3	1	0.96
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	2	0.96
(2,322)	1:54:B:GLU:H	1:52:B:ARG:HB2	7	0.96
(2,297)	1:16:A:ALA:H	1:39:A:LEU:HB2	6	0.96
(2,253)	1:27:A:LEU:HD12	1:32:A:ARG:HB2	9	0.96
(2,248)	1:63:B:GLN:HG2	1:57:B:ILE:H	1	0.96
(2,247)	1:63:A:GLN:HG2	1:57:A:ILE:H	1	0.96
(2,240)	1:49:B:TRP:HB3	1:52:B:ARG:HG2	5	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,239)	1:49:A:TRP:HB3	1:52:A:ARG:HG2	5	0.96
(2,162)	1:39:B:LEU:HG	1:13:B:GLN:H	6	0.96
(2,93)	1:32:A:ARG:HD2	1:34:A:TYR:H	7	0.96
(1,8)	1:34:A:TYR:H	1:30:A:GLU:O	10	0.96
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	10	0.95
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	10	0.95
(3,67)	1:63:A:GLN:HG2	1:54:A:GLU:HA	4	0.95
(2,2256)	1:64:B:PHE:H	1:61:B:HIS:HA	7	0.95
(2,1948)	1:61:B:HIS:H	1:60:B:SER:HG	9	0.95
(2,1700)	1:12:B:GLU:HB3	1:13:B:GLN:H	4	0.95
(2,1553)	1:27:A:LEU:HB3	1:50:A:PHE:HB2	10	0.95
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	2	0.95
(2,1496)	1:61:B:HIS:HA	1:54:B:GLU:HB2	3	0.95
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD13	10	0.95
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	4	0.95
(2,1062)	1:27:B:LEU:HD23	1:50:B:PHE:HB3	10	0.95
(2,1061)	1:27:A:LEU:HD23	1:50:A:PHE:HB3	10	0.95
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD13	5	0.95
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	2	0.95
(2,462)	1:49:B:TRP:HD1	1:14:B:LYS:HE3	8	0.95
(2,461)	1:49:A:TRP:HD1	1:14:A:LYS:HE3	8	0.95
(2,371)	1:51:A:ARG:H	1:55:A:GLN:HG3	7	0.95
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	2	0.95
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD12	2	0.95
(2,199)	1:20:A:ALA:HB1	1:17:A:LEU:HB3	7	0.95
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	1	0.95
(1,49)	1:33:B:ARG:H	1:29:B:PRO:O	1	0.95
(2,2394)	1:7:B:THR:H	1:4:B:ARG:HG3	9	0.94
(2,2167)	1:14:A:LYS:H	1:14:A:LYS:HD3	5	0.94
(2,2084)	1:14:B:LYS:H	1:9:B:PHE:HB3	10	0.94
(2,1554)	1:27:B:LEU:HB3	1:50:B:PHE:HB2	10	0.94
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	3	0.94
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD21	9	0.94
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG22	3	0.94
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG22	3	0.94
(2,1344)	1:41:B:LEU:HD12	1:17:B:LEU:HD22	3	0.94
(2,1195)	1:16:A:ALA:HB2	1:13:A:GLN:HG2	9	0.94
(2,1150)	1:20:B:ALA:HB1	1:35:B:LEU:HD23	2	0.94
(2,1149)	1:20:A:ALA:HB1	1:35:A:LEU:HD23	2	0.94
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB2	10	0.94
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	6	0.94
(2,474)	1:19:B:LEU:HD22	1:19:A:LEU:HB3	10	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,372)	1:51:B:ARG:H	1:55:B:GLN:HG3	7	0.94
(2,204)	1:28:B:THR:HB	1:32:B:ARG:HB2	2	0.94
(2,187)	1:17:A:LEU:HD23	1:45:A:GLN:HB3	6	0.94
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	6	0.94
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	7	0.94
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB2	4	0.94
(1,7)	1:33:A:ARG:H	1:29:A:PRO:O	1	0.94
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	7	0.93
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	9	0.93
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	7	0.93
(3,62)	1:27:B:LEU:HB2	1:21:B:PHE:H	5	0.93
(3,62)	1:27:B:LEU:HB2	1:21:B:PHE:H	6	0.93
(2,2168)	1:14:B:LYS:H	1:14:B:LYS:HD3	5	0.93
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	4	0.93
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	4	0.93
(2,1910)	1:59:B:TRP:H	1:57:B:ILE:HG12	5	0.93
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	2	0.93
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD21	7	0.93
(2,772)	1:54:B:GLU:HA	1:21:B:PHE:HE1	4	0.93
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD22	3	0.93
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD12	9	0.93
(2,254)	1:27:B:LEU:HD11	1:32:B:ARG:HB2	4	0.93
(2,254)	1:27:B:LEU:HD12	1:32:B:ARG:HB2	9	0.93
(2,203)	1:28:A:THR:HB	1:32:A:ARG:HB2	2	0.93
(2,200)	1:20:B:ALA:HB1	1:17:B:LEU:HB3	7	0.93
(2,192)	1:17:B:LEU:HD23	1:14:B:LYS:HB3	3	0.93
(2,162)	1:39:B:LEU:HG	1:13:B:GLN:H	7	0.93
(3,160)	1:43:B:GLU:H	1:44:B:GLU:HG2	6	0.92
(3,159)	1:43:A:GLU:H	1:44:A:GLU:HG2	6	0.92
(3,158)	1:16:B:ALA:H	1:17:B:LEU:HG	8	0.92
(3,157)	1:16:A:ALA:H	1:17:A:LEU:HG	8	0.92
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	2	0.92
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	9	0.92
(2,2200)	1:33:B:ARG:H	1:33:B:ARG:HD3	2	0.92
(2,2199)	1:33:A:ARG:H	1:33:A:ARG:HD3	2	0.92
(2,2199)	1:33:A:ARG:H	1:33:A:ARG:HD3	3	0.92
(2,2152)	1:15:B:LYS:HG3	1:15:B:LYS:H	5	0.92
(2,2151)	1:15:A:LYS:HG3	1:15:A:LYS:H	5	0.92
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD13	10	0.92
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD12	5	0.92
(2,1909)	1:59:A:TRP:H	1:57:A:ILE:HG12	5	0.92
(2,1621)	1:39:A:LEU:HD11	1:18:A:ASP:H	7	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1606)	1:54:B:GLU:HB3	1:21:B:PHE:HZ	6	0.92
(2,1588)	1:54:B:GLU:HB3	1:59:B:TRP:HB2	3	0.92
(2,1587)	1:54:A:GLU:HB3	1:59:A:TRP:HB2	3	0.92
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD21	7	0.92
(2,1398)	1:46:B:ILE:HD13	1:35:B:LEU:H	8	0.92
(2,1397)	1:46:A:ILE:HD13	1:35:A:LEU:H	8	0.92
(2,1394)	1:46:B:ILE:HD11	1:36:B:SER:HG	5	0.92
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD11	7	0.92
(2,1201)	1:17:A:LEU:HD23	1:46:A:ILE:HG12	4	0.92
(2,1196)	1:16:B:ALA:HB2	1:13:B:GLN:HG2	9	0.92
(2,1020)	1:57:B:ILE:HG12	1:57:B:ILE:HG23	4	0.92
(2,1019)	1:57:A:ILE:HG12	1:57:A:ILE:HG23	4	0.92
(2,479)	1:19:A:LEU:HD23	1:17:B:LEU:HD13	4	0.92
(2,371)	1:51:A:ARG:H	1:55:A:GLN:HG3	2	0.92
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	5	0.92
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD13	3	0.92
(3,159)	1:43:A:GLU:H	1:44:A:GLU:HG2	3	0.91
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	2	0.91
(3,76)	1:57:B:ILE:HG12	1:61:B:HIS:HB2	7	0.91
(2,2426)	1:55:B:GLN:HB3	1:56:B:GLN:H	3	0.91
(2,2425)	1:55:A:GLN:HB3	1:56:A:GLN:H	3	0.91
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	3	0.91
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD23	4	0.91
(2,1801)	1:65:A:GLU:H	1:64:A:PHE:HD1	9	0.91
(2,1146)	1:39:B:LEU:HD12	1:16:B:ALA:HB1	5	0.91
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	5	0.91
(2,850)	1:33:B:ARG:HD3	1:34:B:TYR:HD1	8	0.91
(2,849)	1:33:A:ARG:HD3	1:34:A:TYR:HD1	8	0.91
(2,463)	1:49:A:TRP:HD1	1:63:A:GLN:HE21	4	0.91
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	7	0.91
(2,94)	1:32:B:ARG:HD2	1:34:B:TYR:H	8	0.91
(2,93)	1:32:A:ARG:HD2	1:34:A:TYR:H	3	0.91
(2,93)	1:32:A:ARG:HD2	1:34:A:TYR:H	8	0.91
(3,160)	1:43:B:GLU:H	1:44:B:GLU:HG2	3	0.9
(3,61)	1:27:A:LEU:HB2	1:21:A:PHE:H	6	0.9
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	1	0.9
(2,2200)	1:33:B:ARG:H	1:33:B:ARG:HD3	3	0.9
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	5	0.9
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG23	1	0.9
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG23	3	0.9
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG22	6	0.9
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG21	7	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG23	1	0.9
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG23	3	0.9
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG22	6	0.9
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG21	7	0.9
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD13	10	0.9
(2,1616)	1:27:B:LEU:HD13	1:35:B:LEU:HD13	9	0.9
(2,1605)	1:54:A:GLU:HB3	1:21:A:PHE:HZ	6	0.9
(2,1393)	1:46:A:ILE:HD11	1:36:A:SER:HG	5	0.9
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	7	0.9
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD11	7	0.9
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	5	0.9
(2,863)	1:35:A:LEU:HB3	1:39:A:LEU:HD21	3	0.9
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	5	0.9
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG22	3	0.9
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	10	0.89
(2,2436)	1:27:B:LEU:HD13	1:47:B:GLU:H	7	0.89
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	1	0.89
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	8	0.89
(2,2075)	1:48:A:ARG:H	1:47:A:GLU:HG2	8	0.89
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG23	5	0.89
(2,1554)	1:27:B:LEU:HB3	1:50:B:PHE:HB2	8	0.89
(2,1553)	1:27:A:LEU:HB3	1:50:A:PHE:HB2	8	0.89
(2,1496)	1:61:B:HIS:HA	1:54:B:GLU:HB2	5	0.89
(2,1495)	1:61:A:HIS:HA	1:54:A:GLU:HB2	5	0.89
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	7	0.89
(2,1240)	1:20:B:ALA:HB2	1:39:B:LEU:HD22	5	0.89
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD11	3	0.89
(2,1165)	1:46:A:ILE:HD13	1:36:A:SER:H	4	0.89
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD11	7	0.89
(2,1145)	1:39:A:LEU:HD12	1:16:A:ALA:HB1	5	0.89
(2,1059)	1:27:A:LEU:HD22	1:50:A:PHE:HB2	9	0.89
(2,965)	1:55:A:GLN:HG2	1:51:A:ARG:HG3	2	0.89
(2,472)	1:19:B:LEU:HD23	1:19:A:LEU:HG	1	0.89
(2,471)	1:19:A:LEU:HD23	1:19:B:LEU:HG	1	0.89
(2,462)	1:49:B:TRP:HD1	1:14:B:LYS:HE3	6	0.89
(2,443)	1:16:A:ALA:HB2	1:16:B:ALA:H	5	0.89
(2,372)	1:51:B:ARG:H	1:55:B:GLN:HG3	5	0.89
(2,372)	1:51:B:ARG:H	1:47:B:GLU:HG2	10	0.89
(2,277)	1:7:A:THR:HB	1:36:A:SER:HB2	4	0.89
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG22	3	0.89
(2,177)	1:16:A:ALA:HB3	1:20:A:ALA:H	9	0.89
(2,94)	1:32:B:ARG:HD2	1:34:B:TYR:H	3	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,44)	1:53:B:LYS:HA	1:53:B:LYS:HD3	6	0.89
(2,43)	1:53:A:LYS:HA	1:53:A:LYS:HD3	6	0.89
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	7	0.89
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	10	0.88
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	10	0.88
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	3	0.88
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	8	0.88
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	8	0.88
(2,2435)	1:27:A:LEU:HD13	1:47:A:GLU:H	7	0.88
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG23	5	0.88
(2,1626)	1:41:B:LEU:HD12	1:36:B:SER:HA	4	0.88
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD22	1	0.88
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD22	1	0.88
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	10	0.88
(2,1239)	1:20:A:ALA:HB2	1:39:A:LEU:HD22	5	0.88
(2,1210)	1:49:B:TRP:HB3	1:17:B:LEU:HD12	1	0.88
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	5	0.88
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	5	0.88
(2,1146)	1:39:B:LEU:HD13	1:16:B:ALA:HB1	3	0.88
(2,1060)	1:27:B:LEU:HD22	1:50:B:PHE:HB2	9	0.88
(2,847)	1:51:A:ARG:HD2	1:52:A:ARG:HA	8	0.88
(2,371)	1:51:A:ARG:H	1:55:A:GLN:HG3	3	0.88
(2,346)	1:36:B:SER:H	1:41:B:LEU:HD13	7	0.88
(2,295)	1:53:A:LYS:H	1:63:A:GLN:HB3	9	0.88
(2,204)	1:28:B:THR:HB	1:32:B:ARG:HB2	1	0.88
(2,203)	1:28:A:THR:HB	1:32:A:ARG:HB2	1	0.88
(2,44)	1:53:B:LYS:HA	1:53:B:LYS:HD3	5	0.88
(2,43)	1:53:A:LYS:HA	1:53:A:LYS:HD3	5	0.88
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	6	0.88
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	8	0.88
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	8	0.88
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	10	0.87
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	5	0.87
(3,75)	1:57:A:ILE:HG12	1:61:A:HIS:HB2	7	0.87
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	8	0.87
(2,2076)	1:48:B:ARG:H	1:47:B:GLU:HG2	5	0.87
(2,1910)	1:59:B:TRP:H	1:57:B:ILE:HG12	8	0.87
(2,1909)	1:59:A:TRP:H	1:57:A:ILE:HG12	8	0.87
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	10	0.87
(2,1245)	1:20:A:ALA:HB3	1:50:A:PHE:HE1	8	0.87
(2,1192)	1:16:B:ALA:HB2	1:14:B:LYS:HA	9	0.87
(2,1145)	1:39:A:LEU:HD13	1:16:A:ALA:HB1	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,966)	1:55:B:GLN:HG2	1:51:B:ARG:HG3	2	0.87
(2,848)	1:51:B:ARG:HD2	1:52:B:ARG:HA	8	0.87
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	9	0.87
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	10	0.87
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	9	0.87
(2,461)	1:49:A:TRP:HD1	1:14:A:LYS:HE3	6	0.87
(2,444)	1:16:B:ALA:HB2	1:16:A:ALA:H	5	0.87
(2,372)	1:51:B:ARG:H	1:55:B:GLN:HG3	3	0.87
(2,371)	1:51:A:ARG:H	1:47:A:GLU:HG2	10	0.87
(2,345)	1:36:A:SER:H	1:41:A:LEU:HD13	7	0.87
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HD2	10	0.87
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD21	7	0.87
(2,264)	1:39:B:LEU:HD12	1:16:B:ALA:H	9	0.87
(2,87)	1:48:A:ARG:HD3	1:45:A:GLN:HE21	5	0.87
(3,186)	1:13:B:GLN:H	1:17:B:LEU:H	9	0.86
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	3	0.86
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	3	0.86
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	7	0.86
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	1	0.86
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	8	0.86
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG21	9	0.86
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG21	8	0.86
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG21	9	0.86
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG22	8	0.86
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG22	8	0.86
(2,1246)	1:20:B:ALA:HB3	1:50:B:PHE:HE1	8	0.86
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD11	3	0.86
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	4	0.86
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	10	0.86
(2,491)	1:61:A:HIS:HD1	1:61:A:HIS:H	4	0.86
(2,350)	1:27:B:LEU:H	1:24:B:ASP:HB3	2	0.86
(2,349)	1:27:A:LEU:H	1:24:A:ASP:HB3	2	0.86
(2,264)	1:39:B:LEU:HD11	1:16:B:ALA:H	7	0.86
(2,263)	1:39:A:LEU:HD11	1:16:A:ALA:H	7	0.86
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	9	0.86
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	6	0.86
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	7	0.86
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	10	0.85
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	1	0.85
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG21	8	0.85
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG21	4	0.85
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	4	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1513)	1:9:A:PHE:HA	1:17:A:LEU:HD22	8	0.85
(2,1209)	1:49:A:TRP:HB3	1:17:A:LEU:HD12	1	0.85
(2,1146)	1:39:B:LEU:HD12	1:16:B:ALA:HB2	9	0.85
(2,864)	1:35:B:LEU:HB3	1:39:B:LEU:HD21	3	0.85
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD12	6	0.85
(2,492)	1:61:B:HIS:HD1	1:61:B:HIS:H	4	0.85
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD11	9	0.85
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD13	3	0.85
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	6	0.85
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	1	0.85
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	8	0.85
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	1	0.85
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	8	0.85
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	7	0.85
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	9	0.85
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	1	0.84
(3,74)	1:39:B:LEU:HG	1:15:A:LYS:HE3	8	0.84
(3,73)	1:39:A:LEU:HG	1:15:B:LYS:HE3	8	0.84
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	1	0.84
(2,2168)	1:14:B:LYS:H	1:14:B:LYS:HD3	1	0.84
(2,2167)	1:14:A:LYS:H	1:14:A:LYS:HD3	1	0.84
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG21	4	0.84
(2,1912)	1:59:B:TRP:H	1:57:B:ILE:HG13	8	0.84
(2,1911)	1:59:A:TRP:H	1:57:A:ILE:HG13	8	0.84
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	5	0.84
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	5	0.84
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	5	0.84
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	5	0.84
(2,1689)	1:9:A:PHE:HB3	1:14:A:LYS:HG3	10	0.84
(2,1615)	1:27:A:LEU:HD13	1:35:A:LEU:HD13	9	0.84
(2,1548)	1:27:B:LEU:HB3	1:50:B:PHE:HD1	8	0.84
(2,1547)	1:27:A:LEU:HB3	1:50:A:PHE:HD1	8	0.84
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD21	3	0.84
(2,1514)	1:9:B:PHE:HA	1:17:B:LEU:HD22	8	0.84
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD12	8	0.84
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	4	0.84
(2,1156)	1:57:B:ILE:HG22	1:58:B:GLY:H	5	0.84
(2,1155)	1:57:A:ILE:HG22	1:58:A:GLY:H	5	0.84
(2,1145)	1:39:A:LEU:HD11	1:16:A:ALA:HB3	2	0.84
(2,981)	1:33:A:ARG:HB2	1:33:A:ARG:HD3	4	0.84
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	8	0.84
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	8	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,704)	1:64:B:PHE:HA	1:64:B:PHE:HD1	5	0.84
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD12	6	0.84
(2,374)	1:56:B:GLN:H	1:57:B:ILE:HG13	9	0.84
(2,371)	1:51:A:ARG:H	1:47:A:GLU:HG2	4	0.84
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	6	0.84
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	7	0.84
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	3	0.83
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	5	0.83
(2,2294)	1:60:B:SER:H	1:57:B:ILE:HG22	1	0.83
(2,2293)	1:60:A:SER:H	1:57:A:ILE:HG22	1	0.83
(2,1625)	1:41:A:LEU:HD12	1:36:A:SER:HA	4	0.83
(2,1403)	1:46:A:ILE:HG22	1:35:A:LEU:HD13	10	0.83
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD12	8	0.83
(2,1166)	1:46:B:ILE:HD12	1:36:B:SER:H	3	0.83
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD13	4	0.83
(2,1146)	1:39:B:LEU:HD11	1:16:B:ALA:HB3	2	0.83
(2,982)	1:33:B:ARG:HB2	1:33:B:ARG:HD3	4	0.83
(2,703)	1:64:A:PHE:HA	1:64:A:PHE:HD1	5	0.83
(2,662)	1:52:B:ARG:HA	1:55:B:GLN:HG2	1	0.83
(2,442)	1:16:B:ALA:HB2	1:20:A:ALA:H	1	0.83
(2,441)	1:16:A:ALA:HB2	1:20:B:ALA:H	1	0.83
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD22	3	0.83
(2,352)	1:4:B:ARG:H	1:12:B:GLU:HG3	5	0.83
(2,351)	1:4:A:ARG:H	1:12:A:GLU:HG3	5	0.83
(2,278)	1:7:B:THR:HB	1:36:B:SER:HB2	4	0.83
(2,199)	1:20:A:ALA:HB1	1:17:A:LEU:HB3	3	0.83
(2,88)	1:48:B:ARG:HD3	1:45:B:GLN:HE21	5	0.83
(3,185)	1:13:A:GLN:H	1:17:A:LEU:H	9	0.82
(3,181)	1:64:A:PHE:H	1:62:A:PRO:HB3	9	0.82
(3,136)	1:27:B:LEU:H	1:31:B:TRP:HA	3	0.82
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	2	0.82
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	2	0.82
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	3	0.82
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	1	0.82
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	5	0.82
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	7	0.82
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	7	0.82
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	6	0.82
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	6	0.82
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	7	0.82
(2,1622)	1:39:B:LEU:HD11	1:18:B:ASP:H	4	0.82
(2,1615)	1:27:A:LEU:HD12	1:35:A:LEU:HD13	2	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD21	3	0.82
(2,1387)	1:46:A:ILE:HD12	1:45:A:GLN:HG3	4	0.82
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD12	5	0.82
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	8	0.82
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	8	0.82
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD11	7	0.82
(2,808)	1:4:B:ARG:HA	1:4:B:ARG:HG3	8	0.82
(2,807)	1:4:A:ARG:HA	1:4:A:ARG:HG3	8	0.82
(2,661)	1:52:A:ARG:HA	1:55:A:GLN:HG2	1	0.82
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD12	9	0.82
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HD2	10	0.82
(2,239)	1:49:A:TRP:HB3	1:52:A:ARG:HG2	2	0.82
(2,203)	1:28:A:THR:HB	1:32:A:ARG:HB2	9	0.82
(2,178)	1:16:B:ALA:HB3	1:20:B:ALA:H	8	0.82
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	1	0.81
(3,91)	1:27:A:LEU:HA	1:50:A:PHE:HB3	2	0.81
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	1	0.81
(3,28)	1:2:B:GLU:HA	1:12:B:GLU:H	10	0.81
(2,1882)	1:63:B:GLN:H	1:62:B:PRO:HD2	3	0.81
(2,1695)	1:7:A:THR:HB	1:45:A:GLN:HB2	10	0.81
(2,1616)	1:27:B:LEU:HD12	1:35:B:LEU:HD13	2	0.81
(2,1411)	1:46:A:ILE:HG22	1:50:A:PHE:HD2	5	0.81
(2,1191)	1:16:A:ALA:HB2	1:14:A:LYS:HA	9	0.81
(2,1166)	1:46:B:ILE:HD11	1:36:B:SER:H	1	0.81
(2,1145)	1:39:A:LEU:HD12	1:16:A:ALA:HB2	9	0.81
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	2	0.81
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD11	9	0.81
(2,468)	1:19:B:LEU:HD22	1:35:A:LEU:HB2	1	0.81
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD22	5	0.81
(2,371)	1:51:A:ARG:H	1:47:A:GLU:HG2	5	0.81
(2,321)	1:54:A:GLU:H	1:52:A:ARG:HB2	4	0.81
(2,226)	1:46:B:ILE:HD12	1:9:B:PHE:HB2	10	0.81
(2,225)	1:46:A:ILE:HD12	1:9:A:PHE:HB2	10	0.81
(2,177)	1:16:A:ALA:HB3	1:20:A:ALA:H	8	0.81
(2,126)	1:48:B:ARG:HB3	1:48:B:ARG:HD2	8	0.81
(2,125)	1:48:A:ARG:HB3	1:48:A:ARG:HD2	8	0.81
(2,94)	1:32:B:ARG:HD2	1:34:B:TYR:H	6	0.81
(2,93)	1:32:A:ARG:HD2	1:34:A:TYR:H	6	0.81
(2,49)	1:49:A:TRP:HA	1:9:A:PHE:HE2	5	0.81
(1,43)	1:15:B:LYS:H	1:11:B:GLU:O	6	0.81
(1,1)	1:15:A:LYS:H	1:11:A:GLU:O	6	0.81
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	9	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,192)	1:44:B:GLU:H	1:36:B:SER:HB2	6	0.8
(3,191)	1:44:A:GLU:H	1:36:A:SER:HB2	6	0.8
(3,158)	1:16:B:ALA:H	1:17:B:LEU:HG	5	0.8
(3,157)	1:16:A:ALA:H	1:17:A:LEU:HG	5	0.8
(3,78)	1:37:B:GLN:HB3	1:34:B:TYR:HB2	3	0.8
(3,65)	1:55:A:GLN:HG2	1:54:A:GLU:HA	2	0.8
(3,45)	1:6:A:ARG:HD3	1:8:A:GLU:HG3	3	0.8
(3,4)	1:12:B:GLU:HG3	1:12:A:GLU:HB2	7	0.8
(2,1881)	1:63:A:GLN:H	1:62:A:PRO:HD2	3	0.8
(2,1651)	1:28:A:THR:HB	1:31:A:TRP:HB3	3	0.8
(2,1576)	1:27:B:LEU:HD12	1:51:B:ARG:H	6	0.8
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	1	0.8
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	4	0.8
(2,1165)	1:46:A:ILE:HD11	1:36:A:SER:H	1	0.8
(2,1165)	1:46:A:ILE:HD12	1:36:A:SER:H	3	0.8
(2,467)	1:19:A:LEU:HD22	1:35:B:LEU:HB2	1	0.8
(2,372)	1:51:B:ARG:H	1:47:B:GLU:HG2	4	0.8
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	1	0.8
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	1	0.8
(2,251)	1:27:A:LEU:HD13	1:44:A:GLU:HA	4	0.8
(2,226)	1:46:B:ILE:HD11	1:9:B:PHE:HB2	2	0.8
(2,225)	1:46:A:ILE:HD11	1:9:A:PHE:HB2	2	0.8
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	5	0.8
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	5	0.8
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	9	0.8
(2,50)	1:49:B:TRP:HA	1:9:B:PHE:HE2	5	0.8
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	8	0.79
(3,116)	1:3:B:LYS:HG3	1:1:B:MET:HA	6	0.79
(3,115)	1:3:A:LYS:HG3	1:1:A:MET:HA	6	0.79
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	1	0.79
(3,92)	1:27:B:LEU:HA	1:50:B:PHE:HB3	2	0.79
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	9	0.79
(3,46)	1:6:B:ARG:HD3	1:8:B:GLU:HG3	3	0.79
(3,27)	1:2:A:GLU:HA	1:12:A:GLU:H	10	0.79
(2,2442)	1:14:B:LYS:H	1:17:B:LEU:HD21	6	0.79
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	7	0.79
(2,1896)	1:65:B:GLU:HB2	1:65:B:GLU:H	3	0.79
(2,1895)	1:65:A:GLU:HB2	1:65:A:GLU:H	3	0.79
(2,1735)	1:64:A:PHE:H	1:64:A:PHE:HD1	9	0.79
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	2	0.79
(2,1621)	1:39:A:LEU:HD11	1:18:A:ASP:H	4	0.79
(2,1588)	1:54:B:GLU:HB3	1:59:B:TRP:HB2	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1404)	1:46:B:ILE:HG22	1:35:B:LEU:HD13	10	0.79
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	5	0.79
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	5	0.79
(2,1166)	1:46:B:ILE:HD12	1:36:B:SER:H	2	0.79
(2,1002)	1:44:B:GLU:HB3	1:45:B:GLN:H	4	0.79
(2,982)	1:33:B:ARG:HB2	1:33:B:ARG:HD3	2	0.79
(2,981)	1:33:A:ARG:HB2	1:33:A:ARG:HD3	2	0.79
(2,467)	1:19:A:LEU:HD22	1:35:B:LEU:HB2	8	0.79
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD21	2	0.79
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD11	8	0.79
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD11	8	0.79
(2,336)	1:15:B:LYS:H	1:15:B:LYS:HD3	9	0.79
(2,322)	1:54:B:GLU:H	1:52:B:ARG:HB2	4	0.79
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD11	4	0.79
(2,263)	1:39:A:LEU:HD12	1:16:A:ALA:H	9	0.79
(2,204)	1:28:B:THR:HB	1:32:B:ARG:HB2	9	0.79
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	8	0.79
(3,186)	1:13:B:GLN:H	1:17:B:LEU:H	2	0.78
(3,185)	1:13:A:GLN:H	1:17:A:LEU:H	2	0.78
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	5	0.78
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	8	0.78
(3,3)	1:12:A:GLU:HG3	1:12:B:GLU:HB2	7	0.78
(2,2436)	1:27:B:LEU:HD12	1:47:B:GLU:H	6	0.78
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	3	0.78
(2,2255)	1:64:A:PHE:H	1:61:A:HIS:HA	9	0.78
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD13	3	0.78
(2,1700)	1:12:B:GLU:HB3	1:13:B:GLN:H	3	0.78
(2,1699)	1:12:A:GLU:HB3	1:13:A:GLN:H	3	0.78
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	2	0.78
(2,1678)	1:30:B:GLU:HA	1:33:B:ARG:HD3	7	0.78
(2,1587)	1:54:A:GLU:HB3	1:59:A:TRP:HB2	10	0.78
(2,1575)	1:27:A:LEU:HD12	1:51:A:ARG:H	6	0.78
(2,1520)	1:18:B:ASP:HA	1:17:B:LEU:HD23	8	0.78
(2,1519)	1:18:A:ASP:HA	1:17:A:LEU:HD23	8	0.78
(2,1415)	1:46:A:ILE:HG21	1:32:A:ARG:H	5	0.78
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	1	0.78
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	7	0.78
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	7	0.78
(2,1165)	1:46:A:ILE:HD12	1:36:A:SER:H	2	0.78
(2,981)	1:33:A:ARG:HB2	1:33:A:ARG:HD3	3	0.78
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD21	10	0.78
(2,468)	1:19:B:LEU:HD22	1:35:A:LEU:HB2	8	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,407)	1:9:A:PHE:HD1	1:41:A:LEU:HD22	5	0.78
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD12	3	0.78
(2,192)	1:17:B:LEU:HD23	1:14:B:LYS:HB3	9	0.78
(2,189)	1:17:A:LEU:HD22	1:53:A:LYS:HE3	4	0.78
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	1	0.78
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	8	0.78
(3,185)	1:13:A:GLN:H	1:17:A:LEU:H	10	0.77
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	10	0.77
(2,2435)	1:27:A:LEU:HD12	1:47:A:GLU:H	6	0.77
(2,2119)	1:28:A:THR:H	1:32:A:ARG:HE	9	0.77
(2,1876)	1:63:B:GLN:H	1:63:B:GLN:HB2	4	0.77
(2,1850)	1:52:B:ARG:HB3	1:53:B:LYS:H	7	0.77
(2,1698)	1:7:B:THR:HB	1:45:B:GLN:HG3	2	0.77
(2,1696)	1:7:B:THR:HB	1:45:B:GLN:HB2	10	0.77
(2,1602)	1:53:B:LYS:HG3	1:21:B:PHE:HZ	4	0.77
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	7	0.77
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	7	0.77
(2,1326)	1:40:B:GLY:HA3	1:4:B:ARG:HD3	10	0.77
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	10	0.77
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	9	0.77
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	9	0.77
(2,982)	1:33:B:ARG:HB2	1:33:B:ARG:HD3	3	0.77
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	6	0.77
(2,808)	1:4:B:ARG:HA	1:4:B:ARG:HG3	1	0.77
(2,807)	1:4:A:ARG:HA	1:4:A:ARG:HG3	1	0.77
(2,647)	1:53:A:LYS:HA	1:63:A:GLN:HG3	10	0.77
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD13	9	0.77
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD21	10	0.77
(2,548)	1:57:B:ILE:HA	1:57:B:ILE:HG13	4	0.77
(2,547)	1:57:A:ILE:HA	1:57:A:ILE:HG13	4	0.77
(2,408)	1:9:B:PHE:HD1	1:41:B:LEU:HD21	2	0.77
(2,381)	1:34:A:TYR:HD1	1:64:B:PHE:HD1	6	0.77
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	4	0.77
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	10	0.77
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	10	0.77
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	9	0.77
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	9	0.77
(2,19)	1:5:A:PRO:HA	1:6:A:ARG:HG3	10	0.77
(2,14)	1:36:B:SER:HB2	1:45:B:GLN:HB2	2	0.77
(1,23)	1:15:A:LYS:N	1:11:A:GLU:O	4	0.77
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	9	0.76
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	4	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	3	0.76
(3,95)	1:59:A:TRP:HB2	1:55:A:GLN:H	2	0.76
(3,66)	1:55:B:GLN:HG2	1:54:B:GLU:HA	2	0.76
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD23	8	0.76
(2,2072)	1:55:B:GLN:H	1:55:B:GLN:HB3	7	0.76
(2,2071)	1:55:A:GLN:H	1:55:A:GLN:HB3	7	0.76
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD23	7	0.76
(2,1959)	1:34:A:TYR:H	1:33:A:ARG:HG3	4	0.76
(2,1875)	1:63:A:GLN:H	1:63:A:GLN:HB2	4	0.76
(2,1849)	1:52:A:ARG:HB3	1:53:A:LYS:H	7	0.76
(2,1615)	1:27:A:LEU:HD11	1:35:A:LEU:HD13	4	0.76
(2,1388)	1:46:B:ILE:HD12	1:45:B:GLN:HG3	4	0.76
(2,1325)	1:40:A:GLY:HA3	1:4:A:ARG:HD3	10	0.76
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	10	0.76
(2,1195)	1:16:A:ALA:HB3	1:13:A:GLN:HG2	6	0.76
(2,1176)	1:3:B:LYS:HE2	1:3:B:LYS:HB3	4	0.76
(2,1175)	1:3:A:LYS:HE2	1:3:A:LYS:HB3	4	0.76
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	9	0.76
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	9	0.76
(2,1088)	1:15:B:LYS:HG3	1:15:B:LYS:HE3	7	0.76
(2,1087)	1:15:A:LYS:HG3	1:15:A:LYS:HE3	7	0.76
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	6	0.76
(2,943)	1:54:A:GLU:HG2	1:21:A:PHE:HZ	7	0.76
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	10	0.76
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	10	0.76
(2,648)	1:53:B:LYS:HA	1:63:B:GLN:HG3	10	0.76
(2,317)	1:59:A:TRP:HB2	1:55:A:GLN:H	2	0.76
(2,296)	1:53:B:LYS:H	1:63:B:GLN:HB3	9	0.76
(2,240)	1:49:B:TRP:HB3	1:52:B:ARG:HG2	2	0.76
(2,225)	1:46:A:ILE:HD11	1:9:A:PHE:HB2	3	0.76
(2,200)	1:20:B:ALA:HB1	1:17:B:LEU:HB3	3	0.76
(2,189)	1:17:A:LEU:HD23	1:53:A:LYS:HE2	5	0.76
(2,13)	1:36:A:SER:HB2	1:45:A:GLN:HB2	2	0.76
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	5	0.76
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	1	0.76
(3,186)	1:13:B:GLN:H	1:17:B:LEU:H	6	0.75
(3,186)	1:13:B:GLN:H	1:17:B:LEU:H	10	0.75
(3,185)	1:13:A:GLN:H	1:17:A:LEU:H	6	0.75
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	10	0.75
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	2	0.75
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	9	0.75
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD23	8	0.75
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	3	0.75
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	9	0.75
(2,1690)	1:9:B:PHE:HB3	1:14:B:LYS:HG3	3	0.75
(2,1677)	1:30:A:GLU:HA	1:33:A:ARG:HD3	7	0.75
(2,1343)	1:41:A:LEU:HD12	1:17:A:LEU:HD22	3	0.75
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	2	0.75
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	2	0.75
(2,1193)	1:16:A:ALA:HB2	1:13:A:GLN:HB3	10	0.75
(2,1001)	1:44:A:GLU:HB3	1:45:A:GLN:H	4	0.75
(2,944)	1:54:B:GLU:HG2	1:21:B:PHE:HZ	7	0.75
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD13	9	0.75
(2,351)	1:4:A:ARG:H	1:12:B:GLU:HG3	4	0.75
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD11	6	0.75
(2,263)	1:39:A:LEU:HD11	1:16:A:ALA:H	2	0.75
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	3	0.75
(2,191)	1:17:A:LEU:HD21	1:14:A:LYS:HB3	4	0.75
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	7	0.75
(2,49)	1:49:A:TRP:HA	1:9:A:PHE:HE1	10	0.75
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	3	0.75
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	3	0.74
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	2	0.74
(3,77)	1:37:A:GLN:HB3	1:34:A:TYR:HB2	3	0.74
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	5	0.74
(2,2441)	1:14:A:LYS:H	1:17:A:LEU:HD21	6	0.74
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	10	0.74
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	3	0.74
(2,2071)	1:55:A:GLN:H	1:55:A:GLN:HB3	4	0.74
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD23	7	0.74
(2,1896)	1:65:B:GLU:HB2	1:65:B:GLU:H	10	0.74
(2,1895)	1:65:A:GLU:HB2	1:65:A:GLU:H	10	0.74
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD13	5	0.74
(2,1697)	1:7:A:THR:HB	1:45:A:GLN:HG3	2	0.74
(2,1635)	1:41:A:LEU:HD12	1:13:A:GLN:HG2	3	0.74
(2,1514)	1:9:B:PHE:HA	1:17:B:LEU:HD21	6	0.74
(2,1496)	1:61:B:HIS:HA	1:54:B:GLU:HB2	8	0.74
(2,1495)	1:61:A:HIS:HA	1:54:A:GLU:HB2	8	0.74
(2,1336)	1:27:B:LEU:HD22	1:47:B:GLU:H	1	0.74
(2,1335)	1:27:A:LEU:HD22	1:47:A:GLU:H	1	0.74
(2,1196)	1:16:B:ALA:HB3	1:13:B:GLN:HG2	6	0.74
(2,1147)	1:16:A:ALA:HB3	1:19:B:LEU:HD22	9	0.74
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	2	0.74
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	7	0.74
(2,662)	1:52:B:ARG:HA	1:55:B:GLN:HG2	3	0.74
(2,661)	1:52:A:ARG:HA	1:55:A:GLN:HG2	3	0.74
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD11	2	0.74
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD11	6	0.74
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	8	0.74
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	8	0.74
(2,264)	1:39:B:LEU:HD11	1:16:B:ALA:H	2	0.74
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	3	0.74
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	7	0.74
(2,20)	1:5:B:PRO:HA	1:6:B:ARG:HG3	10	0.74
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	5	0.74
(3,192)	1:44:B:GLU:H	1:36:B:SER:HB2	2	0.73
(3,150)	1:2:B:GLU:H	1:4:B:ARG:HA	3	0.73
(3,149)	1:2:A:GLU:H	1:4:A:ARG:HA	3	0.73
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	10	0.73
(3,135)	1:27:A:LEU:H	1:31:A:TRP:HA	3	0.73
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	5	0.73
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	7	0.73
(2,2120)	1:28:B:THR:H	1:32:B:ARG:HE	9	0.73
(2,2072)	1:55:B:GLN:H	1:55:B:GLN:HB3	4	0.73
(2,2072)	1:55:B:GLN:H	1:55:B:GLN:HB3	6	0.73
(2,2071)	1:55:A:GLN:H	1:55:A:GLN:HB3	6	0.73
(2,1960)	1:34:B:TYR:H	1:33:B:ARG:HG3	4	0.73
(2,1832)	1:53:B:LYS:H	1:52:B:ARG:HE	6	0.73
(2,1831)	1:53:A:LYS:H	1:52:A:ARG:HE	6	0.73
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD11	5	0.73
(2,1689)	1:9:A:PHE:HB3	1:14:A:LYS:HG3	3	0.73
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	5	0.73
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	5	0.73
(2,1652)	1:28:B:THR:HB	1:31:B:TRP:HB3	3	0.73
(2,1202)	1:17:B:LEU:HD23	1:46:B:ILE:HG12	4	0.73
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	2	0.73
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	2	0.73
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD13	8	0.73
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD13	8	0.73
(2,1064)	1:27:B:LEU:HD21	1:43:B:GLU:HB3	8	0.73
(2,1063)	1:27:A:LEU:HD22	1:43:A:GLU:HB3	4	0.73
(2,1063)	1:27:A:LEU:HD21	1:43:A:GLU:HB3	8	0.73
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	6	0.73
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	10	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	6	0.73
(2,807)	1:4:A:ARG:HA	1:4:A:ARG:HG3	10	0.73
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD11	2	0.73
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	9	0.73
(2,335)	1:15:A:LYS:H	1:15:A:LYS:HD3	9	0.73
(2,182)	1:16:B:ALA:HB1	1:15:A:LYS:HB3	2	0.73
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	7	0.73
(2,124)	1:15:B:LYS:HB3	1:15:B:LYS:HE3	2	0.73
(2,123)	1:15:A:LYS:HB3	1:15:A:LYS:HE3	2	0.73
(2,50)	1:49:B:TRP:HA	1:9:B:PHE:HE1	10	0.73
(3,191)	1:44:A:GLU:H	1:36:A:SER:HB2	2	0.72
(3,182)	1:64:B:PHE:H	1:62:B:PRO:HB3	9	0.72
(3,96)	1:59:B:TRP:HB2	1:55:B:GLN:H	2	0.72
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	5	0.72
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	10	0.72
(2,1876)	1:63:B:GLN:H	1:63:B:GLN:HB2	2	0.72
(2,1875)	1:63:A:GLN:H	1:63:A:GLN:HB2	2	0.72
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	7	0.72
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	9	0.72
(2,1672)	1:57:B:ILE:HA	1:56:B:GLN:HG3	9	0.72
(2,1548)	1:27:B:LEU:HB3	1:50:B:PHE:HD2	5	0.72
(2,1412)	1:46:B:ILE:HG22	1:50:B:PHE:HD2	5	0.72
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD11	10	0.72
(2,1210)	1:49:B:TRP:HB3	1:17:B:LEU:HD12	7	0.72
(2,1124)	1:20:B:ALA:HB1	1:21:B:PHE:H	3	0.72
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	5	0.72
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	7	0.72
(2,808)	1:4:B:ARG:HA	1:4:B:ARG:HG3	10	0.72
(2,484)	1:50:B:PHE:HD1	1:27:B:LEU:HD13	5	0.72
(2,318)	1:59:B:TRP:HB2	1:55:B:GLN:H	2	0.72
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	4	0.72
(2,190)	1:17:B:LEU:HD23	1:53:B:LYS:HE2	5	0.72
(2,181)	1:16:A:ALA:HB1	1:15:B:LYS:HB3	2	0.72
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	7	0.72
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	6	0.72
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	6	0.72
(3,153)	1:11:A:GLU:H	1:13:A:GLN:HG3	6	0.71
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	1	0.71
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	1	0.71
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	1	0.71
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	1	0.71
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2250)	1:63:B:GLN:H	1:61:B:HIS:HB2	3	0.71
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	7	0.71
(2,1636)	1:41:B:LEU:HD12	1:13:B:GLN:HG2	3	0.71
(2,1625)	1:41:A:LEU:HD13	1:36:A:SER:HA	10	0.71
(2,1332)	1:27:B:LEU:HD23	1:50:B:PHE:H	8	0.71
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	5	0.71
(2,1194)	1:16:B:ALA:HB2	1:13:B:GLN:HB3	9	0.71
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB2	9	0.71
(2,1123)	1:20:A:ALA:HB1	1:21:A:PHE:H	3	0.71
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	10	0.71
(2,896)	1:42:B:ASN:HB3	1:44:B:GLU:HB3	9	0.71
(2,895)	1:42:A:ASN:HB3	1:44:A:GLU:HB3	9	0.71
(2,584)	1:32:B:ARG:HA	1:27:B:LEU:HD11	1	0.71
(2,583)	1:32:A:ARG:HA	1:27:A:LEU:HD11	1	0.71
(2,472)	1:19:B:LEU:HD23	1:19:A:LEU:HG	6	0.71
(2,471)	1:19:A:LEU:HD23	1:19:B:LEU:HG	6	0.71
(2,458)	1:49:B:TRP:HD1	1:17:B:LEU:HD12	1	0.71
(2,382)	1:34:B:TYR:HD1	1:64:A:PHE:HD1	6	0.71
(2,336)	1:15:B:LYS:H	1:15:B:LYS:HD3	2	0.71
(2,335)	1:15:A:LYS:H	1:15:A:LYS:HD3	2	0.71
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD11	4	0.71
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	8	0.71
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	8	0.71
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	6	0.71
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	6	0.71
(3,64)	1:8:B:GLU:HG3	1:45:B:GLN:HE22	1	0.7
(2,2249)	1:63:A:GLN:H	1:61:A:HIS:HB2	3	0.7
(2,2072)	1:55:B:GLN:H	1:55:B:GLN:HB3	9	0.7
(2,2071)	1:55:A:GLN:H	1:55:A:GLN:HB3	9	0.7
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD23	8	0.7
(2,1936)	1:61:B:HIS:H	1:57:B:ILE:HG22	1	0.7
(2,1935)	1:61:A:HIS:H	1:57:A:ILE:HG22	1	0.7
(2,1836)	1:53:B:LYS:H	1:53:B:LYS:HD2	3	0.7
(2,1804)	1:65:B:GLU:H	1:64:B:PHE:HB3	9	0.7
(2,1690)	1:9:B:PHE:HB3	1:14:B:LYS:HG3	10	0.7
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	6	0.7
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	4	0.7
(2,1331)	1:27:A:LEU:HD23	1:50:A:PHE:H	8	0.7
(2,1288)	1:32:B:ARG:HB3	1:27:B:LEU:HD13	9	0.7
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD11	10	0.7
(2,1209)	1:49:A:TRP:HB3	1:17:A:LEU:HD12	7	0.7
(2,1192)	1:16:B:ALA:HB2	1:14:B:LYS:HA	8	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1191)	1:16:A:ALA:HB2	1:14:A:LYS:HA	8	0.7
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD12	2	0.7
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD12	2	0.7
(2,1147)	1:16:A:ALA:HB2	1:19:B:LEU:HD23	5	0.7
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB2	9	0.7
(2,1108)	1:39:B:LEU:HD21	1:17:B:LEU:HG	1	0.7
(2,1064)	1:27:B:LEU:HD21	1:43:B:GLU:HB3	4	0.7
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	9	0.7
(2,226)	1:46:B:ILE:HD11	1:9:B:PHE:HB2	3	0.7
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	3	0.7
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	1	0.7
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	3	0.7
(2,9)	1:16:A:ALA:HB2	1:15:B:LYS:HD3	5	0.7
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	3	0.7
(3,146)	1:4:B:ARG:H	1:12:B:GLU:H	3	0.69
(3,63)	1:8:A:GLU:HG3	1:45:A:GLN:HE22	1	0.69
(2,2456)	1:7:B:THR:H	1:6:B:ARG:H	9	0.69
(2,2455)	1:7:A:THR:H	1:6:A:ARG:H	9	0.69
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	6	0.69
(2,2348)	1:16:B:ALA:H	1:17:B:LEU:HD21	4	0.69
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD23	8	0.69
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD12	2	0.69
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD12	5	0.69
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD12	2	0.69
(2,1835)	1:53:A:LYS:H	1:53:A:LYS:HD2	3	0.69
(2,1824)	1:8:B:GLU:H	1:9:B:PHE:HB3	10	0.69
(2,1803)	1:65:A:GLU:H	1:64:A:PHE:HB3	9	0.69
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	6	0.69
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD23	7	0.69
(2,1513)	1:9:A:PHE:HA	1:17:A:LEU:HD21	6	0.69
(2,1287)	1:32:A:ARG:HB3	1:27:A:LEU:HD13	9	0.69
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD21	9	0.69
(2,1192)	1:16:B:ALA:HB1	1:14:B:LYS:HA	1	0.69
(2,1191)	1:16:A:ALA:HB1	1:14:A:LYS:HA	1	0.69
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	1	0.69
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	1	0.69
(2,1156)	1:57:B:ILE:HG23	1:58:B:GLY:H	10	0.69
(2,1155)	1:57:A:ILE:HG23	1:58:A:GLY:H	10	0.69
(2,1148)	1:16:B:ALA:HB2	1:19:A:LEU:HD23	5	0.69
(2,1148)	1:16:B:ALA:HB3	1:19:A:LEU:HD22	9	0.69
(2,1002)	1:44:B:GLU:HB3	1:45:B:GLN:H	9	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	2	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	3	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	4	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	5	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	6	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	7	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	8	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	9	0.69
(2,842)	1:48:B:ARG:HD3	1:48:B:ARG:HG3	10	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	1	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	2	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	3	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	4	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	5	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	6	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	7	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	8	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	9	0.69
(2,841)	1:48:A:ARG:HD3	1:48:A:ARG:HG3	10	0.69
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	4	0.69
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD12	3	0.69
(2,332)	1:14:B:LYS:H	1:12:B:GLU:HA	1	0.69
(2,260)	1:54:B:GLU:HG3	1:59:B:TRP:HB2	9	0.69
(2,255)	1:53:A:LYS:HG2	1:21:A:PHE:HE1	5	0.69
(2,240)	1:49:B:TRP:HB3	1:46:B:ILE:HG12	7	0.69
(2,239)	1:49:A:TRP:HB3	1:46:A:ILE:HG12	7	0.69
(2,191)	1:17:A:LEU:HD23	1:14:A:LYS:HB3	9	0.69
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	1	0.69
(2,102)	1:19:B:LEU:HB3	1:16:B:ALA:HA	8	0.69
(2,101)	1:19:A:LEU:HB3	1:16:A:ALA:HA	8	0.69
(2,94)	1:32:B:ARG:HD2	1:34:B:TYR:H	1	0.69
(2,93)	1:32:A:ARG:HD2	1:34:A:TYR:H	1	0.69
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	3	0.69
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	4	0.69
(1,48)	1:20:B:ALA:H	1:16:B:ALA:O	3	0.69
(1,6)	1:20:A:ALA:H	1:16:A:ALA:O	3	0.69
(3,154)	1:11:B:GLU:H	1:13:B:GLN:HG3	6	0.68
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	9	0.68
(3,61)	1:27:A:LEU:HB2	1:21:A:PHE:H	5	0.68
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	5	0.68
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	6	0.68
(2,2072)	1:55:B:GLN:H	1:55:B:GLN:HB3	1	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2071)	1:55:A:GLN:H	1:55:A:GLN:HB3	1	0.68
(2,1896)	1:65:B:GLU:HB2	1:65:B:GLU:H	1	0.68
(2,1896)	1:65:B:GLU:HB2	1:65:B:GLU:H	9	0.68
(2,1895)	1:65:A:GLU:HB2	1:65:A:GLU:H	1	0.68
(2,1823)	1:8:A:GLU:H	1:9:A:PHE:HB3	10	0.68
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD13	7	0.68
(2,1474)	1:58:B:GLY:HA3	1:57:B:ILE:HB	6	0.68
(2,1473)	1:58:A:GLY:HA3	1:57:A:ILE:HB	6	0.68
(2,1268)	1:10:B:SER:HB2	1:12:B:GLU:H	6	0.68
(2,1267)	1:10:A:SER:HB2	1:12:A:GLU:H	6	0.68
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	2	0.68
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	3	0.68
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	2	0.68
(2,1193)	1:16:A:ALA:HB2	1:13:A:GLN:HB3	9	0.68
(2,1192)	1:16:B:ALA:HB2	1:14:B:LYS:HA	10	0.68
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	3	0.68
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	7	0.68
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	3	0.68
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	7	0.68
(2,1107)	1:39:A:LEU:HD21	1:17:A:LEU:HG	1	0.68
(2,1001)	1:44:A:GLU:HB3	1:45:A:GLN:H	9	0.68
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	1	0.68
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	1	0.68
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	4	0.68
(2,800)	1:42:B:ASN:HA	1:43:B:GLU:HG3	10	0.68
(2,799)	1:42:A:ASN:HA	1:43:A:GLU:HG3	10	0.68
(2,457)	1:49:A:TRP:HD1	1:17:A:LEU:HD12	1	0.68
(2,331)	1:14:A:LYS:H	1:12:A:GLU:HA	1	0.68
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	5	0.68
(2,178)	1:16:B:ALA:HB3	1:20:B:ALA:H	9	0.68
(2,163)	1:19:A:LEU:HD23	1:24:B:ASP:HB2	2	0.68
(2,100)	1:51:B:ARG:HD2	1:55:B:GLN:HG3	10	0.68
(2,99)	1:51:A:ARG:HD2	1:55:A:GLN:HG3	10	0.68
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	10	0.68
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	10	0.68
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB2	6	0.68
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB2	6	0.68
(2,10)	1:16:B:ALA:HB2	1:15:A:LYS:HD3	5	0.68
(1,74)	1:33:B:ARG:N	1:29:B:PRO:O	1	0.68
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	3	0.68
(1,32)	1:33:A:ARG:N	1:29:A:PRO:O	1	0.68
(3,145)	1:4:A:ARG:H	1:12:A:GLU:H	3	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	9	0.67
(3,128)	1:8:B:GLU:H	1:41:B:LEU:H	9	0.67
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	6	0.67
(2,2256)	1:64:B:PHE:H	1:61:B:HIS:HA	9	0.67
(2,2128)	1:55:B:GLN:H	1:53:B:LYS:HB2	9	0.67
(2,2072)	1:55:B:GLN:H	1:55:B:GLN:HB3	3	0.67
(2,2071)	1:55:A:GLN:H	1:55:A:GLN:HB3	3	0.67
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD11	6	0.67
(2,1804)	1:65:B:GLU:H	1:64:B:PHE:HB3	6	0.67
(2,1803)	1:65:A:GLU:H	1:64:A:PHE:HB3	6	0.67
(2,1671)	1:57:A:ILE:HA	1:56:A:GLN:HG3	9	0.67
(2,1626)	1:41:B:LEU:HD13	1:36:B:SER:HA	10	0.67
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD22	8	0.67
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD22	8	0.67
(2,1416)	1:46:B:ILE:HG22	1:32:B:ARG:H	2	0.67
(2,1415)	1:46:A:ILE:HG22	1:32:A:ARG:H	2	0.67
(2,1388)	1:46:B:ILE:HD12	1:45:B:GLN:HG3	8	0.67
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD21	9	0.67
(2,1194)	1:16:B:ALA:HB2	1:13:B:GLN:HB3	10	0.67
(2,1191)	1:16:A:ALA:HB2	1:14:A:LYS:HA	10	0.67
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	4	0.67
(2,373)	1:56:A:GLN:H	1:57:A:ILE:HG13	9	0.67
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD21	2	0.67
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD21	2	0.67
(2,305)	1:49:A:TRP:H	1:17:A:LEU:HD13	6	0.67
(2,256)	1:53:B:LYS:HG2	1:21:B:PHE:HE1	5	0.67
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	2	0.67
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	2	0.67
(2,106)	1:9:B:PHE:HB3	1:8:B:GLU:HB3	6	0.67
(2,105)	1:9:A:PHE:HB3	1:8:A:GLU:HB3	6	0.67
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	7	0.67
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB2	1	0.67
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB3	10	0.67
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB2	1	0.67
(3,146)	1:4:B:ARG:H	1:12:B:GLU:H	7	0.66
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	10	0.66
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	6	0.66
(2,2277)	1:9:A:PHE:H	1:41:A:LEU:HA	2	0.66
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD11	6	0.66
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD11	6	0.66
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD13	7	0.66
(2,1547)	1:27:A:LEU:HB3	1:50:A:PHE:HD2	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1547)	1:27:A:LEU:HB3	1:50:A:PHE:HD1	7	0.66
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD22	4	0.66
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD23	7	0.66
(2,1387)	1:46:A:ILE:HD12	1:45:A:GLN:HG3	8	0.66
(2,1387)	1:46:A:ILE:HD12	1:45:A:GLN:HG3	9	0.66
(2,1174)	1:3:B:LYS:HD3	1:3:B:LYS:HB3	8	0.66
(2,1173)	1:3:A:LYS:HD3	1:3:A:LYS:HB3	8	0.66
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	2	0.66
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	2	0.66
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD11	3	0.66
(2,584)	1:32:B:ARG:HA	1:27:B:LEU:HD11	8	0.66
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD13	6	0.66
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	6	0.66
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	6	0.66
(2,252)	1:27:B:LEU:HD13	1:44:B:GLU:HA	4	0.66
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	9	0.66
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	9	0.66
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	7	0.66
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB3	10	0.66
(1,62)	1:56:B:GLN:H	1:52:B:ARG:O	7	0.66
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	4	0.66
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	1	0.65
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	1	0.65
(2,2397)	1:42:A:ASN:H	1:36:A:SER:HB2	1	0.65
(2,2246)	1:66:B:LYS:H	1:64:B:PHE:H	5	0.65
(2,2245)	1:66:A:LYS:H	1:64:A:PHE:H	5	0.65
(2,2127)	1:55:A:GLN:H	1:53:A:LYS:HB2	9	0.65
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG21	10	0.65
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG21	10	0.65
(2,1895)	1:65:A:GLU:HB2	1:65:A:GLU:H	9	0.65
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD11	6	0.65
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	7	0.65
(2,1626)	1:41:B:LEU:HD11	1:36:B:SER:HA	3	0.65
(2,1625)	1:41:A:LEU:HD11	1:36:A:SER:HA	3	0.65
(2,1548)	1:27:B:LEU:HB3	1:50:B:PHE:HD1	7	0.65
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD23	7	0.65
(2,1411)	1:46:A:ILE:HG23	1:50:A:PHE:HD1	9	0.65
(2,1388)	1:46:B:ILE:HD12	1:45:B:GLN:HG3	6	0.65
(2,1388)	1:46:B:ILE:HD12	1:45:B:GLN:HG3	9	0.65
(2,1146)	1:39:B:LEU:HD11	1:16:B:ALA:HB2	10	0.65
(2,583)	1:32:A:ARG:HA	1:27:A:LEU:HD11	8	0.65
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD22	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD13	6	0.65
(2,528)	1:57:B:ILE:HA	1:57:B:ILE:HG23	9	0.65
(2,372)	1:51:B:ARG:H	1:47:B:GLU:HG2	9	0.65
(2,306)	1:49:B:TRP:H	1:17:B:LEU:HD13	6	0.65
(2,206)	1:49:B:TRP:HB2	1:52:B:ARG:H	9	0.65
(2,164)	1:19:B:LEU:HD23	1:24:A:ASP:HB2	2	0.65
(2,141)	1:47:A:GLU:HB3	1:27:A:LEU:HD22	9	0.65
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	5	0.65
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	5	0.65
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	2	0.65
(1,65)	1:15:B:LYS:N	1:11:B:GLU:O	4	0.65
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	2	0.65
(3,145)	1:4:A:ARG:H	1:12:A:GLU:H	7	0.64
(2,2398)	1:42:B:ASN:H	1:36:B:SER:HB2	1	0.64
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	7	0.64
(2,2278)	1:9:B:PHE:H	1:41:B:LEU:HA	2	0.64
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD21	9	0.64
(2,1956)	1:64:B:PHE:HB2	1:64:B:PHE:H	5	0.64
(2,1928)	1:6:B:ARG:H	1:6:B:ARG:HG3	5	0.64
(2,1927)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.64
(2,1850)	1:52:B:ARG:HB3	1:53:B:LYS:H	1	0.64
(2,1849)	1:52:A:ARG:HB3	1:53:A:LYS:H	1	0.64
(2,1789)	1:8:A:GLU:H	1:4:A:ARG:HG3	10	0.64
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	7	0.64
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD23	7	0.64
(2,1412)	1:46:B:ILE:HG21	1:50:B:PHE:HD1	4	0.64
(2,1412)	1:46:B:ILE:HG23	1:50:B:PHE:HD1	9	0.64
(2,1387)	1:46:A:ILE:HD12	1:45:A:GLN:HG3	6	0.64
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	3	0.64
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	3	0.64
(2,1240)	1:20:B:ALA:HB3	1:39:B:LEU:HD22	6	0.64
(2,1239)	1:20:A:ALA:HB3	1:39:A:LEU:HD22	6	0.64
(2,1143)	1:46:A:ILE:HG22	1:46:A:ILE:HG12	4	0.64
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD23	9	0.64
(2,371)	1:51:A:ARG:H	1:47:A:GLU:HG2	9	0.64
(2,342)	1:60:B:SER:H	1:59:B:TRP:HA	10	0.64
(2,341)	1:60:A:SER:H	1:59:A:TRP:HA	10	0.64
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	5	0.64
(2,205)	1:49:A:TRP:HB2	1:52:A:ARG:H	9	0.64
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	10	0.64
(1,6)	1:20:A:ALA:H	1:16:A:ALA:O	5	0.64
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	2	0.63
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	2	0.63
(3,127)	1:8:A:GLU:H	1:41:A:LEU:H	9	0.63
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	6	0.63
(2,2398)	1:42:B:ASN:H	1:36:B:SER:HB2	6	0.63
(2,2397)	1:42:A:ASN:H	1:36:A:SER:HB2	6	0.63
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD21	9	0.63
(2,1998)	1:44:B:GLU:H	1:44:B:GLU:HB3	4	0.63
(2,1997)	1:44:A:GLU:H	1:44:A:GLU:HB3	4	0.63
(2,1955)	1:64:A:PHE:HB2	1:64:A:PHE:H	5	0.63
(2,1626)	1:41:B:LEU:HD12	1:36:B:SER:HA	8	0.63
(2,1625)	1:41:A:LEU:HD12	1:36:A:SER:HA	8	0.63
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE1	1	0.63
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE1	1	0.63
(2,1542)	1:17:B:LEU:HD21	1:13:B:GLN:HB3	6	0.63
(2,1495)	1:61:A:HIS:HA	1:54:A:GLU:HB2	10	0.63
(2,1189)	1:16:A:ALA:HB2	1:17:A:LEU:HA	9	0.63
(2,1145)	1:39:A:LEU:HD11	1:16:A:ALA:HB2	10	0.63
(2,1144)	1:46:B:ILE:HG22	1:46:B:ILE:HG12	4	0.63
(2,1144)	1:46:B:ILE:HG21	1:46:B:ILE:HG12	5	0.63
(2,1144)	1:46:B:ILE:HG22	1:46:B:ILE:HG12	8	0.63
(2,1143)	1:46:A:ILE:HG21	1:46:A:ILE:HG12	5	0.63
(2,1143)	1:46:A:ILE:HG22	1:46:A:ILE:HG12	8	0.63
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB3	7	0.63
(2,856)	1:6:B:ARG:HD3	1:6:B:ARG:HG3	5	0.63
(2,855)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	5	0.63
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	1	0.63
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	1	0.63
(2,479)	1:19:A:LEU:HD22	1:17:B:LEU:HD13	9	0.63
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD21	1	0.63
(2,382)	1:34:B:TYR:HD2	1:64:A:PHE:HD2	3	0.63
(2,352)	1:4:B:ARG:H	1:12:B:GLU:HG3	2	0.63
(2,142)	1:47:B:GLU:HB3	1:27:B:LEU:HD22	9	0.63
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	2	0.63
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	10	0.63
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	2	0.63
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	10	0.63
(2,105)	1:9:A:PHE:HB3	1:8:A:GLU:HB3	10	0.63
(2,93)	1:32:A:ARG:HD3	1:45:A:GLN:H	2	0.63
(2,10)	1:16:B:ALA:HB3	1:15:A:LYS:HD3	3	0.63
(1,48)	1:20:B:ALA:H	1:16:B:ALA:O	5	0.63
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	9	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:56:A:GLN:H	1:52:A:ARG:O	7	0.63
(3,184)	1:13:B:GLN:H	1:4:B:ARG:HA	7	0.62
(3,158)	1:16:B:ALA:H	1:17:B:LEU:HG	2	0.62
(3,122)	1:14:B:LYS:HE3	1:49:B:TRP:HB2	4	0.62
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	6	0.62
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	5	0.62
(2,2064)	1:45:B:GLN:H	1:46:B:ILE:HG21	2	0.62
(2,2063)	1:45:A:GLN:H	1:46:A:ILE:HG21	2	0.62
(2,1998)	1:44:B:GLU:H	1:44:B:GLU:HB3	9	0.62
(2,1997)	1:44:A:GLU:H	1:44:A:GLU:HB3	9	0.62
(2,1892)	1:65:B:GLU:HG2	1:65:B:GLU:H	5	0.62
(2,1824)	1:8:B:GLU:H	1:9:B:PHE:HB3	5	0.62
(2,1823)	1:8:A:GLU:H	1:9:A:PHE:HB3	5	0.62
(2,1690)	1:9:B:PHE:HB3	1:14:B:LYS:HG3	1	0.62
(2,1626)	1:41:B:LEU:HD11	1:36:B:SER:HA	6	0.62
(2,1625)	1:41:A:LEU:HD11	1:36:A:SER:HA	6	0.62
(2,1625)	1:41:A:LEU:HD13	1:36:A:SER:HA	7	0.62
(2,1616)	1:27:B:LEU:HD12	1:35:B:LEU:HD12	5	0.62
(2,1474)	1:58:B:GLY:HA3	1:57:B:ILE:HB	9	0.62
(2,1388)	1:46:B:ILE:HD11	1:45:B:GLN:HG3	2	0.62
(2,1387)	1:46:A:ILE:HD11	1:45:A:GLN:HG3	2	0.62
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	3	0.62
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD21	3	0.62
(2,1192)	1:16:B:ALA:HB1	1:14:B:LYS:HA	5	0.62
(2,1165)	1:46:A:ILE:HD11	1:36:A:SER:H	7	0.62
(2,1144)	1:46:B:ILE:HG23	1:46:B:ILE:HG12	3	0.62
(2,1144)	1:46:B:ILE:HG21	1:46:B:ILE:HG12	7	0.62
(2,1144)	1:46:B:ILE:HG21	1:46:B:ILE:HG12	9	0.62
(2,1143)	1:46:A:ILE:HG23	1:46:A:ILE:HG12	3	0.62
(2,1143)	1:46:A:ILE:HG21	1:46:A:ILE:HG12	7	0.62
(2,1143)	1:46:A:ILE:HG21	1:46:A:ILE:HG12	9	0.62
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB2	4	0.62
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB3	7	0.62
(2,1024)	1:12:B:GLU:HB2	1:12:B:GLU:HA	3	0.62
(2,1023)	1:12:A:GLU:HB2	1:12:A:GLU:HA	3	0.62
(2,956)	1:8:B:GLU:HG3	1:9:B:PHE:H	2	0.62
(2,955)	1:8:A:GLU:HG3	1:9:A:PHE:H	2	0.62
(2,856)	1:6:B:ARG:HD3	1:6:B:ARG:HG3	1	0.62
(2,856)	1:6:B:ARG:HD3	1:6:B:ARG:HG3	2	0.62
(2,856)	1:6:B:ARG:HD3	1:6:B:ARG:HG3	6	0.62
(2,856)	1:6:B:ARG:HD3	1:6:B:ARG:HG3	10	0.62
(2,855)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	1	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,855)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	2	0.62
(2,855)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	6	0.62
(2,855)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	10	0.62
(2,662)	1:52:B:ARG:HA	1:55:B:GLN:HG2	7	0.62
(2,661)	1:52:A:ARG:HA	1:55:A:GLN:HG2	7	0.62
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD22	6	0.62
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD22	6	0.62
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD13	4	0.62
(2,410)	1:9:B:PHE:HD2	1:17:B:LEU:HD21	1	0.62
(2,351)	1:4:A:ARG:H	1:12:A:GLU:HG3	2	0.62
(2,346)	1:36:B:SER:H	1:41:B:LEU:HD13	9	0.62
(2,345)	1:36:A:SER:H	1:41:A:LEU:HD13	9	0.62
(2,336)	1:15:B:LYS:H	1:15:B:LYS:HD3	8	0.62
(2,335)	1:15:A:LYS:H	1:15:A:LYS:HD3	8	0.62
(2,240)	1:49:B:TRP:HB3	1:52:B:ARG:HG2	10	0.62
(2,239)	1:49:A:TRP:HB3	1:52:A:ARG:HG2	10	0.62
(2,199)	1:20:A:ALA:HB2	1:17:A:LEU:HB3	4	0.62
(2,177)	1:16:A:ALA:HB2	1:20:A:ALA:H	3	0.62
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	5	0.62
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	5	0.62
(2,94)	1:32:B:ARG:HD3	1:45:B:GLN:H	2	0.62
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB1	8	0.62
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB1	8	0.62
(3,157)	1:16:A:ALA:H	1:17:A:LEU:HG	2	0.61
(3,2)	1:12:B:GLU:HB2	1:39:A:LEU:HA	8	0.61
(2,2435)	1:27:A:LEU:HD13	1:47:A:GLU:H	10	0.61
(2,2347)	1:16:A:ALA:H	1:17:A:LEU:HD21	4	0.61
(2,1891)	1:65:A:GLU:HG2	1:65:A:GLU:H	5	0.61
(2,1824)	1:8:B:GLU:H	1:9:B:PHE:HB3	3	0.61
(2,1823)	1:8:A:GLU:H	1:9:A:PHE:HB3	3	0.61
(2,1691)	1:7:A:THR:HB	1:42:A:ASN:HB2	10	0.61
(2,1689)	1:9:A:PHE:HB3	1:14:A:LYS:HG3	1	0.61
(2,1616)	1:27:B:LEU:HD11	1:35:B:LEU:HD13	4	0.61
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE2	5	0.61
(2,1496)	1:61:B:HIS:HA	1:54:B:GLU:HB2	10	0.61
(2,1388)	1:46:B:ILE:HD13	1:45:B:GLN:HG3	7	0.61
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD23	2	0.61
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD21	3	0.61
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD23	5	0.61
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD23	2	0.61
(2,1191)	1:16:A:ALA:HB1	1:14:A:LYS:HA	5	0.61
(2,1156)	1:57:B:ILE:HG22	1:58:B:GLY:H	8	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1155)	1:57:A:ILE:HG22	1:58:A:GLY:H	8	0.61
(2,1144)	1:46:B:ILE:HG21	1:46:B:ILE:HG12	1	0.61
(2,1144)	1:46:B:ILE:HG21	1:46:B:ILE:HG12	2	0.61
(2,1144)	1:46:B:ILE:HG23	1:46:B:ILE:HG12	6	0.61
(2,1143)	1:46:A:ILE:HG21	1:46:A:ILE:HG12	1	0.61
(2,1143)	1:46:A:ILE:HG21	1:46:A:ILE:HG12	2	0.61
(2,1143)	1:46:A:ILE:HG23	1:46:A:ILE:HG12	6	0.61
(2,1024)	1:12:B:GLU:HB2	1:12:B:GLU:HA	4	0.61
(2,1023)	1:12:A:GLU:HB2	1:12:A:GLU:HA	4	0.61
(2,988)	1:4:B:ARG:HB2	1:4:B:ARG:H	10	0.61
(2,987)	1:4:A:ARG:HB2	1:4:A:ARG:H	10	0.61
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	5	0.61
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	5	0.61
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD21	5	0.61
(2,527)	1:57:A:ILE:HA	1:57:A:ILE:HG23	9	0.61
(2,477)	1:19:A:LEU:HD22	1:19:B:LEU:HA	7	0.61
(2,320)	1:9:B:PHE:H	1:45:B:GLN:HB2	5	0.61
(2,319)	1:9:A:PHE:H	1:45:A:GLN:HB2	5	0.61
(2,310)	1:42:B:ASN:H	1:45:B:GLN:HA	2	0.61
(2,309)	1:42:A:ASN:H	1:45:A:GLN:HA	2	0.61
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD21	7	0.61
(2,258)	1:54:B:GLU:HG2	1:59:B:TRP:HB2	1	0.61
(2,257)	1:54:A:GLU:HG2	1:59:A:TRP:HB2	1	0.61
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	7	0.61
(2,182)	1:16:B:ALA:HB2	1:15:A:LYS:HB3	3	0.61
(2,106)	1:9:B:PHE:HB3	1:8:B:GLU:HB3	10	0.61
(3,1)	1:12:A:GLU:HB2	1:39:B:LEU:HA	8	0.6
(2,2436)	1:27:B:LEU:HD13	1:47:B:GLU:H	10	0.6
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	6	0.6
(2,1790)	1:8:B:GLU:H	1:4:B:ARG:HG3	10	0.6
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD12	1	0.6
(2,1692)	1:7:B:THR:HB	1:42:B:ASN:HB2	10	0.6
(2,1626)	1:41:B:LEU:HD13	1:36:B:SER:HA	7	0.6
(2,1541)	1:17:A:LEU:HD21	1:13:A:GLN:HB3	6	0.6
(2,1486)	1:60:B:SER:HB2	1:60:B:SER:HA	9	0.6
(2,1485)	1:60:A:SER:HB2	1:60:A:SER:HA	9	0.6
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	5	0.6
(2,1232)	1:18:B:ASP:HA	1:49:B:TRP:HE1	3	0.6
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD23	5	0.6
(2,1124)	1:20:B:ALA:HB2	1:21:B:PHE:H	9	0.6
(2,1123)	1:20:A:ALA:HB2	1:21:A:PHE:H	9	0.6
(2,1047)	1:57:A:ILE:HG13	1:57:A:ILE:H	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,992)	1:11:B:GLU:HB3	1:11:B:GLU:H	2	0.6
(2,991)	1:11:A:GLU:HB3	1:11:A:GLU:H	2	0.6
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	9	0.6
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD22	3	0.6
(2,478)	1:19:B:LEU:HD22	1:19:A:LEU:HA	7	0.6
(2,468)	1:19:B:LEU:HD22	1:35:A:LEU:HB2	4	0.6
(2,352)	1:4:B:ARG:H	1:12:A:GLU:HG3	4	0.6
(2,350)	1:27:B:LEU:H	1:32:B:ARG:HB2	1	0.6
(2,349)	1:27:A:LEU:H	1:32:A:ARG:HB2	1	0.6
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	1	0.6
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	1	0.6
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	7	0.6
(2,178)	1:16:B:ALA:HB2	1:20:B:ALA:H	3	0.6
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	6	0.6
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	6	0.6
(2,16)	1:36:B:SER:HB3	1:46:B:ILE:HD13	9	0.6
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	4	0.59
(3,183)	1:13:A:GLN:H	1:4:A:ARG:HA	7	0.59
(3,150)	1:2:B:GLU:H	1:4:B:ARG:HA	9	0.59
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	8	0.59
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	8	0.59
(3,45)	1:6:A:ARG:HD3	1:8:A:GLU:HG3	9	0.59
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	10	0.59
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	10	0.59
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	6	0.59
(2,2006)	1:64:B:PHE:H	1:63:B:GLN:H	10	0.59
(2,2005)	1:64:A:PHE:H	1:63:A:GLN:H	10	0.59
(2,1850)	1:52:B:ARG:HB3	1:53:B:LYS:H	3	0.59
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD13	1	0.59
(2,1615)	1:27:A:LEU:HD12	1:35:A:LEU:HD12	5	0.59
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE2	5	0.59
(2,1547)	1:27:A:LEU:HB3	1:50:A:PHE:HD1	4	0.59
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD22	4	0.59
(2,1486)	1:60:B:SER:HB2	1:60:B:SER:HA	5	0.59
(2,1485)	1:60:A:SER:HB2	1:60:A:SER:HA	5	0.59
(2,1473)	1:58:A:GLY:HA3	1:57:A:ILE:HB	9	0.59
(2,1397)	1:46:A:ILE:HD13	1:35:A:LEU:H	9	0.59
(2,1388)	1:46:B:ILE:HD13	1:45:B:GLN:HG3	1	0.59
(2,1387)	1:46:A:ILE:HD13	1:45:A:GLN:HG3	1	0.59
(2,1387)	1:46:A:ILE:HD13	1:45:A:GLN:HG3	7	0.59
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD21	10	0.59
(2,1048)	1:57:B:ILE:HG13	1:57:B:ILE:H	8	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,970)	1:55:B:GLN:HG2	1:55:B:GLN:HB3	3	0.59
(2,970)	1:55:B:GLN:HG2	1:55:B:GLN:HB3	4	0.59
(2,970)	1:55:B:GLN:HG2	1:55:B:GLN:HB3	7	0.59
(2,970)	1:55:B:GLN:HG2	1:55:B:GLN:HB3	9	0.59
(2,969)	1:55:A:GLN:HG2	1:55:A:GLN:HB3	3	0.59
(2,969)	1:55:A:GLN:HG2	1:55:A:GLN:HB3	4	0.59
(2,969)	1:55:A:GLN:HG2	1:55:A:GLN:HB3	7	0.59
(2,969)	1:55:A:GLN:HG2	1:55:A:GLN:HB3	9	0.59
(2,808)	1:4:B:ARG:HA	1:4:B:ARG:HG3	6	0.59
(2,807)	1:4:A:ARG:HA	1:4:A:ARG:HG3	6	0.59
(2,618)	1:12:B:GLU:HA	1:15:B:LYS:HE3	3	0.59
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD11	3	0.59
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD11	1	0.59
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	8	0.59
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	8	0.59
(2,372)	1:51:B:ARG:H	1:55:B:GLN:HG3	1	0.59
(2,371)	1:51:A:ARG:H	1:55:A:GLN:HG3	1	0.59
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	1	0.59
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	1	0.59
(2,322)	1:54:B:GLU:H	1:52:B:ARG:HB2	1	0.59
(2,321)	1:54:A:GLU:H	1:52:A:ARG:HB2	1	0.59
(2,282)	1:7:B:THR:HB	1:41:B:LEU:H	9	0.59
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD22	6	0.59
(2,196)	1:18:B:ASP:HA	1:53:B:LYS:HD2	5	0.59
(2,181)	1:16:A:ALA:HB2	1:15:B:LYS:HB3	3	0.59
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	9	0.59
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	9	0.59
(2,76)	1:25:B:ARG:HA	1:20:B:ALA:HA	2	0.59
(2,6)	1:49:B:TRP:HD1	1:53:B:LYS:H	7	0.59
(3,181)	1:64:A:PHE:H	1:62:A:PRO:HB3	7	0.58
(3,154)	1:11:B:GLU:H	1:13:B:GLN:HG3	7	0.58
(3,149)	1:2:A:GLU:H	1:4:A:ARG:HA	9	0.58
(3,77)	1:37:A:GLN:HB3	1:34:A:TYR:HB2	9	0.58
(3,46)	1:6:B:ARG:HD3	1:8:B:GLU:HG3	5	0.58
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	9	0.58
(2,1851)	1:53:A:LYS:H	1:52:A:ARG:HG3	7	0.58
(2,1849)	1:52:A:ARG:HB3	1:53:A:LYS:H	3	0.58
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	2	0.58
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	2	0.58
(2,1782)	1:66:B:LYS:H	1:65:B:GLU:HG2	4	0.58
(2,1781)	1:66:A:LYS:H	1:65:A:GLU:HG2	4	0.58
(2,1781)	1:66:A:LYS:H	1:65:A:GLU:HG2	6	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD11	9	0.58
(2,1416)	1:46:B:ILE:HG21	1:32:B:ARG:H	3	0.58
(2,1335)	1:27:A:LEU:HD23	1:47:A:GLU:H	5	0.58
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD21	10	0.58
(2,1202)	1:17:B:LEU:HD23	1:46:B:ILE:HG12	1	0.58
(2,1192)	1:16:B:ALA:HB3	1:14:B:LYS:HA	2	0.58
(2,1191)	1:16:A:ALA:HB3	1:14:A:LYS:HA	2	0.58
(2,1064)	1:27:B:LEU:HD22	1:43:B:GLU:HB3	2	0.58
(2,970)	1:55:B:GLN:HG2	1:55:B:GLN:HB3	1	0.58
(2,969)	1:55:A:GLN:HG2	1:55:A:GLN:HB3	1	0.58
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD11	1	0.58
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	5	0.58
(2,195)	1:18:A:ASP:HA	1:53:A:LYS:HD2	5	0.58
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	2	0.58
(2,105)	1:9:A:PHE:HB3	1:8:A:GLU:HB3	3	0.58
(2,75)	1:25:A:ARG:HA	1:20:A:ALA:HA	2	0.58
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG3	6	0.58
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG3	6	0.58
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB3	9	0.58
(3,184)	1:13:B:GLN:H	1:4:B:ARG:HA	3	0.57
(3,153)	1:11:A:GLU:H	1:13:A:GLN:HG3	7	0.57
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	1	0.57
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	3	0.57
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	1	0.57
(3,46)	1:6:B:ARG:HD3	1:8:B:GLU:HG3	9	0.57
(3,45)	1:6:A:ARG:HD3	1:8:A:GLU:HG3	5	0.57
(2,2397)	1:42:A:ASN:H	1:36:A:SER:HB2	7	0.57
(2,2256)	1:64:B:PHE:H	1:61:B:HIS:HA	8	0.57
(2,2255)	1:64:A:PHE:H	1:61:A:HIS:HA	8	0.57
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	9	0.57
(2,1910)	1:59:B:TRP:H	1:57:B:ILE:HG12	1	0.57
(2,1909)	1:59:A:TRP:H	1:57:A:ILE:HG12	1	0.57
(2,1850)	1:52:B:ARG:HB3	1:53:B:LYS:H	4	0.57
(2,1782)	1:66:B:LYS:H	1:65:B:GLU:HG2	6	0.57
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD11	9	0.57
(2,1746)	1:9:B:PHE:HD1	1:9:B:PHE:H	7	0.57
(2,1732)	1:28:B:THR:H	1:28:B:THR:HG21	6	0.57
(2,1553)	1:27:A:LEU:HB3	1:50:A:PHE:HB2	3	0.57
(2,1398)	1:46:B:ILE:HD13	1:35:B:LEU:H	9	0.57
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	3	0.57
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	5	0.57
(2,1201)	1:17:A:LEU:HD23	1:46:A:ILE:HG12	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1190)	1:16:B:ALA:HB2	1:17:B:LEU:HA	9	0.57
(2,1166)	1:46:B:ILE:HD11	1:36:B:SER:H	5	0.57
(2,1166)	1:46:B:ILE:HD11	1:36:B:SER:H	7	0.57
(2,1144)	1:46:B:ILE:HG21	1:46:B:ILE:HG12	10	0.57
(2,1143)	1:46:A:ILE:HG21	1:46:A:ILE:HG12	10	0.57
(2,1063)	1:27:A:LEU:HD22	1:43:A:GLU:HB3	2	0.57
(2,992)	1:11:B:GLU:HB3	1:11:B:GLU:H	1	0.57
(2,991)	1:11:A:GLU:HB3	1:11:A:GLU:H	1	0.57
(2,970)	1:55:B:GLN:HG2	1:55:B:GLN:HB3	6	0.57
(2,969)	1:55:A:GLN:HG2	1:55:A:GLN:HB3	6	0.57
(2,637)	1:53:A:LYS:HA	1:53:A:LYS:HD2	6	0.57
(2,464)	1:49:B:TRP:HD1	1:63:B:GLN:HE21	4	0.57
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD13	1	0.57
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD13	1	0.57
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	6	0.57
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	6	0.57
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD22	6	0.57
(2,179)	1:16:A:ALA:HB1	1:15:B:LYS:HE3	10	0.57
(2,162)	1:39:B:LEU:HG	1:13:B:GLN:H	5	0.57
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	5	0.57
(2,150)	1:51:B:ARG:HG3	1:51:B:ARG:HA	2	0.57
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	4	0.57
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	2	0.57
(2,106)	1:9:B:PHE:HB3	1:8:B:GLU:HB3	3	0.57
(3,154)	1:11:B:GLU:H	1:13:B:GLN:HG3	9	0.56
(3,153)	1:11:A:GLU:H	1:13:A:GLN:HG3	9	0.56
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	8	0.56
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	8	0.56
(2,2322)	1:6:B:ARG:H	1:5:B:PRO:HB3	1	0.56
(2,2321)	1:6:A:ARG:H	1:5:A:PRO:HB3	1	0.56
(2,2260)	1:6:B:ARG:H	1:6:B:ARG:HD3	9	0.56
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	9	0.56
(2,2128)	1:55:B:GLN:H	1:53:B:LYS:HB2	3	0.56
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	9	0.56
(2,2036)	1:35:B:LEU:H	1:39:B:LEU:HD21	1	0.56
(2,2035)	1:35:A:LEU:H	1:39:A:LEU:HD21	1	0.56
(2,1854)	1:16:B:ALA:H	1:15:B:LYS:HB3	6	0.56
(2,1853)	1:16:A:ALA:H	1:15:A:LYS:HB3	6	0.56
(2,1852)	1:53:B:LYS:H	1:52:B:ARG:HG3	7	0.56
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	10	0.56
(2,1782)	1:66:B:LYS:H	1:65:B:GLU:HG2	5	0.56
(2,1781)	1:66:A:LYS:H	1:65:A:GLU:HG2	5	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1745)	1:9:A:PHE:HD1	1:9:A:PHE:H	7	0.56
(2,1631)	1:39:A:LEU:HD11	1:9:A:PHE:HB2	1	0.56
(2,992)	1:11:B:GLU:HB3	1:11:B:GLU:H	5	0.56
(2,991)	1:11:A:GLU:HB3	1:11:A:GLU:H	5	0.56
(2,912)	1:42:B:ASN:HB2	1:44:B:GLU:H	9	0.56
(2,911)	1:42:A:ASN:HB2	1:44:A:GLU:H	9	0.56
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	9	0.56
(2,638)	1:53:B:LYS:HA	1:53:B:LYS:HD2	6	0.56
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD12	3	0.56
(2,381)	1:34:A:TYR:HD2	1:64:B:PHE:HD2	3	0.56
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	5	0.56
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	7	0.56
(2,281)	1:7:A:THR:HB	1:41:A:LEU:H	9	0.56
(2,186)	1:17:B:LEU:HD22	1:50:B:PHE:HA	4	0.56
(2,181)	1:16:A:ALA:HB1	1:15:B:LYS:HB3	10	0.56
(2,150)	1:51:B:ARG:HG3	1:51:B:ARG:HA	7	0.56
(2,149)	1:51:A:ARG:HG3	1:51:A:ARG:HA	2	0.56
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	4	0.56
(2,102)	1:19:B:LEU:HB3	1:16:B:ALA:HA	5	0.56
(2,101)	1:19:A:LEU:HB3	1:16:A:ALA:HA	5	0.56
(1,20)	1:56:A:GLN:H	1:52:A:ARG:O	1	0.56
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	2	0.55
(3,183)	1:13:A:GLN:H	1:4:A:ARG:HA	3	0.55
(2,2259)	1:6:A:ARG:H	1:6:A:ARG:HD3	9	0.55
(2,2188)	1:54:B:GLU:H	1:21:B:PHE:HE2	3	0.55
(2,2127)	1:55:A:GLN:H	1:53:A:LYS:HB2	3	0.55
(2,1995)	1:44:A:GLU:H	1:44:A:GLU:HG2	8	0.55
(2,1895)	1:65:A:GLU:HB2	1:65:A:GLU:H	7	0.55
(2,1849)	1:52:A:ARG:HB3	1:53:A:LYS:H	4	0.55
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD11	10	0.55
(2,1731)	1:28:A:THR:H	1:28:A:THR:HG21	6	0.55
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	2	0.55
(2,1388)	1:46:B:ILE:HD11	1:45:B:GLN:HG3	3	0.55
(2,1344)	1:41:B:LEU:HD11	1:17:B:LEU:HD23	10	0.55
(2,1165)	1:46:A:ILE:HD11	1:36:A:SER:H	5	0.55
(2,680)	1:63:B:GLN:HA	1:63:B:GLN:HG2	2	0.55
(2,679)	1:63:A:GLN:HA	1:63:A:GLN:HG2	2	0.55
(2,674)	1:8:B:GLU:HA	1:41:B:LEU:HB2	8	0.55
(2,440)	1:20:B:ALA:HB2	1:20:A:ALA:HB2	1	0.55
(2,439)	1:20:A:ALA:HB2	1:20:B:ALA:HB2	1	0.55
(2,372)	1:51:B:ARG:H	1:47:B:GLU:HG2	6	0.55
(2,346)	1:36:B:SER:H	1:39:B:LEU:HD13	2	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,345)	1:36:A:SER:H	1:39:A:LEU:HD13	2	0.55
(2,203)	1:28:A:THR:HB	1:32:A:ARG:HB2	6	0.55
(2,191)	1:17:A:LEU:HD23	1:14:A:LYS:HB3	7	0.55
(2,150)	1:51:B:ARG:HG3	1:51:B:ARG:HA	4	0.55
(2,150)	1:51:B:ARG:HG3	1:51:B:ARG:HA	9	0.55
(2,149)	1:51:A:ARG:HG3	1:51:A:ARG:HA	7	0.55
(2,149)	1:51:A:ARG:HG3	1:51:A:ARG:HA	9	0.55
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB3	9	0.55
(2,15)	1:36:A:SER:HB3	1:46:A:ILE:HD13	9	0.55
(1,62)	1:56:B:GLN:H	1:52:B:ARG:O	1	0.55
(1,1)	1:15:A:LYS:H	1:11:A:GLU:O	7	0.55
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	2	0.54
(3,121)	1:14:A:LYS:HE3	1:49:A:TRP:HB2	4	0.54
(3,100)	1:59:B:TRP:HB3	1:54:B:GLU:HA	3	0.54
(3,92)	1:27:B:LEU:HA	1:50:B:PHE:HB3	5	0.54
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	4	0.54
(3,78)	1:37:B:GLN:HB3	1:34:B:TYR:HB2	9	0.54
(2,2398)	1:42:B:ASN:H	1:36:B:SER:HB2	7	0.54
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD22	1	0.54
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD22	1	0.54
(2,2180)	1:51:B:ARG:H	1:51:B:ARG:HG2	10	0.54
(2,2179)	1:51:A:ARG:H	1:51:A:ARG:HG2	10	0.54
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	3	0.54
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	9	0.54
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	3	0.54
(2,1996)	1:44:B:GLU:H	1:44:B:GLU:HG2	5	0.54
(2,1996)	1:44:B:GLU:H	1:44:B:GLU:HG2	6	0.54
(2,1996)	1:44:B:GLU:H	1:44:B:GLU:HG2	8	0.54
(2,1995)	1:44:A:GLU:H	1:44:A:GLU:HG2	5	0.54
(2,1995)	1:44:A:GLU:H	1:44:A:GLU:HG2	6	0.54
(2,1910)	1:59:B:TRP:H	1:57:B:ILE:HG12	7	0.54
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD12	4	0.54
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD12	4	0.54
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	2	0.54
(2,1652)	1:28:B:THR:HB	1:31:B:TRP:HB3	5	0.54
(2,1632)	1:39:B:LEU:HD11	1:9:B:PHE:HB2	1	0.54
(2,1620)	1:13:B:GLN:HA	1:39:B:LEU:HD11	4	0.54
(2,1388)	1:46:B:ILE:HD12	1:45:B:GLN:HG3	10	0.54
(2,1387)	1:46:A:ILE:HD12	1:45:A:GLN:HG3	10	0.54
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	2	0.54
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	2	0.54
(2,1228)	1:17:B:LEU:HD21	1:49:B:TRP:HE1	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,673)	1:8:A:GLU:HA	1:41:A:LEU:HB2	8	0.54
(2,617)	1:12:A:GLU:HA	1:15:A:LYS:HE3	3	0.54
(2,382)	1:34:B:TYR:HD2	1:64:A:PHE:HD2	1	0.54
(2,382)	1:34:B:TYR:HD1	1:64:A:PHE:HD2	7	0.54
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	10	0.54
(2,371)	1:51:A:ARG:H	1:47:A:GLU:HG2	6	0.54
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	7	0.54
(2,249)	1:13:A:GLN:HB3	1:9:A:PHE:HD1	6	0.54
(2,204)	1:28:B:THR:HB	1:32:B:ARG:HB2	6	0.54
(2,150)	1:51:B:ARG:HG3	1:51:B:ARG:HA	3	0.54
(2,149)	1:51:A:ARG:HG3	1:51:A:ARG:HA	3	0.54
(2,149)	1:51:A:ARG:HG3	1:51:A:ARG:HA	4	0.54
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	9	0.54
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	4	0.54
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	9	0.54
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG2	5	0.54
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB3	8	0.54
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB3	8	0.54
(2,16)	1:36:B:SER:HB3	1:46:B:ILE:HD13	4	0.54
(2,9)	1:16:A:ALA:HB3	1:15:B:LYS:HD3	3	0.54
(1,67)	1:34:B:TYR:N	1:30:B:GLU:O	10	0.54
(1,49)	1:33:B:ARG:H	1:29:B:PRO:O	10	0.54
(1,43)	1:15:B:LYS:H	1:11:B:GLU:O	7	0.54
(3,222)	1:54:B:GLU:H	1:52:B:ARG:HE	2	0.53
(3,153)	1:11:A:GLU:H	1:13:A:GLN:HG3	1	0.53
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	5	0.53
(3,99)	1:59:A:TRP:HB3	1:54:A:GLU:HA	3	0.53
(3,77)	1:37:A:GLN:HB3	1:34:A:TYR:HB2	4	0.53
(3,61)	1:27:A:LEU:HB2	1:21:A:PHE:H	7	0.53
(2,2348)	1:16:B:ALA:H	1:17:B:LEU:HD22	8	0.53
(2,2347)	1:16:A:ALA:H	1:17:A:LEU:HD22	8	0.53
(2,2278)	1:9:B:PHE:H	1:41:B:LEU:HA	1	0.53
(2,2187)	1:54:A:GLU:H	1:21:A:PHE:HE2	3	0.53
(2,2084)	1:14:B:LYS:H	1:9:B:PHE:HB3	8	0.53
(2,2083)	1:14:A:LYS:H	1:9:A:PHE:HB3	8	0.53
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	3	0.53
(2,2030)	1:32:B:ARG:H	1:32:B:ARG:HD3	10	0.53
(2,2029)	1:32:A:ARG:H	1:32:A:ARG:HD3	10	0.53
(2,1996)	1:44:B:GLU:H	1:44:B:GLU:HG2	1	0.53
(2,1996)	1:44:B:GLU:H	1:44:B:GLU:HG2	3	0.53
(2,1996)	1:44:B:GLU:H	1:44:B:GLU:HG2	7	0.53
(2,1995)	1:44:A:GLU:H	1:44:A:GLU:HG2	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1995)	1:44:A:GLU:H	1:44:A:GLU:HG2	3	0.53
(2,1995)	1:44:A:GLU:H	1:44:A:GLU:HG2	7	0.53
(2,1880)	1:63:B:GLN:H	1:62:B:PRO:HD3	3	0.53
(2,1879)	1:63:A:GLN:H	1:62:A:PRO:HD3	3	0.53
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	1	0.53
(2,1696)	1:7:B:THR:HB	1:45:B:GLN:HB2	6	0.53
(2,1695)	1:7:A:THR:HB	1:45:A:GLN:HB2	6	0.53
(2,1690)	1:9:B:PHE:HB3	1:14:B:LYS:HG3	8	0.53
(2,1689)	1:9:A:PHE:HB3	1:14:A:LYS:HG3	8	0.53
(2,1387)	1:46:A:ILE:HD11	1:45:A:GLN:HG3	3	0.53
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	10	0.53
(2,1343)	1:41:A:LEU:HD11	1:17:A:LEU:HD23	10	0.53
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	8	0.53
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	8	0.53
(2,1236)	1:20:B:ALA:HB1	1:26:B:ARG:HD3	1	0.53
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD23	8	0.53
(2,1168)	1:46:B:ILE:HD12	1:46:B:ILE:HB	5	0.53
(2,1167)	1:46:A:ILE:HD12	1:46:A:ILE:HB	5	0.53
(2,1124)	1:20:B:ALA:HB3	1:21:B:PHE:H	5	0.53
(2,1123)	1:20:A:ALA:HB3	1:21:A:PHE:H	5	0.53
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	9	0.53
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	9	0.53
(2,638)	1:53:B:LYS:HA	1:53:B:LYS:HD2	5	0.53
(2,637)	1:53:A:LYS:HA	1:53:A:LYS:HD2	5	0.53
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD13	8	0.53
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD13	4	0.53
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD11	5	0.53
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD11	7	0.53
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD13	8	0.53
(2,492)	1:61:B:HIS:HD1	1:61:B:HIS:H	6	0.53
(2,491)	1:61:A:HIS:HD1	1:61:A:HIS:H	6	0.53
(2,381)	1:34:A:TYR:HD2	1:64:B:PHE:HD2	1	0.53
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	6	0.53
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	10	0.53
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	6	0.53
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HD2	5	0.53
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HD2	5	0.53
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	1	0.53
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	1	0.53
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	4	0.53
(2,72)	1:16:B:ALA:HA	1:19:B:LEU:HD23	3	0.53
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG2	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB1	1	0.53
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	8	0.53
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	8	0.53
(3,154)	1:11:B:GLU:H	1:13:B:GLN:HG3	1	0.52
(3,154)	1:11:B:GLU:H	1:13:B:GLN:HG3	4	0.52
(3,150)	1:2:B:GLU:H	1:4:B:ARG:HA	8	0.52
(3,149)	1:2:A:GLU:H	1:4:A:ARG:HA	8	0.52
(3,121)	1:14:A:LYS:HE3	1:49:A:TRP:HB2	7	0.52
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	10	0.52
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	3	0.52
(2,2394)	1:7:B:THR:H	1:4:B:ARG:HG3	6	0.52
(2,2393)	1:7:A:THR:H	1:4:A:ARG:HG3	6	0.52
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	7	0.52
(2,2336)	1:12:B:GLU:HB2	1:12:B:GLU:H	6	0.52
(2,2335)	1:12:A:GLU:HB2	1:12:A:GLU:H	6	0.52
(2,2321)	1:6:A:ARG:H	1:5:A:PRO:HB3	10	0.52
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	3	0.52
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	10	0.52
(2,2006)	1:64:B:PHE:H	1:63:B:GLN:H	2	0.52
(2,1850)	1:52:B:ARG:HB3	1:53:B:LYS:H	9	0.52
(2,1849)	1:52:A:ARG:HB3	1:53:A:LYS:H	9	0.52
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	1	0.52
(2,1804)	1:65:B:GLU:H	1:64:B:PHE:HB3	5	0.52
(2,1803)	1:65:A:GLU:H	1:64:A:PHE:HB3	5	0.52
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	1	0.52
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	1	0.52
(2,1625)	1:41:A:LEU:HD11	1:36:A:SER:HA	1	0.52
(2,1614)	1:16:B:ALA:HB3	1:35:B:LEU:HD11	10	0.52
(2,1599)	1:53:A:LYS:HG2	1:21:A:PHE:HZ	7	0.52
(2,1498)	1:63:B:GLN:HG2	1:64:B:PHE:HD1	10	0.52
(2,1497)	1:63:A:GLN:HG2	1:64:A:PHE:HD1	10	0.52
(2,1235)	1:20:A:ALA:HB1	1:26:A:ARG:HD3	1	0.52
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD22	1	0.52
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD22	1	0.52
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD23	8	0.52
(2,1196)	1:16:B:ALA:HB3	1:13:B:GLN:HG2	7	0.52
(2,1191)	1:16:A:ALA:HB3	1:14:A:LYS:HA	7	0.52
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD11	7	0.52
(2,374)	1:56:B:GLN:H	1:57:B:ILE:HG13	3	0.52
(2,373)	1:56:A:GLN:H	1:57:A:ILE:HG13	3	0.52
(2,341)	1:60:A:SER:H	1:59:A:TRP:HA	2	0.52
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	3	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	3	0.52
(2,331)	1:14:A:LYS:H	1:12:A:GLU:HA	9	0.52
(2,192)	1:17:B:LEU:HD23	1:14:B:LYS:HB3	7	0.52
(2,150)	1:51:B:ARG:HG3	1:51:B:ARG:HA	8	0.52
(2,149)	1:51:A:ARG:HG3	1:51:A:ARG:HA	8	0.52
(2,87)	1:48:A:ARG:HD3	1:45:A:GLN:HE21	7	0.52
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB1	1	0.52
(2,50)	1:49:B:TRP:HA	1:9:B:PHE:HZ	3	0.52
(2,10)	1:16:B:ALA:HB1	1:15:A:LYS:HD3	2	0.52
(2,9)	1:16:A:ALA:HB1	1:15:B:LYS:HD3	2	0.52
(2,5)	1:49:A:TRP:HD1	1:53:A:LYS:H	7	0.52
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	6	0.52
(1,49)	1:33:B:ARG:H	1:29:B:PRO:O	7	0.52
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	6	0.52
(3,177)	1:49:A:TRP:H	1:45:A:GLN:H	9	0.51
(3,145)	1:4:A:ARG:H	1:12:A:GLU:H	4	0.51
(3,122)	1:14:B:LYS:HE3	1:49:B:TRP:HB2	7	0.51
(3,78)	1:37:B:GLN:HB3	1:34:B:TYR:HB2	4	0.51
(3,62)	1:27:B:LEU:HB2	1:21:B:PHE:H	7	0.51
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	10	0.51
(2,2322)	1:6:B:ARG:H	1:5:B:PRO:HB3	10	0.51
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	8	0.51
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	8	0.51
(2,2005)	1:64:A:PHE:H	1:63:A:GLN:H	2	0.51
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	8	0.51
(2,1901)	1:59:A:TRP:H	1:62:A:PRO:HD2	8	0.51
(2,1896)	1:65:B:GLU:HB2	1:65:B:GLU:H	7	0.51
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	4	0.51
(2,1626)	1:41:B:LEU:HD11	1:36:B:SER:HA	1	0.51
(2,1600)	1:53:B:LYS:HG2	1:21:B:PHE:HZ	7	0.51
(2,1334)	1:27:B:LEU:HD21	1:32:B:ARG:H	10	0.51
(2,1196)	1:16:B:ALA:HB1	1:13:B:GLN:HG2	1	0.51
(2,1195)	1:16:A:ALA:HB3	1:13:A:GLN:HG2	7	0.51
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	4	0.51
(2,874)	1:14:B:LYS:HE3	1:14:B:LYS:HG3	8	0.51
(2,873)	1:14:A:LYS:HE3	1:14:A:LYS:HG3	8	0.51
(2,800)	1:42:B:ASN:HA	1:43:B:GLU:HG3	3	0.51
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD11	5	0.51
(2,462)	1:49:B:TRP:HD1	1:14:B:LYS:HE3	2	0.51
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	7	0.51
(2,342)	1:60:B:SER:H	1:59:B:TRP:HA	2	0.51
(2,264)	1:39:B:LEU:HD12	1:16:B:ALA:H	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	8	0.51
(2,180)	1:16:B:ALA:HB1	1:15:A:LYS:HE3	10	0.51
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	3	0.51
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	7	0.51
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	3	0.51
(2,88)	1:48:B:ARG:HD3	1:45:B:GLN:HE21	7	0.51
(2,49)	1:49:A:TRP:HA	1:9:A:PHE:HZ	3	0.51
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	5	0.51
(1,25)	1:34:A:TYR:N	1:30:A:GLU:O	10	0.51
(1,11)	1:37:A:GLN:H	1:33:A:ARG:O	4	0.51
(3,221)	1:54:A:GLU:H	1:52:A:ARG:HE	7	0.5
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	3	0.5
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	1	0.5
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE1	4	0.5
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	8	0.5
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	8	0.5
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	3	0.5
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	6	0.5
(2,2277)	1:9:A:PHE:H	1:41:A:LEU:HA	1	0.5
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	4	0.5
(2,1909)	1:59:A:TRP:H	1:57:A:ILE:HG12	7	0.5
(2,1801)	1:65:A:GLU:H	1:64:A:PHE:HD1	6	0.5
(2,1782)	1:66:B:LYS:H	1:65:B:GLU:HG2	8	0.5
(2,1781)	1:66:A:LYS:H	1:65:A:GLU:HG2	8	0.5
(2,1609)	1:35:A:LEU:HB2	1:39:A:LEU:HD22	6	0.5
(2,1554)	1:27:B:LEU:HB3	1:50:B:PHE:HB2	3	0.5
(2,1195)	1:16:A:ALA:HB1	1:13:A:GLN:HG2	1	0.5
(2,1168)	1:46:B:ILE:HD12	1:46:B:ILE:HB	1	0.5
(2,1168)	1:46:B:ILE:HD13	1:46:B:ILE:HB	3	0.5
(2,1168)	1:46:B:ILE:HD11	1:46:B:ILE:HB	4	0.5
(2,1168)	1:46:B:ILE:HD11	1:46:B:ILE:HB	6	0.5
(2,1168)	1:46:B:ILE:HD12	1:46:B:ILE:HB	7	0.5
(2,1168)	1:46:B:ILE:HD11	1:46:B:ILE:HB	8	0.5
(2,1168)	1:46:B:ILE:HD11	1:46:B:ILE:HB	10	0.5
(2,1167)	1:46:A:ILE:HD12	1:46:A:ILE:HB	1	0.5
(2,1167)	1:46:A:ILE:HD13	1:46:A:ILE:HB	3	0.5
(2,1167)	1:46:A:ILE:HD11	1:46:A:ILE:HB	4	0.5
(2,1167)	1:46:A:ILE:HD11	1:46:A:ILE:HB	6	0.5
(2,1167)	1:46:A:ILE:HD12	1:46:A:ILE:HB	7	0.5
(2,1167)	1:46:A:ILE:HD11	1:46:A:ILE:HB	8	0.5
(2,1167)	1:46:A:ILE:HD11	1:46:A:ILE:HB	10	0.5
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	2	0.5
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	8	0.5
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	9	0.5
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	2	0.5
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	8	0.5
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	9	0.5
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	8	0.5
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	8	0.5
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	7	0.5
(2,874)	1:14:B:LYS:HE3	1:14:B:LYS:HG3	7	0.5
(2,873)	1:14:A:LYS:HE3	1:14:A:LYS:HG3	7	0.5
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG23	7	0.5
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG23	7	0.5
(2,661)	1:52:A:ARG:HA	1:55:A:GLN:HG2	4	0.5
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD12	3	0.5
(2,461)	1:49:A:TRP:HD1	1:14:A:LYS:HE3	2	0.5
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	1	0.5
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	7	0.5
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	1	0.5
(2,263)	1:39:A:LEU:HD12	1:16:A:ALA:H	6	0.5
(2,250)	1:13:B:GLN:HB3	1:9:B:PHE:HD1	6	0.5
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	8	0.5
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	9	0.5
(2,126)	1:51:B:ARG:HB3	1:51:B:ARG:HD3	1	0.5
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	1	0.5
(2,125)	1:51:A:ARG:HB3	1:51:A:ARG:HD3	7	0.5
(2,124)	1:15:B:LYS:HB3	1:15:B:LYS:HE3	4	0.5
(2,123)	1:15:A:LYS:HB3	1:15:A:LYS:HE3	4	0.5
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	4	0.5
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	4	0.5
(1,7)	1:33:A:ARG:H	1:29:A:PRO:O	10	0.5
(3,216)	1:7:B:THR:H	1:4:B:ARG:HA	5	0.49
(3,215)	1:7:A:THR:H	1:4:A:ARG:HA	5	0.49
(3,100)	1:59:B:TRP:HB3	1:54:B:GLU:HA	1	0.49
(3,99)	1:59:A:TRP:HB3	1:54:A:GLU:HA	1	0.49
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	1	0.49
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE1	2	0.49
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	6	0.49
(2,2332)	1:7:B:THR:HA	1:7:B:THR:H	5	0.49
(2,2331)	1:7:A:THR:HA	1:7:A:THR:H	5	0.49
(2,2245)	1:66:A:LYS:H	1:64:A:PHE:H	7	0.49
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	9	0.49
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	1	0.49
(2,1928)	1:6:B:ARG:H	1:6:B:ARG:HG3	2	0.49
(2,1927)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.49
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	5	0.49
(2,1802)	1:65:B:GLU:H	1:64:B:PHE:HD1	6	0.49
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD11	8	0.49
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD11	8	0.49
(2,1610)	1:35:B:LEU:HB2	1:39:B:LEU:HD22	6	0.49
(2,1608)	1:16:B:ALA:HB3	1:35:B:LEU:HD22	10	0.49
(2,1607)	1:16:A:ALA:HB3	1:35:A:LEU:HD22	10	0.49
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD21	1	0.49
(2,1339)	1:27:A:LEU:HD23	1:46:A:ILE:H	5	0.49
(2,1333)	1:27:A:LEU:HD21	1:32:A:ARG:H	10	0.49
(2,1244)	1:20:B:ALA:HB2	1:35:B:LEU:HD13	8	0.49
(2,1243)	1:20:A:ALA:HB2	1:35:A:LEU:HD13	8	0.49
(2,1168)	1:46:B:ILE:HD13	1:46:B:ILE:HB	2	0.49
(2,1167)	1:46:A:ILE:HD13	1:46:A:ILE:HB	2	0.49
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	4	0.49
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	5	0.49
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	7	0.49
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	4	0.49
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	5	0.49
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	7	0.49
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	10	0.49
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	10	0.49
(2,799)	1:42:A:ASN:HA	1:43:A:GLU:HG3	3	0.49
(2,680)	1:63:B:GLN:HA	1:63:B:GLN:HG2	4	0.49
(2,679)	1:63:A:GLN:HA	1:63:A:GLN:HG2	4	0.49
(2,662)	1:52:B:ARG:HA	1:55:B:GLN:HG2	4	0.49
(2,600)	1:50:B:PHE:HA	1:53:B:LYS:HB3	2	0.49
(2,332)	1:14:B:LYS:H	1:12:B:GLU:HA	9	0.49
(2,312)	1:17:B:LEU:H	1:14:B:LYS:HB3	8	0.49
(2,311)	1:17:A:LEU:H	1:14:A:LYS:HB3	8	0.49
(2,259)	1:54:A:GLU:HG3	1:59:A:TRP:HB2	9	0.49
(2,182)	1:16:B:ALA:HB1	1:15:A:LYS:HB3	10	0.49
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	5	0.49
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	5	0.49
(2,55)	1:60:A:SER:HB3	1:61:A:HIS:H	7	0.49
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	1	0.49
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	1	0.49
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	4	0.48
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE1	4	0.48
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE1	2	0.48
(2,2327)	1:39:A:LEU:H	1:38:A:ARG:HG3	1	0.48
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG23	10	0.48
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	5	0.48
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	5	0.48
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	10	0.48
(2,2027)	1:32:A:ARG:H	1:27:A:LEU:HD13	7	0.48
(2,1932)	1:49:B:TRP:H	1:52:B:ARG:HB2	10	0.48
(2,1901)	1:59:A:TRP:H	1:62:A:PRO:HD2	5	0.48
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD11	10	0.48
(2,1652)	1:28:B:THR:HB	1:31:B:TRP:HB3	1	0.48
(2,1652)	1:28:B:THR:HB	1:31:B:TRP:HB3	2	0.48
(2,1651)	1:28:A:THR:HB	1:31:A:TRP:HB3	2	0.48
(2,1626)	1:41:B:LEU:HD13	1:36:B:SER:HA	9	0.48
(2,1613)	1:16:A:ALA:HB3	1:35:A:LEU:HD11	10	0.48
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD21	1	0.48
(2,1331)	1:27:A:LEU:HD23	1:50:A:PHE:H	5	0.48
(2,1192)	1:16:B:ALA:HB3	1:14:B:LYS:HA	7	0.48
(2,1168)	1:46:B:ILE:HD11	1:46:B:ILE:HB	9	0.48
(2,1167)	1:46:A:ILE:HD11	1:46:A:ILE:HB	9	0.48
(2,1138)	1:17:B:LEU:HA	1:20:B:ALA:HB3	8	0.48
(2,1137)	1:17:A:LEU:HA	1:20:A:ALA:HB3	8	0.48
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	7	0.48
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	7	0.48
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	7	0.48
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	10	0.48
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	7	0.48
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	10	0.48
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	1	0.48
(2,986)	1:51:B:ARG:HB2	1:51:B:ARG:H	3	0.48
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	1	0.48
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	3	0.48
(2,985)	1:51:A:ARG:HB2	1:51:A:ARG:H	7	0.48
(2,874)	1:14:B:LYS:HE3	1:14:B:LYS:HG3	9	0.48
(2,873)	1:14:A:LYS:HE3	1:14:A:LYS:HG3	9	0.48
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	8	0.48
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	8	0.48
(2,673)	1:8:A:GLU:HA	1:41:A:LEU:HB2	1	0.48
(2,472)	1:19:B:LEU:HD23	1:19:A:LEU:HG	8	0.48
(2,471)	1:19:A:LEU:HD23	1:19:B:LEU:HG	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,438)	1:20:B:ALA:HB1	1:20:A:ALA:H	2	0.48
(2,437)	1:20:A:ALA:HB1	1:20:B:ALA:H	2	0.48
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	2	0.48
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	2	0.48
(2,352)	1:4:B:ARG:H	1:5:B:PRO:HB2	10	0.48
(2,351)	1:4:A:ARG:H	1:5:A:PRO:HB2	10	0.48
(2,264)	1:39:B:LEU:HD11	1:16:B:ALA:H	4	0.48
(2,243)	1:58:A:GLY:HA3	1:57:A:ILE:HG21	9	0.48
(2,56)	1:60:B:SER:HB3	1:61:B:HIS:H	7	0.48
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	5	0.48
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	1	0.48
(1,53)	1:37:B:GLN:H	1:33:B:ARG:O	4	0.48
(1,44)	1:16:B:ALA:H	1:12:B:GLU:O	2	0.48
(1,7)	1:33:A:ARG:H	1:29:A:PRO:O	7	0.48
(1,2)	1:16:A:ALA:H	1:12:A:GLU:O	2	0.48
(3,186)	1:13:B:GLN:H	1:17:B:LEU:H	7	0.47
(3,185)	1:13:A:GLN:H	1:17:A:LEU:H	7	0.47
(3,182)	1:64:B:PHE:H	1:62:B:PRO:HB3	7	0.47
(3,158)	1:16:B:ALA:H	1:17:B:LEU:HG	1	0.47
(3,146)	1:4:B:ARG:H	1:12:B:GLU:H	4	0.47
(3,116)	1:3:B:LYS:HG3	1:1:B:MET:HA	2	0.47
(3,115)	1:3:A:LYS:HG3	1:1:A:MET:HA	2	0.47
(3,93)	1:64:A:PHE:HA	1:49:A:TRP:HE1	10	0.47
(3,74)	1:39:B:LEU:HG	1:15:A:LYS:HE3	9	0.47
(3,48)	1:33:B:ARG:HD3	1:31:B:TRP:HA	10	0.47
(3,46)	1:6:B:ARG:HD3	1:8:B:GLU:HG3	8	0.47
(3,4)	1:12:B:GLU:HG3	1:12:A:GLU:HB2	10	0.47
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE1	8	0.47
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE1	8	0.47
(2,2328)	1:39:B:LEU:H	1:38:B:ARG:HG3	1	0.47
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG23	10	0.47
(2,1931)	1:49:A:TRP:H	1:52:A:ARG:HB2	10	0.47
(2,1801)	1:65:A:GLU:H	1:64:A:PHE:HD1	4	0.47
(2,1651)	1:28:A:THR:HB	1:31:A:TRP:HB3	1	0.47
(2,1625)	1:41:A:LEU:HD13	1:36:A:SER:HA	9	0.47
(2,1619)	1:13:A:GLN:HA	1:39:A:LEU:HD11	4	0.47
(2,1614)	1:16:B:ALA:HB2	1:35:B:LEU:HD13	5	0.47
(2,1434)	1:52:B:ARG:HG3	1:52:B:ARG:H	6	0.47
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	5	0.47
(2,1182)	1:6:B:ARG:HD3	1:6:B:ARG:HB2	6	0.47
(2,1181)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	6	0.47
(2,1087)	1:15:A:LYS:HG3	1:15:A:LYS:HE3	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	1	0.47
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	1	0.47
(2,674)	1:8:B:GLU:HA	1:41:B:LEU:HB2	1	0.47
(2,638)	1:53:B:LYS:HA	1:53:B:LYS:HD2	9	0.47
(2,637)	1:53:A:LYS:HA	1:53:A:LYS:HD2	9	0.47
(2,605)	1:54:A:GLU:HA	1:57:A:ILE:HG23	7	0.47
(2,304)	1:59:B:TRP:H	1:62:B:PRO:HD3	9	0.47
(2,134)	1:12:B:GLU:HB2	1:12:B:GLU:H	6	0.47
(2,133)	1:12:A:GLU:HB2	1:12:A:GLU:H	6	0.47
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	10	0.47
(2,13)	1:36:A:SER:HB2	1:32:A:ARG:HB2	1	0.47
(2,11)	1:36:A:SER:HB2	1:32:A:ARG:HB2	1	0.47
(3,222)	1:54:B:GLU:H	1:52:B:ARG:HE	7	0.46
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	1	0.46
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	1	0.46
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	6	0.46
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	6	0.46
(3,178)	1:49:B:TRP:H	1:45:B:GLN:H	9	0.46
(3,157)	1:16:A:ALA:H	1:17:A:LEU:HG	1	0.46
(3,153)	1:11:A:GLU:H	1:13:A:GLN:HG3	4	0.46
(3,100)	1:59:B:TRP:HB3	1:54:B:GLU:HA	2	0.46
(3,94)	1:64:B:PHE:HA	1:49:B:TRP:HE1	10	0.46
(3,92)	1:27:B:LEU:HA	1:50:B:PHE:HB3	1	0.46
(3,91)	1:27:A:LEU:HA	1:50:A:PHE:HB3	1	0.46
(3,47)	1:33:A:ARG:HD3	1:31:A:TRP:HA	10	0.46
(3,45)	1:6:A:ARG:HD3	1:8:A:GLU:HG3	8	0.46
(2,2435)	1:27:A:LEU:HD11	1:47:A:GLU:H	3	0.46
(2,2245)	1:66:A:LYS:H	1:64:A:PHE:H	6	0.46
(2,2173)	1:17:A:LEU:HG	1:17:A:LEU:H	9	0.46
(2,2128)	1:55:B:GLN:H	1:53:B:LYS:HB2	8	0.46
(2,2127)	1:55:A:GLN:H	1:53:A:LYS:HB2	8	0.46
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	4	0.46
(2,2028)	1:32:B:ARG:H	1:27:B:LEU:HD13	7	0.46
(2,1944)	1:61:B:HIS:HB3	1:61:B:HIS:H	3	0.46
(2,1943)	1:61:A:HIS:HB3	1:61:A:HIS:H	3	0.46
(2,1932)	1:49:B:TRP:H	1:52:B:ARG:HB2	6	0.46
(2,1931)	1:49:A:TRP:H	1:52:A:ARG:HB2	6	0.46
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG23	10	0.46
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG23	10	0.46
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	4	0.46
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	4	0.46
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD12	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1539)	1:13:A:GLN:HB3	1:41:A:LEU:HD23	7	0.46
(2,1433)	1:52:A:ARG:HG3	1:52:A:ARG:H	6	0.46
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	8	0.46
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	8	0.46
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD12	6	0.46
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD12	6	0.46
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD13	9	0.46
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB2	4	0.46
(2,1088)	1:15:B:LYS:HG3	1:15:B:LYS:HE3	1	0.46
(2,922)	1:43:B:GLU:HG3	1:32:B:ARG:HB2	7	0.46
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	2	0.46
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	2	0.46
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG23	1	0.46
(2,688)	1:55:B:GLN:HA	1:55:B:GLN:HB2	3	0.46
(2,688)	1:55:B:GLN:HA	1:55:B:GLN:HB2	7	0.46
(2,687)	1:55:A:GLN:HA	1:55:A:GLN:HB2	3	0.46
(2,687)	1:55:A:GLN:HA	1:55:A:GLN:HB2	7	0.46
(2,618)	1:12:B:GLU:HA	1:15:B:LYS:HE3	6	0.46
(2,606)	1:54:B:GLU:HA	1:57:B:ILE:HG23	7	0.46
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD13	9	0.46
(2,409)	1:9:A:PHE:HD2	1:17:A:LEU:HD23	9	0.46
(2,196)	1:18:B:ASP:HA	1:53:B:LYS:HD2	10	0.46
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	9	0.46
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	6	0.46
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	6	0.46
(1,39)	1:20:A:ALA:N	1:16:A:ALA:O	9	0.46
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	1	0.46
(1,3)	1:17:A:LEU:H	1:13:A:GLN:O	10	0.46
(3,215)	1:7:A:THR:H	1:4:A:ARG:HA	9	0.45
(3,157)	1:16:A:ALA:H	1:17:A:LEU:HG	10	0.45
(3,121)	1:14:A:LYS:HE3	1:49:A:TRP:HB2	5	0.45
(3,76)	1:57:B:ILE:HG12	1:61:B:HIS:HB2	4	0.45
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	2	0.45
(2,2277)	1:9:A:PHE:H	1:41:A:LEU:HA	6	0.45
(2,2246)	1:66:B:LYS:H	1:64:B:PHE:H	6	0.45
(2,2197)	1:60:A:SER:H	1:58:A:GLY:HA2	5	0.45
(2,2103)	1:9:A:PHE:H	1:13:A:GLN:HG2	10	0.45
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	1	0.45
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	1	0.45
(2,1862)	1:53:B:LYS:H	1:55:B:GLN:H	10	0.45
(2,1861)	1:53:A:LYS:H	1:55:A:GLN:H	10	0.45
(2,1602)	1:53:B:LYS:HG3	1:21:B:PHE:HZ	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1601)	1:53:A:LYS:HG3	1:21:A:PHE:HZ	1	0.45
(2,1540)	1:13:B:GLN:HB3	1:41:B:LEU:HD23	7	0.45
(2,1230)	1:18:B:ASP:HA	1:21:B:PHE:H	9	0.45
(2,1146)	1:39:B:LEU:HD11	1:16:B:ALA:HB3	7	0.45
(2,1038)	1:51:B:ARG:HG3	1:52:B:ARG:HA	10	0.45
(2,1037)	1:51:A:ARG:HG3	1:52:A:ARG:HA	10	0.45
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	3	0.45
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	2	0.45
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	8	0.45
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	2	0.45
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	8	0.45
(2,921)	1:43:A:GLU:HG3	1:32:A:ARG:HB2	7	0.45
(2,790)	1:16:B:ALA:HA	1:15:B:LYS:HB3	6	0.45
(2,755)	1:43:A:GLU:HA	1:36:A:SER:HB2	9	0.45
(2,708)	1:59:B:TRP:HA	1:55:B:GLN:H	3	0.45
(2,707)	1:59:A:TRP:HA	1:55:A:GLN:H	3	0.45
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG23	2	0.45
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG23	1	0.45
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG23	2	0.45
(2,688)	1:55:B:GLN:HA	1:55:B:GLN:HB2	1	0.45
(2,688)	1:55:B:GLN:HA	1:55:B:GLN:HB2	4	0.45
(2,688)	1:55:B:GLN:HA	1:55:B:GLN:HB2	6	0.45
(2,688)	1:55:B:GLN:HA	1:55:B:GLN:HB2	9	0.45
(2,687)	1:55:A:GLN:HA	1:55:A:GLN:HB2	1	0.45
(2,687)	1:55:A:GLN:HA	1:55:A:GLN:HB2	4	0.45
(2,687)	1:55:A:GLN:HA	1:55:A:GLN:HB2	9	0.45
(2,617)	1:12:A:GLU:HA	1:15:A:LYS:HE3	6	0.45
(2,599)	1:50:A:PHE:HA	1:53:A:LYS:HB3	2	0.45
(2,353)	1:47:A:GLU:H	1:45:A:GLN:HB3	9	0.45
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	10	0.45
(2,247)	1:63:A:GLN:HG2	1:57:A:ILE:H	10	0.45
(2,220)	1:43:B:GLU:HA	1:44:B:GLU:HG2	9	0.45
(2,219)	1:43:A:GLU:HA	1:44:A:GLU:HG2	4	0.45
(2,219)	1:43:A:GLU:HA	1:44:A:GLU:HG2	9	0.45
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	7	0.45
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	7	0.45
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	9	0.45
(2,14)	1:36:B:SER:HB2	1:32:B:ARG:HB2	1	0.45
(2,12)	1:36:B:SER:HB2	1:32:B:ARG:HB2	1	0.45
(3,216)	1:7:B:THR:H	1:4:B:ARG:HA	9	0.44
(3,158)	1:16:B:ALA:H	1:17:B:LEU:HG	9	0.44
(3,158)	1:16:B:ALA:H	1:17:B:LEU:HG	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,140)	1:27:B:LEU:H	1:24:B:ASP:H	10	0.44
(3,99)	1:59:A:TRP:HB3	1:54:A:GLU:HA	2	0.44
(3,27)	1:2:A:GLU:HA	1:12:A:GLU:H	9	0.44
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	2	0.44
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	7	0.44
(2,2278)	1:9:B:PHE:H	1:41:B:LEU:HA	6	0.44
(2,2198)	1:60:B:SER:H	1:58:B:GLY:HA2	5	0.44
(2,2030)	1:32:B:ARG:H	1:32:B:ARG:HD3	5	0.44
(2,1876)	1:63:B:GLN:H	1:63:B:GLN:HB2	6	0.44
(2,1875)	1:63:A:GLN:H	1:63:A:GLN:HB2	6	0.44
(2,1852)	1:53:B:LYS:H	1:52:B:ARG:HG3	1	0.44
(2,1851)	1:53:A:LYS:H	1:52:A:ARG:HG3	1	0.44
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	4	0.44
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	8	0.44
(2,1660)	1:57:B:ILE:HG12	1:60:B:SER:HG	8	0.44
(2,1659)	1:57:A:ILE:HG12	1:60:A:SER:HG	8	0.44
(2,1636)	1:41:B:LEU:HD11	1:13:B:GLN:HG2	10	0.44
(2,1613)	1:16:A:ALA:HB2	1:35:A:LEU:HD13	5	0.44
(2,1474)	1:58:B:GLY:HA3	1:57:B:ILE:HB	3	0.44
(2,1473)	1:58:A:GLY:HA3	1:57:A:ILE:HB	3	0.44
(2,1344)	1:41:B:LEU:HD11	1:17:B:LEU:HD22	9	0.44
(2,1229)	1:18:A:ASP:HA	1:21:A:PHE:H	9	0.44
(2,1206)	1:17:B:LEU:HD21	1:17:B:LEU:H	4	0.44
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD22	6	0.44
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD22	6	0.44
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	5	0.44
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	5	0.44
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	5	0.44
(2,948)	1:54:B:GLU:HG2	1:21:B:PHE:HE2	3	0.44
(2,926)	1:36:B:SER:HB2	1:43:B:GLU:HG3	10	0.44
(2,789)	1:16:A:ALA:HA	1:15:A:LYS:HB3	6	0.44
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	8	0.44
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	8	0.44
(2,687)	1:55:A:GLN:HA	1:55:A:GLN:HB2	6	0.44
(2,661)	1:52:A:ARG:HA	1:55:A:GLN:HG2	10	0.44
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD13	9	0.44
(2,467)	1:19:A:LEU:HD22	1:35:B:LEU:HB2	4	0.44
(2,381)	1:34:A:TYR:HD1	1:64:B:PHE:HD2	7	0.44
(2,354)	1:47:B:GLU:H	1:45:B:GLN:HB3	9	0.44
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	10	0.44
(2,220)	1:43:B:GLU:HA	1:44:B:GLU:HG2	4	0.44
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	4	0.44
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	5	0.44
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	8	0.44
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	9	0.44
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	10	0.44
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	1	0.44
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	4	0.44
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	5	0.44
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	8	0.44
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	10	0.44
(2,124)	1:14:B:LYS:HB2	1:14:B:LYS:HE3	9	0.44
(2,94)	1:32:B:ARG:HD3	1:45:B:GLN:H	5	0.44
(2,72)	1:16:B:ALA:HA	1:19:B:LEU:HD23	5	0.44
(2,71)	1:16:A:ALA:HA	1:19:A:LEU:HD23	5	0.44
(2,67)	1:25:A:ARG:HA	1:19:B:LEU:HD21	3	0.44
(2,56)	1:60:B:SER:HB3	1:61:B:HIS:H	1	0.44
(2,56)	1:60:B:SER:HB2	1:61:B:HIS:H	2	0.44
(2,56)	1:60:B:SER:HB3	1:61:B:HIS:H	10	0.44
(2,55)	1:60:A:SER:HB3	1:61:A:HIS:H	1	0.44
(2,55)	1:60:A:SER:HB2	1:61:A:HIS:H	2	0.44
(2,55)	1:60:A:SER:HB3	1:61:A:HIS:H	10	0.44
(2,40)	1:15:B:LYS:HA	1:15:B:LYS:HB3	5	0.44
(2,39)	1:15:A:LYS:HA	1:15:A:LYS:HB3	5	0.44
(3,146)	1:4:B:ARG:H	1:12:B:GLU:H	8	0.43
(3,145)	1:4:A:ARG:H	1:12:A:GLU:H	8	0.43
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	5	0.43
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE1	3	0.43
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE2	5	0.43
(2,2393)	1:7:A:THR:H	1:4:A:ARG:HG3	10	0.43
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	7	0.43
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD21	2	0.43
(2,2216)	1:36:B:SER:HB2	1:36:B:SER:H	2	0.43
(2,2215)	1:36:A:SER:HB2	1:36:A:SER:H	2	0.43
(2,2215)	1:36:A:SER:HB2	1:36:A:SER:H	10	0.43
(2,2174)	1:17:B:LEU:HG	1:17:B:LEU:H	9	0.43
(2,2104)	1:9:B:PHE:H	1:13:B:GLN:HG2	10	0.43
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	7	0.43
(2,1802)	1:65:B:GLU:H	1:64:B:PHE:HD1	4	0.43
(2,1788)	1:66:B:LYS:H	1:66:B:LYS:HG2	6	0.43
(2,1787)	1:66:A:LYS:H	1:66:A:LYS:HG2	6	0.43
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD12	3	0.43
(2,1696)	1:7:B:THR:HB	1:45:B:GLN:HB2	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	8	0.43
(2,1626)	1:41:B:LEU:HD11	1:36:B:SER:HA	2	0.43
(2,1625)	1:41:A:LEU:HD11	1:36:A:SER:HA	2	0.43
(2,1191)	1:16:A:ALA:HB2	1:14:A:LYS:HA	4	0.43
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD13	9	0.43
(2,1145)	1:39:A:LEU:HD11	1:16:A:ALA:HB3	7	0.43
(2,1137)	1:17:A:LEU:HA	1:20:A:ALA:HB1	3	0.43
(2,1078)	1:52:B:ARG:HB2	1:52:B:ARG:HG3	6	0.43
(2,1077)	1:52:A:ARG:HB2	1:52:A:ARG:HG3	6	0.43
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	8	0.43
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	8	0.43
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	5	0.43
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	1	0.43
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	4	0.43
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	5	0.43
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	10	0.43
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	1	0.43
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	4	0.43
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	5	0.43
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	6	0.43
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	10	0.43
(2,925)	1:36:A:SER:HB2	1:43:A:GLU:HG3	10	0.43
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	3	0.43
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	3	0.43
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	9	0.43
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG23	8	0.43
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG23	10	0.43
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG23	8	0.43
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG23	10	0.43
(2,662)	1:52:B:ARG:HA	1:55:B:GLN:HG2	10	0.43
(2,391)	1:34:A:TYR:HD2	1:35:A:LEU:HD23	6	0.43
(2,303)	1:59:A:TRP:H	1:62:A:PRO:HD3	9	0.43
(2,248)	1:63:B:GLN:HG2	1:57:B:ILE:H	10	0.43
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	6	0.43
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	6	0.43
(2,195)	1:18:A:ASP:HA	1:53:A:LYS:HD2	10	0.43
(2,156)	1:62:B:PRO:HA	1:62:B:PRO:HG2	2	0.43
(2,155)	1:62:A:PRO:HA	1:62:A:PRO:HG2	2	0.43
(2,123)	1:14:A:LYS:HB2	1:14:A:LYS:HE3	9	0.43
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	3	0.42
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	8	0.42
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,139)	1:27:A:LEU:H	1:24:A:ASP:H	10	0.42
(3,122)	1:14:B:LYS:HE3	1:49:B:TRP:HB2	5	0.42
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE1	3	0.42
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE2	5	0.42
(2,2216)	1:36:B:SER:HB2	1:36:B:SER:H	10	0.42
(2,2215)	1:36:A:SER:HB2	1:36:A:SER:H	4	0.42
(2,2029)	1:32:A:ARG:H	1:32:A:ARG:HD3	5	0.42
(2,1853)	1:16:A:ALA:H	1:15:A:LYS:HB3	3	0.42
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	10	0.42
(2,1635)	1:41:A:LEU:HD13	1:13:A:GLN:HG2	10	0.42
(2,1415)	1:46:A:ILE:HG21	1:32:A:ARG:H	3	0.42
(2,1145)	1:39:A:LEU:HD11	1:16:A:ALA:HB1	6	0.42
(2,1049)	1:41:A:LEU:HD21	1:41:A:LEU:H	5	0.42
(2,994)	1:12:B:GLU:HB3	1:12:B:GLU:H	4	0.42
(2,993)	1:12:A:GLU:HB3	1:12:A:GLU:H	4	0.42
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	6	0.42
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	6	0.42
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	3	0.42
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	6	0.42
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	7	0.42
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	8	0.42
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	9	0.42
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	3	0.42
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	7	0.42
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	8	0.42
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	9	0.42
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	10	0.42
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	10	0.42
(2,947)	1:54:A:GLU:HG2	1:21:A:PHE:HE2	3	0.42
(2,617)	1:12:A:GLU:HA	1:15:A:LYS:HE3	4	0.42
(2,528)	1:57:B:ILE:HA	1:57:B:ILE:HG21	3	0.42
(2,527)	1:57:A:ILE:HA	1:57:A:ILE:HG21	3	0.42
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	3	0.42
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	6	0.42
(2,515)	1:62:A:PRO:HA	1:62:A:PRO:HB2	3	0.42
(2,515)	1:62:A:PRO:HA	1:62:A:PRO:HB2	6	0.42
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	5	0.42
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	5	0.42
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	8	0.42
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	8	0.42
(2,342)	1:60:B:SER:H	1:59:B:TRP:HA	1	0.42
(2,341)	1:60:A:SER:H	1:59:A:TRP:HA	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,263)	1:39:A:LEU:HD11	1:16:A:ALA:H	4	0.42
(2,250)	1:13:B:GLN:HB3	1:41:B:LEU:H	4	0.42
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	4	0.42
(2,71)	1:16:A:ALA:HA	1:19:B:LEU:HD23	3	0.42
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	5	0.42
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	5	0.42
(2,43)	1:53:A:LYS:HA	1:53:A:LYS:HD3	3	0.42
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	9	0.42
(3,186)	1:13:B:GLN:H	1:17:B:LEU:H	1	0.41
(3,186)	1:13:B:GLN:H	1:17:B:LEU:H	3	0.41
(3,185)	1:13:A:GLN:H	1:17:A:LEU:H	1	0.41
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	7	0.41
(2,2322)	1:6:B:ARG:H	1:5:B:PRO:HB3	5	0.41
(2,2321)	1:6:A:ARG:H	1:5:A:PRO:HB3	5	0.41
(2,2216)	1:36:B:SER:HB2	1:36:B:SER:H	4	0.41
(2,2215)	1:36:A:SER:HB2	1:36:A:SER:H	5	0.41
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	5	0.41
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	5	0.41
(2,1854)	1:16:B:ALA:H	1:15:B:LYS:HB3	3	0.41
(2,1846)	1:53:B:LYS:H	1:54:B:GLU:HG2	6	0.41
(2,1845)	1:53:A:LYS:H	1:54:A:GLU:HG2	6	0.41
(2,1636)	1:41:B:LEU:HD13	1:13:B:GLN:HG2	8	0.41
(2,1586)	1:35:B:LEU:HD21	1:35:B:LEU:HA	10	0.41
(2,1585)	1:35:A:LEU:HD21	1:35:A:LEU:HA	10	0.41
(2,1415)	1:46:A:ILE:HG21	1:32:A:ARG:H	6	0.41
(2,1331)	1:27:A:LEU:HD21	1:50:A:PHE:H	3	0.41
(2,1254)	1:28:B:THR:HB	1:30:B:GLU:HB2	1	0.41
(2,1253)	1:28:A:THR:HB	1:30:A:GLU:HB2	1	0.41
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD13	5	0.41
(2,1166)	1:46:B:ILE:HD13	1:36:B:SER:H	8	0.41
(2,1165)	1:46:A:ILE:HD13	1:36:A:SER:H	8	0.41
(2,1146)	1:39:B:LEU:HD11	1:16:B:ALA:HB1	6	0.41
(2,1050)	1:41:B:LEU:HD21	1:41:B:LEU:H	5	0.41
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD22	1	0.41
(2,990)	1:48:B:ARG:HB3	1:48:B:ARG:H	3	0.41
(2,989)	1:48:A:ARG:HB3	1:48:A:ARG:H	3	0.41
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	1	0.41
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	6	0.41
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	8	0.41
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	9	0.41
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	1	0.41
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	8	0.41
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	9	0.41
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	10	0.41
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG23	6	0.41
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG23	6	0.41
(2,392)	1:34:B:TYR:HD2	1:35:B:LEU:HD23	6	0.41
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	4	0.41
(2,342)	1:60:B:SER:H	1:59:B:TRP:HA	4	0.41
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HE2	6	0.41
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HE2	6	0.41
(2,281)	1:7:A:THR:HB	1:41:A:LEU:H	7	0.41
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	3	0.41
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	4	0.41
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	3	0.41
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	2	0.41
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	2	0.41
(2,66)	1:24:B:ASP:HA	1:20:B:ALA:HB3	2	0.41
(2,44)	1:53:B:LYS:HA	1:53:B:LYS:HD3	3	0.41
(1,81)	1:20:B:ALA:N	1:16:B:ALA:O	8	0.41
(1,50)	1:34:B:TYR:H	1:30:B:GLU:O	5	0.41
(1,39)	1:20:A:ALA:N	1:16:A:ALA:O	8	0.41
(1,8)	1:34:A:TYR:H	1:30:A:GLU:O	5	0.41
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	3	0.4
(3,91)	1:27:A:LEU:HA	1:50:A:PHE:HB3	3	0.4
(3,75)	1:57:A:ILE:HG12	1:61:A:HIS:HB2	4	0.4
(3,73)	1:39:A:LEU:HG	1:15:B:LYS:HE3	9	0.4
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	7	0.4
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE2	6	0.4
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE2	6	0.4
(2,2436)	1:27:B:LEU:HD11	1:47:B:GLU:H	3	0.4
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	5	0.4
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	5	0.4
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	8	0.4
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	8	0.4
(2,2394)	1:7:B:THR:H	1:4:B:ARG:HG3	10	0.4
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD21	2	0.4
(2,2224)	1:57:B:ILE:HG12	1:58:B:GLY:H	2	0.4
(2,2216)	1:36:B:SER:HB2	1:36:B:SER:H	5	0.4
(2,2215)	1:36:A:SER:HB2	1:36:A:SER:H	3	0.4
(2,1804)	1:65:B:GLU:H	1:64:B:PHE:HB3	3	0.4
(2,1803)	1:65:A:GLU:H	1:64:A:PHE:HB3	3	0.4
(2,1695)	1:7:A:THR:HB	1:45:A:GLN:HB2	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1635)	1:41:A:LEU:HD13	1:13:A:GLN:HG2	8	0.4
(2,1547)	1:27:A:LEU:HB3	1:50:A:PHE:HD2	3	0.4
(2,1539)	1:13:A:GLN:HB3	1:41:A:LEU:HD22	4	0.4
(2,1483)	1:59:A:TRP:HB3	1:57:A:ILE:HG21	9	0.4
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	6	0.4
(2,1227)	1:17:A:LEU:HD23	1:49:A:TRP:HE1	9	0.4
(2,1192)	1:16:B:ALA:HB2	1:14:B:LYS:HA	4	0.4
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB3	2	0.4
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB3	2	0.4
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD22	1	0.4
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	3	0.4
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	3	0.4
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	7	0.4
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	3	0.4
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	7	0.4
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	9	0.4
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	9	0.4
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	10	0.4
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	4	0.4
(2,618)	1:12:B:GLU:HA	1:15:B:LYS:HE3	4	0.4
(2,615)	1:15:A:LYS:HA	1:18:A:ASP:HB2	4	0.4
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD13	10	0.4
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD13	10	0.4
(2,381)	1:34:A:TYR:HD1	1:64:B:PHE:HD2	8	0.4
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	9	0.4
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	8	0.4
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	8	0.4
(2,341)	1:60:A:SER:H	1:59:A:TRP:HA	4	0.4
(2,322)	1:54:B:GLU:H	1:52:B:ARG:HB2	3	0.4
(2,282)	1:7:B:THR:HB	1:41:B:LEU:H	7	0.4
(2,220)	1:43:B:GLU:HA	1:44:B:GLU:HG2	2	0.4
(2,219)	1:43:A:GLU:HA	1:44:A:GLU:HG2	2	0.4
(2,124)	1:14:B:LYS:HB2	1:14:B:LYS:HE3	7	0.4
(2,44)	1:53:B:LYS:HA	1:53:B:LYS:HD3	8	0.4
(2,43)	1:53:A:LYS:HA	1:53:A:LYS:HD3	8	0.4
(3,119)	1:9:A:PHE:HB3	1:45:A:GLN:HA	7	0.39
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE1	9	0.39
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	2	0.39
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	2	0.39
(2,2226)	1:58:B:GLY:H	1:57:B:ILE:HG13	8	0.39
(2,2225)	1:58:A:GLY:H	1:57:A:ILE:HG13	8	0.39
(2,2223)	1:57:A:ILE:HG12	1:58:A:GLY:H	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2216)	1:36:B:SER:HB2	1:36:B:SER:H	3	0.39
(2,2216)	1:36:B:SER:HB2	1:36:B:SER:H	8	0.39
(2,2215)	1:36:A:SER:HB2	1:36:A:SER:H	8	0.39
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG21	3	0.39
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	5	0.39
(2,2045)	1:34:A:TYR:HD1	1:35:A:LEU:H	5	0.39
(2,1901)	1:59:A:TRP:H	1:62:A:PRO:HD2	9	0.39
(2,1891)	1:65:A:GLU:HG2	1:65:A:GLU:H	6	0.39
(2,1666)	1:57:B:ILE:HG12	1:60:B:SER:H	1	0.39
(2,1665)	1:57:A:ILE:HG12	1:60:A:SER:H	1	0.39
(2,1620)	1:13:B:GLN:HA	1:39:B:LEU:HD11	7	0.39
(2,1540)	1:13:B:GLN:HB3	1:41:B:LEU:HD22	6	0.39
(2,1416)	1:46:B:ILE:HG21	1:32:B:ARG:H	6	0.39
(2,1370)	1:13:B:GLN:HB3	1:4:B:ARG:HA	6	0.39
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD11	3	0.39
(2,1190)	1:16:B:ALA:HB2	1:17:B:LEU:HA	4	0.39
(2,1165)	1:46:A:ILE:HD13	1:36:A:SER:H	10	0.39
(2,1123)	1:20:A:ALA:HB2	1:21:A:PHE:H	4	0.39
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD21	7	0.39
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	6	0.39
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	6	0.39
(2,382)	1:34:B:TYR:HD1	1:64:A:PHE:HD2	8	0.39
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	9	0.39
(2,353)	1:47:A:GLU:H	1:45:A:GLN:HB3	4	0.39
(2,333)	1:52:A:ARG:HB2	1:56:A:GLN:H	4	0.39
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD23	10	0.39
(2,321)	1:54:A:GLU:H	1:52:A:ARG:HB2	3	0.39
(2,239)	1:49:A:TRP:HB3	1:46:A:ILE:HG12	1	0.39
(2,178)	1:16:B:ALA:HB2	1:20:B:ALA:H	5	0.39
(2,177)	1:16:A:ALA:HB2	1:20:A:ALA:H	5	0.39
(2,123)	1:14:A:LYS:HB2	1:14:A:LYS:HE3	7	0.39
(2,120)	1:47:B:GLU:HG2	1:27:B:LEU:HD23	8	0.39
(2,119)	1:47:A:GLU:HG2	1:27:A:LEU:HD23	8	0.39
(2,70)	1:61:B:HIS:HA	1:62:B:PRO:HG3	3	0.39
(2,69)	1:61:A:HIS:HA	1:62:A:PRO:HG3	3	0.39
(2,65)	1:24:A:ASP:HA	1:20:A:ALA:HB3	2	0.39
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	10	0.39
(1,50)	1:34:B:TYR:H	1:30:B:GLU:O	1	0.39
(1,8)	1:34:A:TYR:H	1:30:A:GLU:O	1	0.39
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	3	0.38
(3,100)	1:59:B:TRP:HB3	1:54:B:GLU:HA	9	0.38
(3,99)	1:59:A:TRP:HB3	1:54:A:GLU:HA	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	3	0.38
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	3	0.38
(3,78)	1:37:B:GLN:HB3	1:34:B:TYR:HB2	8	0.38
(3,77)	1:37:A:GLN:HB3	1:34:A:TYR:HB2	8	0.38
(3,28)	1:2:B:GLU:HA	1:12:B:GLU:H	9	0.38
(3,4)	1:12:B:GLU:HG3	1:12:A:GLU:HB2	4	0.38
(3,3)	1:12:A:GLU:HG3	1:12:B:GLU:HB2	10	0.38
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE1	9	0.38
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE1	7	0.38
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	5	0.38
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	8	0.38
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	10	0.38
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	8	0.38
(2,2216)	1:36:B:SER:HB2	1:36:B:SER:H	9	0.38
(2,2215)	1:36:A:SER:HB2	1:36:A:SER:H	9	0.38
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG21	3	0.38
(2,2006)	1:64:B:PHE:H	1:63:B:GLN:H	9	0.38
(2,1892)	1:65:B:GLU:HG2	1:65:B:GLU:H	6	0.38
(2,1852)	1:53:B:LYS:H	1:52:B:ARG:HG3	3	0.38
(2,1851)	1:53:A:LYS:H	1:52:A:ARG:HG3	3	0.38
(2,1786)	1:66:B:LYS:H	1:64:B:PHE:HB3	5	0.38
(2,1785)	1:66:A:LYS:H	1:64:A:PHE:HB3	5	0.38
(2,1619)	1:13:A:GLN:HA	1:39:A:LEU:HD11	7	0.38
(2,1540)	1:13:B:GLN:HB3	1:41:B:LEU:HD22	4	0.38
(2,1390)	1:46:B:ILE:HD12	1:35:B:LEU:HA	3	0.38
(2,1338)	1:27:B:LEU:HD21	1:50:B:PHE:HD1	9	0.38
(2,1337)	1:27:A:LEU:HD21	1:50:A:PHE:HD1	9	0.38
(2,1331)	1:27:A:LEU:HD21	1:50:A:PHE:H	2	0.38
(2,1189)	1:16:A:ALA:HB2	1:17:A:LEU:HA	10	0.38
(2,1088)	1:15:B:LYS:HG3	1:15:B:LYS:HE3	10	0.38
(2,1087)	1:15:A:LYS:HG3	1:15:A:LYS:HE3	10	0.38
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD23	6	0.38
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD22	2	0.38
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD23	6	0.38
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD21	7	0.38
(2,996)	1:33:B:ARG:HB2	1:34:B:TYR:H	2	0.38
(2,995)	1:33:A:ARG:HB2	1:34:A:TYR:H	2	0.38
(2,960)	1:45:B:GLN:HG3	1:45:B:GLN:HA	4	0.38
(2,959)	1:45:A:GLN:HG3	1:45:A:GLN:HA	4	0.38
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	2	0.38
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	2	0.38
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG22	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG22	4	0.38
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD22	2	0.38
(2,573)	1:32:A:ARG:HA	1:27:A:LEU:HD22	2	0.38
(2,462)	1:49:B:TRP:HD1	1:14:B:LYS:HE3	1	0.38
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	4	0.38
(2,349)	1:27:A:LEU:H	1:32:A:ARG:HB2	7	0.38
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD23	10	0.38
(2,257)	1:54:A:GLU:HG2	1:21:A:PHE:HB3	6	0.38
(2,240)	1:49:B:TRP:HB3	1:46:B:ILE:HG12	1	0.38
(2,220)	1:43:B:GLU:HA	1:44:B:GLU:HG2	10	0.38
(2,219)	1:43:A:GLU:HA	1:44:A:GLU:HG2	10	0.38
(2,162)	1:39:B:LEU:HG	1:13:B:GLN:H	8	0.38
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	8	0.38
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	10	0.38
(2,14)	1:36:B:SER:HB2	1:45:B:GLN:HB2	9	0.38
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	9	0.38
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	3	0.37
(3,164)	1:6:B:ARG:H	1:4:B:ARG:HA	9	0.37
(3,163)	1:6:A:ARG:H	1:4:A:ARG:HA	9	0.37
(3,157)	1:16:A:ALA:H	1:17:A:LEU:HG	3	0.37
(3,150)	1:2:B:GLU:H	1:4:B:ARG:HA	6	0.37
(3,149)	1:2:A:GLU:H	1:4:A:ARG:HA	6	0.37
(3,120)	1:9:B:PHE:HB3	1:45:B:GLN:HA	7	0.37
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	5	0.37
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	5	0.37
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	8	0.37
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	6	0.37
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	6	0.37
(2,2242)	1:8:B:GLU:HG3	1:8:B:GLU:H	5	0.37
(2,2241)	1:8:A:GLU:HG3	1:8:A:GLU:H	5	0.37
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	2	0.37
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	2	0.37
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	8	0.37
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	8	0.37
(2,2046)	1:34:B:TYR:HD1	1:35:B:LEU:H	7	0.37
(2,1926)	1:6:B:ARG:H	1:5:B:PRO:HB2	7	0.37
(2,1925)	1:6:A:ARG:H	1:5:A:PRO:HB2	7	0.37
(2,1924)	1:63:B:GLN:HG2	1:63:B:GLN:H	1	0.37
(2,1923)	1:63:A:GLN:HG2	1:63:A:GLN:H	1	0.37
(2,1836)	1:53:B:LYS:H	1:53:B:LYS:HD2	4	0.37
(2,1816)	1:4:B:ARG:H	1:10:B:SER:HB3	5	0.37
(2,1651)	1:28:A:THR:HB	1:31:A:TRP:HB3	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1613)	1:16:A:ALA:HB2	1:35:A:LEU:HD11	1	0.37
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE2	8	0.37
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE2	8	0.37
(2,1539)	1:13:A:GLN:HB3	1:41:A:LEU:HD22	6	0.37
(2,1236)	1:20:B:ALA:HB1	1:26:B:ARG:HD3	8	0.37
(2,1235)	1:20:A:ALA:HB1	1:26:A:ARG:HD3	8	0.37
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD21	7	0.37
(2,1202)	1:17:B:LEU:HD21	1:46:B:ILE:HG12	8	0.37
(2,1201)	1:17:A:LEU:HD21	1:46:A:ILE:HG12	8	0.37
(2,1190)	1:16:B:ALA:HB2	1:17:B:LEU:HA	10	0.37
(2,1138)	1:17:B:LEU:HA	1:20:B:ALA:HB1	3	0.37
(2,1062)	1:27:B:LEU:HD23	1:50:B:PHE:HB3	5	0.37
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD22	2	0.37
(2,883)	1:9:A:PHE:HB3	1:39:A:LEU:HG	1	0.37
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	4	0.37
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	9	0.37
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	9	0.37
(2,597)	1:47:A:GLU:HA	1:27:A:LEU:HD13	2	0.37
(2,461)	1:49:A:TRP:HD1	1:14:A:LYS:HE3	1	0.37
(2,94)	1:32:B:ARG:HD3	1:45:B:GLN:H	9	0.37
(2,56)	1:60:B:SER:HB2	1:61:B:HIS:H	4	0.37
(2,55)	1:60:A:SER:HB2	1:61:A:HIS:H	4	0.37
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	9	0.37
(1,50)	1:34:B:TYR:H	1:30:B:GLU:O	6	0.37
(1,8)	1:34:A:TYR:H	1:30:A:GLU:O	6	0.37
(3,158)	1:16:B:ALA:H	1:17:B:LEU:HG	3	0.36
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE1	7	0.36
(2,2419)	1:51:A:ARG:H	1:54:A:GLU:HG3	9	0.36
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	8	0.36
(2,2273)	1:48:A:ARG:H	1:27:A:LEU:HD23	5	0.36
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	10	0.36
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG23	7	0.36
(2,1943)	1:61:A:HIS:HB3	1:61:A:HIS:H	4	0.36
(2,1835)	1:53:A:LYS:H	1:53:A:LYS:HD2	4	0.36
(2,1815)	1:4:A:ARG:H	1:10:A:SER:HB3	5	0.36
(2,1802)	1:65:B:GLU:H	1:64:B:PHE:HD1	2	0.36
(2,1801)	1:65:A:GLU:H	1:64:A:PHE:HD1	2	0.36
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	8	0.36
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	8	0.36
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	8	0.36
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	5	0.36
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1577)	1:27:A:LEU:HD21	1:32:A:ARG:HD2	5	0.36
(2,1548)	1:27:B:LEU:HB3	1:50:B:PHE:HD2	3	0.36
(2,1466)	1:54:B:GLU:HB2	1:54:B:GLU:H	2	0.36
(2,1389)	1:46:A:ILE:HD12	1:35:A:LEU:HA	3	0.36
(2,1369)	1:13:A:GLN:HB3	1:4:A:ARG:HA	10	0.36
(2,1332)	1:27:B:LEU:HD21	1:50:B:PHE:H	2	0.36
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD12	1	0.36
(2,1205)	1:17:A:LEU:HD21	1:17:A:LEU:H	4	0.36
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD21	7	0.36
(2,1189)	1:16:A:ALA:HB2	1:17:A:LEU:HA	4	0.36
(2,1189)	1:16:A:ALA:HB1	1:17:A:LEU:HA	5	0.36
(2,1181)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	9	0.36
(2,1156)	1:57:B:ILE:HG23	1:58:B:GLY:H	7	0.36
(2,1155)	1:57:A:ILE:HG23	1:58:A:GLY:H	7	0.36
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	10	0.36
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	10	0.36
(2,943)	1:54:A:GLU:HG2	1:21:A:PHE:HZ	3	0.36
(2,884)	1:9:B:PHE:HB3	1:39:B:LEU:HG	1	0.36
(2,814)	1:61:B:HIS:HA	1:62:B:PRO:HD3	5	0.36
(2,813)	1:61:A:HIS:HA	1:62:A:PRO:HD3	5	0.36
(2,790)	1:16:B:ALA:HA	1:15:B:LYS:HB3	3	0.36
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	2	0.36
(2,738)	1:60:B:SER:HB3	1:60:B:SER:H	5	0.36
(2,737)	1:60:A:SER:HB3	1:60:A:SER:H	5	0.36
(2,703)	1:64:A:PHE:HA	1:64:A:PHE:HD2	7	0.36
(2,598)	1:47:B:GLU:HA	1:27:B:LEU:HD13	2	0.36
(2,526)	1:36:B:SER:HB2	1:46:B:ILE:HG12	5	0.36
(2,441)	1:16:A:ALA:HB1	1:20:B:ALA:H	7	0.36
(2,402)	1:9:B:PHE:HD2	1:45:B:GLN:HG3	2	0.36
(2,401)	1:9:A:PHE:HD2	1:45:A:GLN:HG3	2	0.36
(2,354)	1:47:B:GLU:H	1:45:B:GLN:HB3	4	0.36
(2,350)	1:27:B:LEU:H	1:32:B:ARG:HB2	7	0.36
(2,249)	1:13:A:GLN:HB3	1:41:A:LEU:H	4	0.36
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	2	0.36
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	2	0.36
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	9	0.36
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	10	0.36
(2,130)	1:33:B:ARG:HB2	1:33:B:ARG:H	9	0.36
(1,3)	1:17:A:LEU:H	1:13:A:GLN:O	6	0.36
(2,2444)	1:50:B:PHE:H	1:50:B:PHE:HE1	1	0.35
(2,2443)	1:50:A:PHE:H	1:50:A:PHE:HE1	1	0.35
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	4	0.35
(2,2322)	1:6:B:ARG:H	1:5:B:PRO:HB3	8	0.35
(2,2321)	1:6:A:ARG:H	1:5:A:PRO:HB3	8	0.35
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD12	2	0.35
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD12	2	0.35
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG23	7	0.35
(2,1944)	1:61:B:HIS:HB3	1:61:B:HIS:H	4	0.35
(2,1862)	1:53:B:LYS:H	1:55:B:GLN:H	8	0.35
(2,1861)	1:53:A:LYS:H	1:55:A:GLN:H	8	0.35
(2,1786)	1:66:B:LYS:H	1:64:B:PHE:HB3	6	0.35
(2,1785)	1:66:A:LYS:H	1:64:A:PHE:HB3	6	0.35
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	5	0.35
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	8	0.35
(2,1614)	1:16:B:ALA:HB2	1:35:B:LEU:HD11	1	0.35
(2,1614)	1:16:B:ALA:HB3	1:35:B:LEU:HD12	8	0.35
(2,1613)	1:16:A:ALA:HB3	1:35:A:LEU:HD12	8	0.35
(2,1497)	1:63:A:GLN:HG2	1:64:A:PHE:HD1	2	0.35
(2,1465)	1:54:A:GLU:HB2	1:54:A:GLU:H	2	0.35
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD12	1	0.35
(2,1190)	1:16:B:ALA:HB1	1:17:B:LEU:HA	5	0.35
(2,1190)	1:16:B:ALA:HB1	1:17:B:LEU:HA	6	0.35
(2,1189)	1:16:A:ALA:HB1	1:17:A:LEU:HA	6	0.35
(2,1182)	1:6:B:ARG:HD3	1:6:B:ARG:HB2	9	0.35
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD23	4	0.35
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD23	8	0.35
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD23	4	0.35
(2,993)	1:12:A:GLU:HB3	1:12:A:GLU:H	3	0.35
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	8	0.35
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	8	0.35
(2,755)	1:43:A:GLU:HA	1:36:A:SER:HB2	2	0.35
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG21	3	0.35
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG21	3	0.35
(2,576)	1:14:B:LYS:HA	1:17:B:LEU:HD22	8	0.35
(2,575)	1:14:A:LYS:HA	1:17:A:LEU:HD22	8	0.35
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	9	0.35
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	9	0.35
(2,458)	1:49:B:TRP:HD1	1:17:B:LEU:HD12	7	0.35
(2,436)	1:16:B:ALA:HB2	1:39:A:LEU:HD11	2	0.35
(2,334)	1:52:B:ARG:HB2	1:56:B:GLN:H	4	0.35
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD22	1	0.35
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD23	5	0.35
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD22	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,324)	1:54:B:GLU:H	1:51:B:ARG:HD2	7	0.35
(2,264)	1:39:B:LEU:HD12	1:16:B:ALA:H	10	0.35
(2,258)	1:54:B:GLU:HG2	1:21:B:PHE:HB3	6	0.35
(2,250)	1:13:B:GLN:HB3	1:9:B:PHE:HD1	3	0.35
(2,217)	1:42:A:ASN:HB3	1:44:A:GLU:HA	9	0.35
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	8	0.35
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	8	0.35
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	9	0.35
(2,129)	1:65:A:GLU:HB2	1:65:A:GLU:H	9	0.35
(2,107)	1:9:A:PHE:HB2	1:4:A:ARG:HB2	6	0.35
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	9	0.35
(2,56)	1:60:B:SER:HB2	1:61:B:HIS:H	6	0.35
(2,55)	1:60:A:SER:HB2	1:61:A:HIS:H	6	0.35
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	4	0.35
(1,47)	1:19:B:LEU:H	1:15:B:LYS:O	8	0.35
(1,45)	1:17:B:LEU:H	1:13:B:GLN:O	6	0.35
(1,45)	1:17:B:LEU:H	1:13:B:GLN:O	10	0.35
(1,5)	1:19:A:LEU:H	1:15:A:LYS:O	8	0.35
(3,222)	1:54:B:GLU:H	1:52:B:ARG:HE	5	0.34
(3,221)	1:54:A:GLU:H	1:52:A:ARG:HE	5	0.34
(3,120)	1:9:B:PHE:HB3	1:45:B:GLN:HA	1	0.34
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	10	0.34
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	10	0.34
(3,95)	1:59:A:TRP:HB2	1:55:A:GLN:H	5	0.34
(3,91)	1:27:A:LEU:HA	1:50:A:PHE:HB3	5	0.34
(3,68)	1:63:B:GLN:HG2	1:54:B:GLU:HA	8	0.34
(3,67)	1:63:A:GLN:HG2	1:54:A:GLU:HA	8	0.34
(3,3)	1:12:A:GLU:HG3	1:12:B:GLU:HB2	4	0.34
(2,2305)	1:58:A:GLY:H	1:60:A:SER:HG	6	0.34
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	9	0.34
(2,2245)	1:66:A:LYS:H	1:64:A:PHE:H	9	0.34
(2,2188)	1:54:B:GLU:H	1:21:B:PHE:HE1	4	0.34
(2,2152)	1:15:B:LYS:HG3	1:15:B:LYS:H	4	0.34
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	2	0.34
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	4	0.34
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	6	0.34
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	2	0.34
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	4	0.34
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	6	0.34
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	8	0.34
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	8	0.34
(2,1514)	1:9:B:PHE:HA	1:17:B:LEU:HD22	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1513)	1:9:A:PHE:HA	1:17:A:LEU:HD22	2	0.34
(2,1498)	1:63:B:GLN:HG2	1:64:B:PHE:HD1	2	0.34
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	3	0.34
(2,1231)	1:18:A:ASP:HA	1:49:A:TRP:HE1	3	0.34
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD11	3	0.34
(2,1202)	1:17:B:LEU:HD23	1:46:B:ILE:HG12	6	0.34
(2,1196)	1:16:B:ALA:HB3	1:13:B:GLN:HG2	2	0.34
(2,1195)	1:16:A:ALA:HB3	1:13:A:GLN:HG2	2	0.34
(2,1152)	1:46:B:ILE:HG21	1:27:B:LEU:HD22	8	0.34
(2,1151)	1:46:A:ILE:HG21	1:27:A:LEU:HD22	8	0.34
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD23	8	0.34
(2,994)	1:12:B:GLU:HB3	1:12:B:GLU:H	3	0.34
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	1	0.34
(2,583)	1:32:A:ARG:HA	1:27:A:LEU:HD13	7	0.34
(2,525)	1:36:A:SER:HB2	1:46:A:ILE:HG12	5	0.34
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD13	5	0.34
(2,486)	1:50:B:PHE:HB2	1:50:B:PHE:HE1	5	0.34
(2,486)	1:50:B:PHE:HB2	1:50:B:PHE:HE1	6	0.34
(2,485)	1:50:A:PHE:HB2	1:50:A:PHE:HE1	5	0.34
(2,485)	1:50:A:PHE:HB2	1:50:A:PHE:HE1	6	0.34
(2,353)	1:47:A:GLU:H	1:44:A:GLU:HG3	10	0.34
(2,332)	1:14:B:LYS:H	1:12:B:GLU:HA	7	0.34
(2,331)	1:14:A:LYS:H	1:12:A:GLU:HA	2	0.34
(2,331)	1:14:A:LYS:H	1:12:A:GLU:HA	7	0.34
(2,323)	1:54:A:GLU:H	1:51:A:ARG:HD2	7	0.34
(2,317)	1:59:A:TRP:HB2	1:55:A:GLN:H	5	0.34
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HD2	3	0.34
(2,263)	1:39:A:LEU:HD12	1:16:A:ALA:H	10	0.34
(2,250)	1:13:B:GLN:HB3	1:9:B:PHE:HD1	5	0.34
(2,250)	1:13:B:GLN:HB3	1:41:B:LEU:H	7	0.34
(2,249)	1:13:A:GLN:HB3	1:9:A:PHE:HD1	3	0.34
(2,249)	1:13:A:GLN:HB3	1:9:A:PHE:HD1	5	0.34
(2,249)	1:13:A:GLN:HB3	1:41:A:LEU:H	7	0.34
(2,238)	1:49:B:TRP:HA	1:52:B:ARG:H	7	0.34
(2,218)	1:42:B:ASN:HB3	1:44:B:GLU:HA	9	0.34
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	7	0.34
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	7	0.34
(2,75)	1:25:A:ARG:HA	1:20:A:ALA:HA	4	0.34
(2,68)	1:25:B:ARG:HA	1:19:A:LEU:HD22	3	0.34
(2,18)	1:60:B:SER:HB2	1:57:B:ILE:HA	5	0.34
(2,17)	1:60:A:SER:HB2	1:57:A:ILE:HA	5	0.34
(2,13)	1:36:A:SER:HB2	1:45:A:GLN:HB2	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,117)	1:39:A:LEU:HG	1:9:A:PHE:H	5	0.33
(3,116)	1:3:B:LYS:HG3	1:1:B:MET:HA	3	0.33
(3,96)	1:59:B:TRP:HB2	1:55:B:GLN:H	5	0.33
(3,64)	1:8:B:GLU:HG3	1:45:B:GLN:HE22	8	0.33
(3,63)	1:8:A:GLU:HG3	1:45:A:GLN:HE22	8	0.33
(2,2306)	1:58:B:GLY:H	1:60:B:SER:HG	6	0.33
(2,2151)	1:15:A:LYS:HG3	1:15:A:LYS:H	4	0.33
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	10	0.33
(2,2032)	1:32:B:ARG:H	1:30:B:GLU:HB2	4	0.33
(2,1939)	1:61:A:HIS:H	1:54:A:GLU:HB2	3	0.33
(2,1678)	1:30:B:GLU:HA	1:33:B:ARG:HD3	4	0.33
(2,1445)	1:53:A:LYS:HB2	1:21:A:PHE:HZ	2	0.33
(2,1343)	1:41:A:LEU:HD11	1:17:A:LEU:HD22	9	0.33
(2,1246)	1:20:B:ALA:HB3	1:50:B:PHE:HE1	10	0.33
(2,1064)	1:27:B:LEU:HD21	1:43:B:GLU:HB3	5	0.33
(2,1048)	1:57:B:ILE:HG13	1:57:B:ILE:H	4	0.33
(2,1047)	1:57:A:ILE:HG13	1:57:A:ILE:H	4	0.33
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD22	3	0.33
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD22	3	0.33
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD21	9	0.33
(2,944)	1:54:B:GLU:HG2	1:21:B:PHE:HZ	3	0.33
(2,789)	1:16:A:ALA:HA	1:15:A:LYS:HB3	3	0.33
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	1	0.33
(2,457)	1:49:A:TRP:HD1	1:17:A:LEU:HD12	7	0.33
(2,435)	1:16:A:ALA:HB2	1:39:B:LEU:HD11	2	0.33
(2,354)	1:47:B:GLU:H	1:44:B:GLU:HG3	10	0.33
(2,332)	1:14:B:LYS:H	1:12:B:GLU:HA	2	0.33
(2,322)	1:54:B:GLU:H	1:52:B:ARG:HB2	9	0.33
(2,321)	1:54:A:GLU:H	1:52:A:ARG:HB2	9	0.33
(2,318)	1:59:B:TRP:HB2	1:55:B:GLN:H	5	0.33
(2,304)	1:59:B:TRP:H	1:62:B:PRO:HD3	5	0.33
(2,303)	1:59:A:TRP:H	1:62:A:PRO:HD3	5	0.33
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HD2	3	0.33
(2,244)	1:58:B:GLY:HA3	1:57:B:ILE:HG21	9	0.33
(2,237)	1:49:A:TRP:HA	1:52:A:ARG:H	7	0.33
(2,199)	1:20:A:ALA:HB2	1:17:A:LEU:HB3	9	0.33
(2,149)	1:33:A:ARG:HG3	1:34:A:TYR:HA	5	0.33
(2,108)	1:9:B:PHE:HB2	1:4:B:ARG:HB2	6	0.33
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	9	0.33
(2,30)	1:53:B:LYS:HA	1:56:B:GLN:HB3	3	0.33
(1,3)	1:17:A:LEU:H	1:13:A:GLN:O	9	0.33
(3,222)	1:54:B:GLU:H	1:52:B:ARG:HE	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,205)	1:57:A:ILE:H	1:54:A:GLU:HB2	2	0.32
(3,185)	1:13:A:GLN:H	1:17:A:LEU:H	3	0.32
(3,119)	1:9:A:PHE:HB3	1:45:A:GLN:HA	1	0.32
(3,115)	1:3:A:LYS:HG3	1:1:A:MET:HA	3	0.32
(3,98)	1:59:B:TRP:HB3	1:55:B:GLN:H	1	0.32
(3,92)	1:27:B:LEU:HA	1:50:B:PHE:HB3	3	0.32
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	8	0.32
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	8	0.32
(2,2441)	1:14:A:LYS:H	1:17:A:LEU:HD22	8	0.32
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	1	0.32
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	9	0.32
(2,2246)	1:66:B:LYS:H	1:64:B:PHE:H	9	0.32
(2,2180)	1:51:B:ARG:H	1:51:B:ARG:HG2	6	0.32
(2,2179)	1:51:A:ARG:H	1:51:A:ARG:HG2	6	0.32
(2,1944)	1:61:B:HIS:HB3	1:61:B:HIS:H	1	0.32
(2,1943)	1:61:A:HIS:HB3	1:61:A:HIS:H	1	0.32
(2,1940)	1:61:B:HIS:H	1:54:B:GLU:HB2	3	0.32
(2,1928)	1:6:B:ARG:H	1:6:B:ARG:HG3	1	0.32
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG22	8	0.32
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG22	8	0.32
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	9	0.32
(2,1736)	1:64:B:PHE:H	1:64:B:PHE:HD1	4	0.32
(2,1604)	1:53:B:LYS:HB3	1:21:B:PHE:HZ	4	0.32
(2,1580)	1:27:B:LEU:HD13	1:47:B:GLU:HG3	5	0.32
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD22	6	0.32
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD22	6	0.32
(2,1514)	1:9:B:PHE:HA	1:17:B:LEU:HD23	9	0.32
(2,1416)	1:46:B:ILE:HG23	1:32:B:ARG:H	4	0.32
(2,1336)	1:27:B:LEU:HD21	1:47:B:GLU:H	2	0.32
(2,1335)	1:27:A:LEU:HD21	1:47:A:GLU:H	2	0.32
(2,1332)	1:27:B:LEU:HD21	1:50:B:PHE:H	3	0.32
(2,1246)	1:20:B:ALA:HB1	1:50:B:PHE:HE1	3	0.32
(2,1201)	1:17:A:LEU:HD23	1:46:A:ILE:HG12	6	0.32
(2,1190)	1:16:B:ALA:HB3	1:17:B:LEU:HA	2	0.32
(2,1189)	1:16:A:ALA:HB3	1:17:A:LEU:HA	2	0.32
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD21	9	0.32
(2,954)	1:54:B:GLU:HG3	1:53:B:LYS:H	5	0.32
(2,828)	1:62:B:PRO:HD3	1:62:B:PRO:HB3	6	0.32
(2,827)	1:62:A:PRO:HD3	1:62:A:PRO:HB3	6	0.32
(2,799)	1:42:A:ASN:HA	1:43:A:GLU:HG3	4	0.32
(2,664)	1:52:B:ARG:HA	1:52:B:ARG:HB3	6	0.32
(2,663)	1:52:A:ARG:HA	1:52:A:ARG:HB3	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,584)	1:32:B:ARG:HA	1:27:B:LEU:HD13	7	0.32
(2,564)	1:43:B:GLU:HA	1:46:B:ILE:HD12	2	0.32
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	4	0.32
(2,332)	1:14:B:LYS:H	1:12:B:GLU:HA	10	0.32
(2,259)	1:54:A:GLU:HG3	1:59:A:TRP:HB2	2	0.32
(2,128)	1:38:B:ARG:HB2	1:15:A:LYS:HE3	1	0.32
(2,120)	1:47:B:GLU:HG2	1:27:B:LEU:HD21	2	0.32
(2,101)	1:19:A:LEU:HB3	1:16:A:ALA:HA	9	0.32
(2,68)	1:65:B:GLU:HA	1:19:B:LEU:HD21	9	0.32
(2,56)	1:60:B:SER:HB2	1:61:B:HIS:H	8	0.32
(2,55)	1:60:A:SER:HB2	1:61:A:HIS:H	8	0.32
(2,9)	1:16:A:ALA:HB3	1:15:B:LYS:HD3	1	0.32
(1,43)	1:15:B:LYS:H	1:11:B:GLU:O	3	0.32
(3,221)	1:54:A:GLU:H	1:52:A:ARG:HE	6	0.31
(3,172)	1:17:B:LEU:H	1:14:B:LYS:HG3	1	0.31
(3,171)	1:17:A:LEU:H	1:14:A:LYS:HG3	1	0.31
(3,143)	1:26:A:ARG:H	1:19:B:LEU:HA	2	0.31
(3,118)	1:39:B:LEU:HG	1:9:B:PHE:H	5	0.31
(3,100)	1:59:B:TRP:HB3	1:54:B:GLU:HA	8	0.31
(3,99)	1:59:A:TRP:HB3	1:54:A:GLU:HA	8	0.31
(3,97)	1:59:A:TRP:HB3	1:55:A:GLN:H	1	0.31
(3,64)	1:8:B:GLU:HG3	1:45:B:GLN:HE22	7	0.31
(2,2442)	1:14:B:LYS:H	1:17:B:LEU:HD22	8	0.31
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	1	0.31
(2,2274)	1:48:B:ARG:H	1:27:B:LEU:HD23	5	0.31
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD11	3	0.31
(2,2031)	1:32:A:ARG:H	1:30:A:GLU:HB2	4	0.31
(2,1927)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.31
(2,1892)	1:65:B:GLU:HG2	1:65:B:GLU:H	4	0.31
(2,1891)	1:65:A:GLU:HG2	1:65:A:GLU:H	4	0.31
(2,1735)	1:64:A:PHE:H	1:64:A:PHE:HD1	4	0.31
(2,1696)	1:7:B:THR:HB	1:45:B:GLN:HB2	4	0.31
(2,1695)	1:7:A:THR:HB	1:45:A:GLN:HB2	4	0.31
(2,1692)	1:7:B:THR:HB	1:42:B:ASN:HB2	6	0.31
(2,1691)	1:7:A:THR:HB	1:42:A:ASN:HB2	6	0.31
(2,1599)	1:53:A:LYS:HG2	1:21:A:PHE:HZ	4	0.31
(2,1554)	1:27:B:LEU:HB3	1:50:B:PHE:HB2	6	0.31
(2,1553)	1:27:A:LEU:HB3	1:50:A:PHE:HB2	6	0.31
(2,1388)	1:46:B:ILE:HD13	1:45:B:GLN:HG3	5	0.31
(2,1276)	1:32:B:ARG:HA	1:36:B:SER:HB2	6	0.31
(2,1275)	1:32:A:ARG:HA	1:36:A:SER:HB2	6	0.31
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1202)	1:17:B:LEU:HD22	1:46:B:ILE:HG12	3	0.31
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD13	10	0.31
(2,1125)	1:16:A:ALA:HB2	1:17:A:LEU:H	9	0.31
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	4	0.31
(2,790)	1:16:B:ALA:HA	1:15:B:LYS:HB3	7	0.31
(2,704)	1:64:B:PHE:HA	1:64:B:PHE:HD2	7	0.31
(2,563)	1:43:A:GLU:HA	1:46:A:ILE:HD12	2	0.31
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD13	6	0.31
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD13	6	0.31
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	4	0.31
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HE2	8	0.31
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HE2	8	0.31
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	1	0.31
(2,130)	1:33:B:ARG:HB2	1:33:B:ARG:H	10	0.31
(2,129)	1:33:A:ARG:HB2	1:33:A:ARG:H	10	0.31
(2,127)	1:38:A:ARG:HB2	1:15:B:LYS:HE3	1	0.31
(2,72)	1:16:B:ALA:HA	1:19:A:LEU:HD22	9	0.31
(1,45)	1:17:B:LEU:H	1:13:B:GLN:O	9	0.31
(3,206)	1:57:B:ILE:H	1:54:B:GLU:HB2	2	0.3
(3,192)	1:44:B:GLU:H	1:36:B:SER:HB2	10	0.3
(3,191)	1:44:A:GLU:H	1:36:A:SER:HB2	10	0.3
(3,144)	1:26:B:ARG:H	1:19:A:LEU:HA	2	0.3
(3,118)	1:39:B:LEU:HG	1:9:B:PHE:H	9	0.3
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	6	0.3
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	6	0.3
(3,63)	1:8:A:GLU:HG3	1:45:A:GLN:HE22	7	0.3
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	10	0.3
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	10	0.3
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD11	3	0.3
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD13	9	0.3
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	6	0.3
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	6	0.3
(2,2029)	1:32:A:ARG:H	1:32:A:ARG:HD3	4	0.3
(2,2006)	1:64:B:PHE:H	1:63:B:GLN:H	6	0.3
(2,1852)	1:53:B:LYS:H	1:52:B:ARG:HG3	9	0.3
(2,1851)	1:53:A:LYS:H	1:52:A:ARG:HG3	9	0.3
(2,1677)	1:30:A:GLU:HA	1:33:A:ARG:HD3	4	0.3
(2,1629)	1:41:A:LEU:HD12	1:9:A:PHE:HB2	3	0.3
(2,1609)	1:35:A:LEU:HB2	1:39:A:LEU:HD22	10	0.3
(2,1608)	1:16:B:ALA:HB1	1:35:B:LEU:HD23	7	0.3
(2,1446)	1:53:B:LYS:HB2	1:21:B:PHE:HZ	2	0.3
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1201)	1:17:A:LEU:HD21	1:46:A:ILE:HG12	5	0.3
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD13	10	0.3
(2,1053)	1:12:A:GLU:HB3	1:12:A:GLU:HG3	9	0.3
(2,1036)	1:41:B:LEU:HB3	1:41:B:LEU:HD21	10	0.3
(2,953)	1:54:A:GLU:HG3	1:53:A:LYS:H	5	0.3
(2,800)	1:42:B:ASN:HA	1:43:B:GLU:HG3	4	0.3
(2,789)	1:16:A:ALA:HA	1:15:A:LYS:HB3	7	0.3
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	10	0.3
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	2	0.3
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	2	0.3
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	10	0.3
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	10	0.3
(2,468)	1:19:B:LEU:HD23	1:35:A:LEU:HB2	10	0.3
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	1	0.3
(2,119)	1:47:A:GLU:HG2	1:27:A:LEU:HD21	2	0.3
(2,29)	1:53:A:LYS:HA	1:56:A:GLN:HB3	3	0.3
(2,20)	1:5:B:PRO:HA	1:4:B:ARG:HG3	5	0.3
(2,19)	1:5:A:PRO:HA	1:4:A:ARG:HG3	5	0.3
(2,12)	1:36:B:SER:HB3	1:45:B:GLN:HB2	9	0.3
(2,10)	1:16:B:ALA:HB3	1:15:A:LYS:HD3	1	0.3
(3,172)	1:17:B:LEU:H	1:14:B:LYS:HG3	3	0.29
(3,56)	1:57:B:ILE:HB	1:58:B:GLY:HA2	9	0.29
(3,41)	1:61:A:HIS:HA	1:60:A:SER:HG	9	0.29
(2,2246)	1:66:B:LYS:H	1:64:B:PHE:H	7	0.29
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD13	9	0.29
(2,2148)	1:15:B:LYS:H	1:14:B:LYS:HB3	8	0.29
(2,2147)	1:15:A:LYS:H	1:14:A:LYS:HB3	8	0.29
(2,2030)	1:32:B:ARG:H	1:32:B:ARG:HD3	4	0.29
(2,2005)	1:64:A:PHE:H	1:63:A:GLN:H	6	0.29
(2,1914)	1:59:B:TRP:H	1:57:B:ILE:HG23	7	0.29
(2,1890)	1:49:B:TRP:H	1:48:B:ARG:HG3	10	0.29
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	6	0.29
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	6	0.29
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	10	0.29
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	10	0.29
(2,1701)	1:66:A:LYS:H	1:66:A:LYS:HE2	5	0.29
(2,1696)	1:7:B:THR:HB	1:45:B:GLN:HB2	3	0.29
(2,1630)	1:41:B:LEU:HD12	1:9:B:PHE:HB2	3	0.29
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	9	0.29
(2,1387)	1:46:A:ILE:HD13	1:45:A:GLN:HG3	5	0.29
(2,1245)	1:20:A:ALA:HB3	1:50:A:PHE:HE1	10	0.29
(2,1228)	1:17:B:LEU:HD23	1:49:B:TRP:HE1	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1210)	1:49:B:TRP:HB3	1:17:B:LEU:HD13	10	0.29
(2,1207)	1:17:A:LEU:HD21	1:18:A:ASP:H	4	0.29
(2,1202)	1:17:B:LEU:HD22	1:46:B:ILE:HG12	10	0.29
(2,1190)	1:16:B:ALA:HB1	1:17:B:LEU:HA	3	0.29
(2,1166)	1:46:B:ILE:HD13	1:36:B:SER:H	10	0.29
(2,1060)	1:27:B:LEU:HD22	1:50:B:PHE:HB2	5	0.29
(2,1054)	1:12:B:GLU:HB3	1:12:B:GLU:HG3	9	0.29
(2,1035)	1:41:A:LEU:HB3	1:41:A:LEU:HD21	10	0.29
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	7	0.29
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	4	0.29
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	7	0.29
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	8	0.29
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	8	0.29
(2,828)	1:62:B:PRO:HD3	1:62:B:PRO:HB3	3	0.29
(2,827)	1:62:A:PRO:HD3	1:62:A:PRO:HB3	3	0.29
(2,755)	1:43:A:GLU:HA	1:36:A:SER:HB2	10	0.29
(2,484)	1:50:B:PHE:HD2	1:27:B:LEU:HD11	10	0.29
(2,483)	1:50:A:PHE:HD2	1:27:A:LEU:HD11	10	0.29
(2,467)	1:19:A:LEU:HD23	1:35:B:LEU:HB2	10	0.29
(2,444)	1:16:B:ALA:HB3	1:16:A:ALA:H	6	0.29
(2,374)	1:56:B:GLN:H	1:57:B:ILE:HG13	8	0.29
(2,373)	1:56:A:GLN:H	1:57:A:ILE:HG13	8	0.29
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	10	0.29
(2,258)	1:54:B:GLU:HG2	1:59:B:TRP:HB2	5	0.29
(2,186)	1:17:B:LEU:HD22	1:50:B:PHE:HA	1	0.29
(2,185)	1:17:A:LEU:HD22	1:50:A:PHE:HA	4	0.29
(2,162)	1:39:B:LEU:HG	1:13:B:GLN:H	9	0.29
(2,150)	1:33:B:ARG:HG3	1:34:B:TYR:HA	5	0.29
(2,124)	1:15:B:LYS:HB3	1:15:B:LYS:HE3	3	0.29
(2,124)	1:14:B:LYS:HB2	1:14:B:LYS:HE3	8	0.29
(2,123)	1:14:A:LYS:HB2	1:14:A:LYS:HE3	8	0.29
(2,93)	1:32:A:ARG:HD3	1:45:A:GLN:H	9	0.29
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	4	0.29
(1,62)	1:56:B:GLN:H	1:52:B:ARG:O	3	0.29
(3,178)	1:49:B:TRP:H	1:45:B:GLN:H	4	0.28
(3,171)	1:17:A:LEU:H	1:14:A:LYS:HG3	3	0.28
(3,171)	1:17:A:LEU:H	1:14:A:LYS:HG3	10	0.28
(3,42)	1:61:B:HIS:HA	1:60:B:SER:HG	5	0.28
(3,41)	1:61:A:HIS:HA	1:60:A:SER:HG	5	0.28
(3,4)	1:12:B:GLU:HG3	1:12:A:GLU:HB2	5	0.28
(3,3)	1:12:A:GLU:HG3	1:12:B:GLU:HB2	5	0.28
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	9	0.28
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	2	0.28
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	2	0.28
(2,2224)	1:57:B:ILE:HG12	1:58:B:GLY:H	1	0.28
(2,2223)	1:57:A:ILE:HG12	1:58:A:GLY:H	1	0.28
(2,2130)	1:33:B:ARG:H	1:30:B:GLU:HA	10	0.28
(2,2074)	1:55:B:GLN:H	1:53:B:LYS:HA	10	0.28
(2,2073)	1:55:A:GLN:H	1:53:A:LYS:HA	10	0.28
(2,2070)	1:54:B:GLU:HB3	1:55:B:GLN:H	1	0.28
(2,2069)	1:54:A:GLU:HB3	1:55:A:GLN:H	1	0.28
(2,1913)	1:59:A:TRP:H	1:57:A:ILE:HG23	7	0.28
(2,1890)	1:49:B:TRP:H	1:48:B:ARG:HG3	7	0.28
(2,1889)	1:49:A:TRP:H	1:48:A:ARG:HG3	7	0.28
(2,1889)	1:49:A:TRP:H	1:48:A:ARG:HG3	10	0.28
(2,1702)	1:66:B:LYS:H	1:66:B:LYS:HE2	5	0.28
(2,1695)	1:7:A:THR:HB	1:45:A:GLN:HB2	3	0.28
(2,1630)	1:41:B:LEU:HD11	1:9:B:PHE:HB2	10	0.28
(2,1412)	1:46:B:ILE:HG22	1:50:B:PHE:HD2	6	0.28
(2,1354)	1:42:B:ASN:HB3	1:43:B:GLU:HA	9	0.28
(2,1353)	1:42:A:ASN:HB3	1:43:A:GLU:HA	9	0.28
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	1	0.28
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	1	0.28
(2,1201)	1:17:A:LEU:HD22	1:46:A:ILE:HG12	3	0.28
(2,1201)	1:17:A:LEU:HD22	1:46:A:ILE:HG12	10	0.28
(2,1189)	1:16:A:ALA:HB1	1:17:A:LEU:HA	3	0.28
(2,1126)	1:16:B:ALA:HB2	1:17:B:LEU:H	9	0.28
(2,1084)	1:15:B:LYS:HG3	1:15:B:LYS:HB3	2	0.28
(2,1084)	1:15:B:LYS:HG3	1:15:B:LYS:HB3	5	0.28
(2,1084)	1:15:B:LYS:HG3	1:15:B:LYS:HB3	8	0.28
(2,1084)	1:15:B:LYS:HG3	1:15:B:LYS:HB3	9	0.28
(2,1083)	1:15:A:LYS:HG3	1:15:A:LYS:HB3	2	0.28
(2,1083)	1:15:A:LYS:HG3	1:15:A:LYS:HB3	5	0.28
(2,1083)	1:15:A:LYS:HG3	1:15:A:LYS:HB3	8	0.28
(2,1083)	1:15:A:LYS:HG3	1:15:A:LYS:HB3	9	0.28
(2,1054)	1:12:B:GLU:HB3	1:12:B:GLU:HG3	6	0.28
(2,1053)	1:12:A:GLU:HB3	1:12:A:GLU:HG3	6	0.28
(2,961)	1:45:A:GLN:HG2	1:45:A:GLN:HE22	2	0.28
(2,714)	1:3:B:LYS:HA	1:4:B:ARG:H	10	0.28
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	4	0.28
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	4	0.28
(2,530)	1:50:B:PHE:HA	1:53:B:LYS:HB2	7	0.28
(2,528)	1:57:B:ILE:HA	1:57:B:ILE:HG22	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,527)	1:57:A:ILE:HA	1:57:A:ILE:HG22	7	0.28
(2,466)	1:19:B:LEU:HD21	1:19:A:LEU:HD21	10	0.28
(2,465)	1:19:A:LEU:HD21	1:19:B:LEU:HD21	10	0.28
(2,450)	1:9:B:PHE:HD1	1:10:B:SER:H	3	0.28
(2,449)	1:9:A:PHE:HD1	1:10:A:SER:H	3	0.28
(2,443)	1:16:A:ALA:HB3	1:16:B:ALA:H	6	0.28
(2,378)	1:34:B:TYR:HD1	1:34:B:TYR:H	3	0.28
(2,377)	1:34:A:TYR:HD1	1:34:A:TYR:H	3	0.28
(2,361)	1:55:A:GLN:HB2	1:58:A:GLY:H	5	0.28
(2,257)	1:54:A:GLU:HG2	1:59:A:TRP:HB2	5	0.28
(2,109)	1:3:A:LYS:HE3	1:4:A:ARG:HA	10	0.28
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	2	0.28
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	8	0.28
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	2	0.28
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	8	0.28
(2,14)	1:36:B:SER:HB2	1:45:B:GLN:HB2	4	0.28
(2,11)	1:36:A:SER:HB3	1:45:A:GLN:HB2	9	0.28
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	3	0.28
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	3	0.28
(1,20)	1:56:A:GLN:H	1:52:A:ARG:O	3	0.28
(1,20)	1:56:A:GLN:H	1:52:A:ARG:O	6	0.28
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	8	0.27
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	8	0.27
(3,172)	1:17:B:LEU:H	1:14:B:LYS:HG3	10	0.27
(3,121)	1:14:A:LYS:HE3	1:49:A:TRP:HB2	10	0.27
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	1	0.27
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	1	0.27
(3,64)	1:8:B:GLU:HG3	1:45:B:GLN:HE22	10	0.27
(3,55)	1:57:A:ILE:HB	1:58:A:GLY:HA2	9	0.27
(3,42)	1:61:B:HIS:HA	1:60:B:SER:HG	9	0.27
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	3	0.27
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	3	0.27
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	9	0.27
(2,2306)	1:58:B:GLY:H	1:60:B:SER:HG	9	0.27
(2,2305)	1:58:A:GLY:H	1:60:A:SER:HG	9	0.27
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	10	0.27
(2,1926)	1:6:B:ARG:H	1:5:B:PRO:HB2	4	0.27
(2,1850)	1:52:B:ARG:HB3	1:53:B:LYS:H	10	0.27
(2,1849)	1:52:A:ARG:HB3	1:53:A:LYS:H	10	0.27
(2,1695)	1:7:A:THR:HB	1:45:A:GLN:HB2	7	0.27
(2,1629)	1:41:A:LEU:HD11	1:9:A:PHE:HB2	10	0.27
(2,1411)	1:46:A:ILE:HG22	1:50:A:PHE:HD2	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1336)	1:27:B:LEU:HD23	1:47:B:GLU:H	5	0.27
(2,1190)	1:16:B:ALA:HB2	1:17:B:LEU:HA	8	0.27
(2,1189)	1:16:A:ALA:HB3	1:17:A:LEU:HA	7	0.27
(2,1189)	1:16:A:ALA:HB2	1:17:A:LEU:HA	8	0.27
(2,962)	1:45:B:GLN:HG2	1:45:B:GLN:HE22	2	0.27
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	9	0.27
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	9	0.27
(2,713)	1:3:A:LYS:HA	1:4:A:ARG:H	10	0.27
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG22	5	0.27
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG22	5	0.27
(2,693)	1:8:A:GLU:HA	1:7:A:THR:HG23	9	0.27
(2,615)	1:15:A:LYS:HA	1:18:A:ASP:HB2	1	0.27
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	7	0.27
(2,600)	1:50:B:PHE:HA	1:53:B:LYS:HB3	8	0.27
(2,599)	1:50:A:PHE:HA	1:53:A:LYS:HB3	8	0.27
(2,529)	1:50:A:PHE:HA	1:53:A:LYS:HB2	7	0.27
(2,450)	1:9:B:PHE:HD1	1:10:B:SER:H	5	0.27
(2,442)	1:16:B:ALA:HB1	1:20:A:ALA:H	7	0.27
(2,440)	1:20:B:ALA:HB2	1:20:A:ALA:HB2	8	0.27
(2,439)	1:20:A:ALA:HB2	1:20:B:ALA:HB2	8	0.27
(2,365)	1:14:A:LYS:H	1:17:A:LEU:HB2	8	0.27
(2,362)	1:55:B:GLN:HB2	1:58:B:GLY:H	5	0.27
(2,362)	1:55:B:GLN:HB3	1:58:B:GLY:H	6	0.27
(2,200)	1:20:B:ALA:HB3	1:17:B:LEU:HB3	8	0.27
(2,199)	1:20:A:ALA:HB3	1:17:A:LEU:HB3	8	0.27
(2,185)	1:17:A:LEU:HD22	1:50:A:PHE:HA	1	0.27
(2,110)	1:3:B:LYS:HE3	1:4:B:ARG:HA	10	0.27
(2,87)	1:48:A:ARG:HD3	1:45:A:GLN:HE21	3	0.27
(2,86)	1:6:B:ARG:HD3	1:4:B:ARG:HA	1	0.27
(2,85)	1:6:A:ARG:HD3	1:4:A:ARG:HA	1	0.27
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	2	0.27
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	3	0.27
(2,13)	1:36:A:SER:HB2	1:32:A:ARG:HB2	7	0.27
(2,11)	1:36:A:SER:HB2	1:32:A:ARG:HB2	7	0.27
(1,84)	1:54:B:GLU:N	1:50:B:PHE:O	4	0.27
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	9	0.27
(3,206)	1:57:B:ILE:H	1:54:B:GLU:HB2	5	0.26
(3,205)	1:57:A:ILE:H	1:54:A:GLU:HB2	5	0.26
(3,202)	1:54:B:GLU:H	1:63:B:GLN:HB2	6	0.26
(3,182)	1:64:B:PHE:H	1:62:B:PRO:HB3	6	0.26
(3,181)	1:64:A:PHE:H	1:62:A:PRO:HB3	6	0.26
(3,157)	1:16:A:ALA:H	1:17:A:LEU:HG	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	2	0.26
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	2	0.26
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	7	0.26
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	4	0.26
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	4	0.26
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	7	0.26
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	5	0.26
(2,2166)	1:33:B:ARG:H	1:33:B:ARG:HG3	4	0.26
(2,2083)	1:14:A:LYS:H	1:9:A:PHE:HB3	4	0.26
(2,1925)	1:6:A:ARG:H	1:5:A:PRO:HB2	4	0.26
(2,1852)	1:53:B:LYS:H	1:52:B:ARG:HG3	4	0.26
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	8	0.26
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	8	0.26
(2,1696)	1:7:B:THR:HB	1:45:B:GLN:HB2	7	0.26
(2,1602)	1:53:B:LYS:HG3	1:21:B:PHE:HZ	3	0.26
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD13	9	0.26
(2,1202)	1:17:B:LEU:HD21	1:46:B:ILE:HG12	5	0.26
(2,1136)	1:13:B:GLN:HA	1:16:B:ALA:HB1	1	0.26
(2,1066)	1:27:B:LEU:HB2	1:27:B:LEU:HD23	4	0.26
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	3	0.26
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	3	0.26
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	6	0.26
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	6	0.26
(2,800)	1:42:B:ASN:HA	1:43:B:GLU:HG3	8	0.26
(2,799)	1:42:A:ASN:HA	1:43:A:GLU:HG3	8	0.26
(2,790)	1:16:B:ALA:HA	1:15:B:LYS:HB3	5	0.26
(2,694)	1:8:B:GLU:HA	1:7:B:THR:HG23	9	0.26
(2,674)	1:8:B:GLU:HA	1:41:B:LEU:HB2	9	0.26
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	7	0.26
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	7	0.26
(2,616)	1:15:B:LYS:HA	1:18:B:ASP:HB2	1	0.26
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	9	0.26
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	9	0.26
(2,449)	1:9:A:PHE:HD1	1:10:A:SER:H	5	0.26
(2,366)	1:14:B:LYS:H	1:17:B:LEU:HB2	3	0.26
(2,366)	1:14:B:LYS:H	1:17:B:LEU:HB2	8	0.26
(2,361)	1:55:A:GLN:HB3	1:58:A:GLY:H	6	0.26
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HE2	1	0.26
(2,169)	1:12:A:GLU:HA	1:15:A:LYS:H	5	0.26
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	10	0.26
(2,140)	1:55:B:GLN:HB2	1:56:B:GLN:H	3	0.26
(2,139)	1:55:A:GLN:HB2	1:56:A:GLN:H	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:33:B:ARG:HB2	1:33:B:ARG:H	1	0.26
(2,129)	1:33:A:ARG:HB2	1:33:A:ARG:H	1	0.26
(2,88)	1:48:B:ARG:HD3	1:45:B:GLN:HE21	3	0.26
(2,50)	1:49:B:TRP:HA	1:9:B:PHE:HZ	4	0.26
(2,33)	1:28:A:THR:HA	1:47:A:GLU:HG2	2	0.26
(2,14)	1:36:B:SER:HB2	1:32:B:ARG:HB2	7	0.26
(2,12)	1:36:B:SER:HB2	1:32:B:ARG:HB2	7	0.26
(1,74)	1:33:B:ARG:N	1:29:B:PRO:O	10	0.26
(1,62)	1:56:B:GLN:H	1:52:B:ARG:O	6	0.26
(1,42)	1:54:A:GLU:N	1:50:A:PHE:O	4	0.26
(3,201)	1:54:A:GLU:H	1:63:A:GLN:HB2	6	0.25
(3,168)	1:59:B:TRP:H	1:61:B:HIS:HB3	5	0.25
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	7	0.25
(3,6)	1:12:B:GLU:HG3	1:12:A:GLU:HA	10	0.25
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	1	0.25
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	7	0.25
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	1	0.25
(2,2318)	1:4:B:ARG:H	1:4:B:ARG:HD3	4	0.25
(2,2317)	1:4:A:ARG:H	1:4:A:ARG:HD3	4	0.25
(2,2165)	1:33:A:ARG:H	1:33:A:ARG:HG3	4	0.25
(2,2119)	1:28:A:THR:H	1:32:A:ARG:HE	5	0.25
(2,2084)	1:14:B:LYS:H	1:9:B:PHE:HB3	4	0.25
(2,2005)	1:64:A:PHE:H	1:63:A:GLN:H	9	0.25
(2,1927)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.25
(2,1890)	1:49:B:TRP:H	1:48:B:ARG:HG3	1	0.25
(2,1889)	1:49:A:TRP:H	1:48:A:ARG:HG3	1	0.25
(2,1851)	1:53:A:LYS:H	1:52:A:ARG:HG3	4	0.25
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	7	0.25
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	7	0.25
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	5	0.25
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	1	0.25
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	1	0.25
(2,1774)	1:38:B:ARG:H	1:39:B:LEU:HD13	2	0.25
(2,1773)	1:38:A:ARG:H	1:39:A:LEU:HD13	2	0.25
(2,1665)	1:57:A:ILE:HG12	1:60:A:SER:H	6	0.25
(2,1579)	1:27:A:LEU:HD12	1:47:A:GLU:HG3	5	0.25
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	9	0.25
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	3	0.25
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	5	0.25
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	8	0.25
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	3	0.25
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	8	0.25
(2,1465)	1:54:A:GLU:HB2	1:54:A:GLU:H	9	0.25
(2,1392)	1:46:B:ILE:HD13	1:9:B:PHE:HB3	7	0.25
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD13	9	0.25
(2,1209)	1:49:A:TRP:HB3	1:17:A:LEU:HD13	10	0.25
(2,1202)	1:17:B:LEU:HD22	1:46:B:ILE:HG12	9	0.25
(2,1190)	1:16:B:ALA:HB3	1:17:B:LEU:HA	7	0.25
(2,1160)	1:36:B:SER:HA	1:46:B:ILE:HD11	5	0.25
(2,1135)	1:13:A:GLN:HA	1:16:A:ALA:HB1	1	0.25
(2,1065)	1:27:A:LEU:HB2	1:27:A:LEU:HD23	4	0.25
(2,1064)	1:27:B:LEU:HD22	1:43:B:GLU:HB3	9	0.25
(2,1063)	1:27:A:LEU:HD22	1:43:A:GLU:HB3	9	0.25
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	1	0.25
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	1	0.25
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	1	0.25
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	1	0.25
(2,950)	1:54:B:GLU:HG2	1:54:B:GLU:H	6	0.25
(2,949)	1:54:A:GLU:HG2	1:54:A:GLU:H	6	0.25
(2,789)	1:16:A:ALA:HA	1:15:A:LYS:HB3	5	0.25
(2,728)	1:36:B:SER:HB3	1:36:B:SER:H	1	0.25
(2,728)	1:36:B:SER:HB3	1:36:B:SER:H	7	0.25
(2,727)	1:36:A:SER:HB3	1:36:A:SER:H	1	0.25
(2,727)	1:36:A:SER:HB3	1:36:A:SER:H	7	0.25
(2,704)	1:64:B:PHE:HA	1:64:B:PHE:HD2	8	0.25
(2,703)	1:64:A:PHE:HA	1:64:A:PHE:HD2	8	0.25
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	10	0.25
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	1	0.25
(2,489)	1:50:A:PHE:HE1	1:27:A:LEU:HD13	1	0.25
(2,449)	1:9:A:PHE:HD1	1:10:A:SER:H	10	0.25
(2,303)	1:59:A:TRP:H	1:62:A:PRO:HD3	2	0.25
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HE2	1	0.25
(2,170)	1:12:B:GLU:HA	1:15:B:LYS:H	5	0.25
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	9	0.25
(2,123)	1:15:A:LYS:HB3	1:15:A:LYS:HE3	3	0.25
(2,108)	1:9:B:PHE:HB2	1:4:B:ARG:HB2	8	0.25
(2,102)	1:19:B:LEU:HB3	1:16:B:ALA:HA	9	0.25
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	10	0.25
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	10	0.25
(3,117)	1:39:A:LEU:HG	1:9:A:PHE:H	9	0.24
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	3	0.24
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	3	0.24
(3,81)	1:39:A:LEU:HG	1:36:A:SER:HB3	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2430)	1:57:B:ILE:H	1:56:B:GLN:HB3	8	0.24
(2,2429)	1:57:A:ILE:H	1:56:A:GLN:HB3	8	0.24
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	9	0.24
(2,2382)	1:32:B:ARG:H	1:34:B:TYR:HD1	2	0.24
(2,2381)	1:32:A:ARG:H	1:34:A:TYR:HD1	2	0.24
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	9	0.24
(2,2129)	1:33:A:ARG:H	1:30:A:GLU:HA	10	0.24
(2,2106)	1:54:B:GLU:HB3	1:54:B:GLU:H	5	0.24
(2,2106)	1:54:B:GLU:HB3	1:54:B:GLU:H	6	0.24
(2,2106)	1:54:B:GLU:HB3	1:54:B:GLU:H	8	0.24
(2,2105)	1:54:A:GLU:HB3	1:54:A:GLU:H	5	0.24
(2,2105)	1:54:A:GLU:HB3	1:54:A:GLU:H	6	0.24
(2,2105)	1:54:A:GLU:HB3	1:54:A:GLU:H	8	0.24
(2,2098)	1:53:B:LYS:HB2	1:54:B:GLU:H	6	0.24
(2,2097)	1:53:A:LYS:HB2	1:54:A:GLU:H	6	0.24
(2,1960)	1:34:B:TYR:H	1:33:B:ARG:HG3	3	0.24
(2,1890)	1:49:B:TRP:H	1:48:B:ARG:HG3	4	0.24
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	5	0.24
(2,1607)	1:16:A:ALA:HB1	1:35:A:LEU:HD23	7	0.24
(2,1601)	1:53:A:LYS:HG3	1:21:A:PHE:HZ	3	0.24
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD21	1	0.24
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	1	0.24
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	2	0.24
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	4	0.24
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	7	0.24
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	9	0.24
(2,1480)	1:59:B:TRP:HA	1:59:B:TRP:HB3	10	0.24
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	1	0.24
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	2	0.24
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	4	0.24
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	7	0.24
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	9	0.24
(2,1479)	1:59:A:TRP:HA	1:59:A:TRP:HB3	10	0.24
(2,1466)	1:54:B:GLU:HB2	1:54:B:GLU:H	9	0.24
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	9	0.24
(2,1245)	1:20:A:ALA:HB1	1:50:A:PHE:HE1	3	0.24
(2,1244)	1:20:B:ALA:HB2	1:35:B:LEU:HD12	1	0.24
(2,1201)	1:17:A:LEU:HD22	1:46:A:ILE:HG12	9	0.24
(2,1084)	1:15:B:LYS:HG3	1:15:B:LYS:HB3	1	0.24
(2,1083)	1:15:A:LYS:HG3	1:15:A:LYS:HB3	1	0.24
(2,1023)	1:12:A:GLU:HB2	1:12:A:GLU:HA	10	0.24
(2,948)	1:54:B:GLU:HG2	1:21:B:PHE:HE1	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,944)	1:54:B:GLU:HG2	1:21:B:PHE:HZ	8	0.24
(2,943)	1:54:A:GLU:HG2	1:21:A:PHE:HZ	8	0.24
(2,926)	1:36:B:SER:HB2	1:43:B:GLU:HG3	1	0.24
(2,728)	1:36:B:SER:HB3	1:36:B:SER:H	6	0.24
(2,727)	1:36:A:SER:HB3	1:36:A:SER:H	6	0.24
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	10	0.24
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	1	0.24
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	3	0.24
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	3	0.24
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	7	0.24
(2,576)	1:14:B:LYS:HA	1:17:B:LEU:HD21	6	0.24
(2,548)	1:57:B:ILE:HA	1:57:B:ILE:HG13	8	0.24
(2,547)	1:57:A:ILE:HA	1:57:A:ILE:HG13	8	0.24
(2,490)	1:50:B:PHE:HE1	1:27:B:LEU:HD13	1	0.24
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	5	0.24
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	5	0.24
(2,304)	1:59:B:TRP:H	1:62:B:PRO:HD3	2	0.24
(2,260)	1:54:B:GLU:HG3	1:59:B:TRP:HB2	2	0.24
(2,107)	1:9:A:PHE:HB2	1:4:A:ARG:HB2	8	0.24
(2,106)	1:9:B:PHE:HB3	1:4:B:ARG:HB2	8	0.24
(2,105)	1:9:A:PHE:HB3	1:4:A:ARG:HB2	8	0.24
(2,34)	1:28:B:THR:HA	1:47:B:GLU:HG2	3	0.24
(2,19)	1:5:A:PRO:HA	1:4:A:ARG:HG3	4	0.24
(2,12)	1:36:B:SER:HB3	1:45:B:GLN:HB2	2	0.24
(1,81)	1:20:B:ALA:N	1:16:B:ALA:O	9	0.24
(1,1)	1:15:A:LYS:H	1:11:A:GLU:O	3	0.24
(3,221)	1:54:A:GLU:H	1:52:A:ARG:HE	2	0.23
(3,198)	1:61:B:HIS:H	1:63:B:GLN:H	3	0.23
(3,177)	1:49:A:TRP:H	1:45:A:GLN:H	4	0.23
(3,172)	1:17:B:LEU:H	1:14:B:LYS:HG3	8	0.23
(3,171)	1:17:A:LEU:H	1:14:A:LYS:HG3	8	0.23
(3,167)	1:59:A:TRP:H	1:61:A:HIS:HB3	5	0.23
(3,122)	1:14:B:LYS:HE3	1:49:B:TRP:HB2	10	0.23
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	5	0.23
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	5	0.23
(3,82)	1:39:B:LEU:HG	1:36:B:SER:HB3	2	0.23
(3,77)	1:37:A:GLN:HB3	1:34:A:TYR:HB2	7	0.23
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	1	0.23
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	9	0.23
(3,5)	1:12:A:GLU:HG3	1:12:B:GLU:HA	10	0.23
(3,3)	1:12:A:GLU:HG3	1:12:B:GLU:HB2	1	0.23
(2,2437)	1:53:A:LYS:H	1:21:A:PHE:HE1	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	9	0.23
(2,2326)	1:7:B:THR:H	1:4:B:ARG:HD3	9	0.23
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	5	0.23
(2,2278)	1:9:B:PHE:H	1:41:B:LEU:HA	9	0.23
(2,2198)	1:60:B:SER:H	1:58:B:GLY:HA2	8	0.23
(2,2197)	1:60:A:SER:H	1:58:A:GLY:HA2	8	0.23
(2,1928)	1:6:B:ARG:H	1:6:B:ARG:HG3	10	0.23
(2,1890)	1:49:B:TRP:H	1:48:B:ARG:HG3	3	0.23
(2,1889)	1:49:A:TRP:H	1:48:A:ARG:HG3	3	0.23
(2,1801)	1:65:A:GLU:H	1:64:A:PHE:HD1	7	0.23
(2,1666)	1:57:B:ILE:HG12	1:60:B:SER:H	6	0.23
(2,1552)	1:27:B:LEU:HB3	1:50:B:PHE:HB3	6	0.23
(2,1551)	1:27:A:LEU:HB3	1:50:A:PHE:HB3	6	0.23
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD21	1	0.23
(2,1515)	1:9:A:PHE:HA	1:41:A:LEU:HD21	2	0.23
(2,1512)	1:39:B:LEU:HD21	1:39:B:LEU:HA	1	0.23
(2,1511)	1:39:A:LEU:HD21	1:39:A:LEU:HA	1	0.23
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	9	0.23
(2,1243)	1:20:A:ALA:HB2	1:35:A:LEU:HD12	1	0.23
(2,1061)	1:27:A:LEU:HD21	1:50:A:PHE:HB3	2	0.23
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	10	0.23
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	10	0.23
(2,925)	1:36:A:SER:HB2	1:43:A:GLU:HG3	1	0.23
(2,818)	1:62:B:PRO:HD2	1:60:B:SER:HG	1	0.23
(2,817)	1:62:A:PRO:HD2	1:60:A:SER:HG	1	0.23
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	4	0.23
(2,704)	1:64:B:PHE:HA	1:64:B:PHE:HD2	10	0.23
(2,703)	1:64:A:PHE:HA	1:64:A:PHE:HD2	10	0.23
(2,674)	1:8:B:GLU:HA	1:41:B:LEU:HB2	6	0.23
(2,673)	1:8:A:GLU:HA	1:41:A:LEU:HB2	6	0.23
(2,529)	1:50:A:PHE:HA	1:53:A:LYS:HB2	5	0.23
(2,472)	1:19:B:LEU:HD21	1:19:A:LEU:HG	4	0.23
(2,450)	1:9:B:PHE:HD1	1:10:B:SER:H	10	0.23
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	2	0.23
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	10	0.23
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	1	0.23
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	1	0.23
(2,15)	1:36:A:SER:HB3	1:46:A:ILE:HD13	4	0.23
(2,11)	1:36:A:SER:HB3	1:45:A:GLN:HB2	2	0.23
(2,9)	1:16:A:ALA:HB1	1:15:B:LYS:HD3	4	0.23
(1,74)	1:33:B:ARG:N	1:29:B:PRO:O	7	0.23
(3,231)	1:60:A:SER:H	1:57:A:ILE:HA	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,222)	1:54:B:GLU:H	1:52:B:ARG:HE	8	0.22
(3,221)	1:54:A:GLU:H	1:52:A:ARG:HE	8	0.22
(3,197)	1:61:A:HIS:H	1:63:A:GLN:H	3	0.22
(3,195)	1:32:A:ARG:HA	1:47:A:GLU:H	7	0.22
(3,120)	1:9:B:PHE:HB3	1:45:B:GLN:HA	2	0.22
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	8	0.22
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	8	0.22
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	1	0.22
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	4	0.22
(3,4)	1:12:B:GLU:HG3	1:12:A:GLU:HB2	1	0.22
(2,2435)	1:27:A:LEU:HD13	1:47:A:GLU:H	2	0.22
(2,2422)	1:52:B:ARG:H	1:51:B:ARG:HB2	6	0.22
(2,2421)	1:52:A:ARG:H	1:51:A:ARG:HB2	6	0.22
(2,2325)	1:7:A:THR:H	1:4:A:ARG:HD3	9	0.22
(2,2294)	1:60:B:SER:H	1:57:B:ILE:HG21	4	0.22
(2,2293)	1:60:A:SER:H	1:57:A:ILE:HG21	4	0.22
(2,2277)	1:9:A:PHE:H	1:41:A:LEU:HA	9	0.22
(2,2174)	1:17:B:LEU:HG	1:17:B:LEU:H	5	0.22
(2,2093)	1:54:A:GLU:H	1:53:A:LYS:HG3	2	0.22
(2,1901)	1:59:A:TRP:H	1:62:A:PRO:HD2	2	0.22
(2,1890)	1:49:B:TRP:H	1:48:B:ARG:HG3	6	0.22
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	2	0.22
(2,1798)	1:65:B:GLU:H	1:66:B:LYS:HB3	10	0.22
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	2	0.22
(2,1797)	1:65:A:GLU:H	1:66:A:LYS:HB3	10	0.22
(2,1651)	1:28:A:THR:HB	1:31:A:TRP:HB3	4	0.22
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE1	7	0.22
(2,1516)	1:9:B:PHE:HA	1:41:B:LEU:HD21	2	0.22
(2,1484)	1:59:B:TRP:HB3	1:57:B:ILE:HG21	9	0.22
(2,1391)	1:46:A:ILE:HD13	1:9:A:PHE:HB3	7	0.22
(2,1204)	1:17:B:LEU:HA	1:17:B:LEU:HD22	4	0.22
(2,1202)	1:17:B:LEU:HD21	1:46:B:ILE:HG12	2	0.22
(2,1201)	1:17:A:LEU:HD21	1:46:A:ILE:HG12	2	0.22
(2,1084)	1:15:B:LYS:HG3	1:15:B:LYS:HB3	10	0.22
(2,1048)	1:57:B:ILE:HG13	1:57:B:ILE:H	9	0.22
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	8	0.22
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	4	0.22
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	7	0.22
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	8	0.22
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	8	0.22
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	3	0.22
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	4	0.22
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	1	0.22
(2,362)	1:55:B:GLN:HB3	1:58:B:GLY:H	4	0.22
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	2	0.22
(2,320)	1:9:B:PHE:H	1:45:B:GLN:HB2	2	0.22
(2,319)	1:9:A:PHE:H	1:45:A:GLN:HB2	2	0.22
(1,4)	1:18:A:ASP:H	1:14:A:LYS:O	4	0.22
(3,119)	1:9:A:PHE:HB3	1:45:A:GLN:HA	2	0.21
(3,118)	1:39:B:LEU:HG	1:9:B:PHE:H	8	0.21
(3,117)	1:39:A:LEU:HG	1:9:A:PHE:H	8	0.21
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	4	0.21
(3,102)	1:42:B:ASN:HB3	1:36:B:SER:HB2	2	0.21
(3,77)	1:37:A:GLN:HB3	1:34:A:TYR:HB2	1	0.21
(2,2436)	1:27:B:LEU:HD13	1:47:B:GLU:H	2	0.21
(2,2318)	1:4:B:ARG:H	1:4:B:ARG:HD3	7	0.21
(2,2317)	1:4:A:ARG:H	1:4:A:ARG:HD3	7	0.21
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD12	1	0.21
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD13	10	0.21
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD12	1	0.21
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	8	0.21
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	8	0.21
(2,2173)	1:17:A:LEU:HG	1:17:A:LEU:H	5	0.21
(2,1944)	1:61:B:HIS:HB3	1:61:B:HIS:H	2	0.21
(2,1943)	1:61:A:HIS:HB3	1:61:A:HIS:H	2	0.21
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	2	0.21
(2,1901)	1:59:A:TRP:H	1:62:A:PRO:HD2	10	0.21
(2,1889)	1:49:A:TRP:H	1:48:A:ARG:HG3	6	0.21
(2,1762)	1:36:B:SER:H	1:36:B:SER:HG	1	0.21
(2,1761)	1:36:A:SER:H	1:36:A:SER:HG	1	0.21
(2,1686)	1:9:B:PHE:HA	1:45:B:GLN:HB2	10	0.21
(2,1610)	1:35:B:LEU:HB2	1:39:B:LEU:HD22	10	0.21
(2,1512)	1:39:B:LEU:HD22	1:39:B:LEU:HA	7	0.21
(2,1511)	1:39:A:LEU:HD22	1:39:A:LEU:HA	7	0.21
(2,1466)	1:54:B:GLU:HB2	1:54:B:GLU:H	10	0.21
(2,1465)	1:54:A:GLU:HB2	1:54:A:GLU:H	10	0.21
(2,1344)	1:41:B:LEU:HD12	1:17:B:LEU:HD23	1	0.21
(2,1343)	1:41:A:LEU:HD12	1:17:A:LEU:HD23	1	0.21
(2,1214)	1:50:B:PHE:HB3	1:27:B:LEU:HD13	9	0.21
(2,1213)	1:50:A:PHE:HB3	1:27:A:LEU:HD13	9	0.21
(2,1203)	1:17:A:LEU:HA	1:17:A:LEU:HD22	4	0.21
(2,1159)	1:36:A:SER:HA	1:46:A:ILE:HD11	5	0.21
(2,1088)	1:15:B:LYS:HG3	1:15:B:LYS:HE3	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1087)	1:15:A:LYS:HG3	1:15:A:LYS:HE3	5	0.21
(2,1083)	1:15:A:LYS:HG3	1:15:A:LYS:HB3	10	0.21
(2,1063)	1:27:A:LEU:HD21	1:43:A:GLU:HB3	10	0.21
(2,1062)	1:27:B:LEU:HD21	1:50:B:PHE:HB3	2	0.21
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	4	0.21
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	7	0.21
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	3	0.21
(2,906)	1:18:B:ASP:HB2	1:19:B:LEU:H	8	0.21
(2,905)	1:18:A:ASP:HB2	1:19:A:LEU:H	3	0.21
(2,905)	1:18:A:ASP:HB2	1:19:A:LEU:H	8	0.21
(2,815)	1:61:A:HIS:HA	1:62:A:PRO:HD2	4	0.21
(2,673)	1:8:A:GLU:HA	1:41:A:LEU:HB2	9	0.21
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	1	0.21
(2,544)	1:57:B:ILE:HA	1:57:B:ILE:HB	8	0.21
(2,543)	1:57:A:ILE:HA	1:57:A:ILE:HB	8	0.21
(2,354)	1:47:B:GLU:H	1:44:B:GLU:HG3	2	0.21
(2,353)	1:47:A:GLU:H	1:44:A:GLU:HG3	2	0.21
(2,286)	1:50:B:PHE:H	1:9:B:PHE:HE2	7	0.21
(2,274)	1:44:B:GLU:HA	1:48:B:ARG:HD3	4	0.21
(2,224)	1:45:B:GLN:HG3	1:41:B:LEU:HA	1	0.21
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	3	0.21
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	3	0.21
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	3	0.21
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	3	0.21
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	4	0.21
(1,42)	1:54:A:GLU:N	1:50:A:PHE:O	5	0.21
(1,32)	1:33:A:ARG:N	1:29:A:PRO:O	10	0.21
(3,232)	1:60:B:SER:H	1:57:B:ILE:HA	2	0.2
(3,177)	1:49:A:TRP:H	1:45:A:GLN:H	10	0.2
(3,121)	1:14:A:LYS:HE3	1:49:A:TRP:HB2	8	0.2
(3,104)	1:45:B:GLN:HB3	1:44:B:GLU:H	9	0.2
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	4	0.2
(3,101)	1:42:A:ASN:HB3	1:36:A:SER:HB2	2	0.2
(3,100)	1:59:B:TRP:HB3	1:54:B:GLU:HA	6	0.2
(3,95)	1:59:A:TRP:HB2	1:55:A:GLN:H	7	0.2
(3,78)	1:37:B:GLN:HB3	1:34:B:TYR:HB2	1	0.2
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	5	0.2
(2,2243)	1:65:A:GLU:H	1:66:A:LYS:H	7	0.2
(2,2154)	1:56:B:GLN:H	1:53:B:LYS:HA	2	0.2
(2,2149)	1:52:A:ARG:HB3	1:56:A:GLN:H	7	0.2
(2,2102)	1:9:B:PHE:H	1:45:B:GLN:HB3	1	0.2
(2,2094)	1:54:B:GLU:H	1:53:B:LYS:HG3	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2090)	1:28:B:THR:H	1:27:B:LEU:HD21	10	0.2
(2,2089)	1:28:A:THR:H	1:27:A:LEU:HD21	10	0.2
(2,1966)	1:13:B:GLN:HB3	1:13:B:GLN:H	4	0.2
(2,1965)	1:13:A:GLN:HB3	1:13:A:GLN:H	4	0.2
(2,1965)	1:13:A:GLN:HB3	1:13:A:GLN:H	6	0.2
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	10	0.2
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD13	7	0.2
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD13	7	0.2
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD22	2	0.2
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD22	2	0.2
(2,1511)	1:39:A:LEU:HD21	1:39:A:LEU:HA	9	0.2
(2,1466)	1:54:B:GLU:HB2	1:54:B:GLU:H	3	0.2
(2,1465)	1:54:A:GLU:HB2	1:54:A:GLU:H	3	0.2
(2,1340)	1:27:B:LEU:HD21	1:46:B:ILE:H	1	0.2
(2,1339)	1:27:A:LEU:HD21	1:46:A:ILE:H	1	0.2
(2,1249)	1:27:A:LEU:HA	1:32:A:ARG:H	7	0.2
(2,1210)	1:49:B:TRP:HB3	1:17:B:LEU:HD13	5	0.2
(2,1194)	1:16:B:ALA:HB3	1:13:B:GLN:HB3	2	0.2
(2,1193)	1:16:A:ALA:HB3	1:13:A:GLN:HB3	2	0.2
(2,816)	1:61:B:HIS:HA	1:62:B:PRO:HD2	4	0.2
(2,790)	1:16:B:ALA:HA	1:15:B:LYS:HB3	8	0.2
(2,789)	1:16:A:ALA:HA	1:15:A:LYS:HB3	8	0.2
(2,789)	1:16:A:ALA:HA	1:15:A:LYS:HB3	9	0.2
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	8	0.2
(2,755)	1:43:A:GLU:HA	1:36:A:SER:HB2	8	0.2
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	2	0.2
(2,583)	1:32:A:ARG:HA	1:27:A:LEU:HD13	3	0.2
(2,575)	1:14:A:LYS:HA	1:17:A:LEU:HD21	6	0.2
(2,530)	1:50:B:PHE:HA	1:53:B:LYS:HB2	5	0.2
(2,366)	1:14:B:LYS:H	1:39:B:LEU:HD12	6	0.2
(2,332)	1:14:B:LYS:H	1:12:B:GLU:HA	8	0.2
(2,331)	1:14:A:LYS:H	1:12:A:GLU:HA	8	0.2
(2,317)	1:59:A:TRP:HB2	1:55:A:GLN:H	7	0.2
(2,311)	1:17:A:LEU:H	1:14:A:LYS:HB3	3	0.2
(2,304)	1:59:B:TRP:H	1:60:B:SER:HB3	10	0.2
(2,303)	1:59:A:TRP:H	1:60:A:SER:HB3	10	0.2
(2,200)	1:20:B:ALA:HB2	1:17:B:LEU:HB3	2	0.2
(2,199)	1:20:A:ALA:HB2	1:17:A:LEU:HB3	2	0.2
(2,113)	1:57:A:ILE:HB	1:58:A:GLY:H	6	0.2
(2,88)	1:48:B:ARG:HD3	1:45:B:GLN:HE21	6	0.2
(2,87)	1:48:A:ARG:HD3	1:45:A:GLN:HE21	6	0.2
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	8	0.2
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	4	0.2
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	8	0.2
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	9	0.2
(2,71)	1:16:A:ALA:HA	1:19:B:LEU:HD22	9	0.2
(2,49)	1:49:A:TRP:HA	1:9:A:PHE:HZ	4	0.2
(2,13)	1:36:A:SER:HB2	1:45:A:GLN:HB2	4	0.2
(3,196)	1:32:B:ARG:HA	1:47:B:GLU:H	7	0.19
(3,122)	1:14:B:LYS:HE3	1:49:B:TRP:HB2	8	0.19
(3,103)	1:45:A:GLN:HB3	1:44:A:GLU:H	9	0.19
(3,102)	1:42:B:ASN:HB3	1:36:B:SER:HB2	6	0.19
(3,101)	1:42:A:ASN:HB3	1:36:A:SER:HB2	6	0.19
(3,99)	1:59:A:TRP:HB3	1:54:A:GLU:HA	6	0.19
(3,96)	1:59:B:TRP:HB2	1:55:B:GLN:H	7	0.19
(3,22)	1:3:B:LYS:HA	1:2:B:GLU:HG3	4	0.19
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	9	0.19
(2,2429)	1:57:A:ILE:H	1:56:A:GLN:HB3	6	0.19
(2,2395)	1:42:A:ASN:H	1:45:A:GLN:HE22	10	0.19
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD13	10	0.19
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	9	0.19
(2,2198)	1:60:B:SER:H	1:58:B:GLY:HA2	1	0.19
(2,2197)	1:60:A:SER:H	1:58:A:GLY:HA2	1	0.19
(2,2153)	1:56:A:GLN:H	1:53:A:LYS:HA	2	0.19
(2,2101)	1:9:A:PHE:H	1:45:A:GLN:HB3	1	0.19
(2,1966)	1:13:B:GLN:HB3	1:13:B:GLN:H	6	0.19
(2,1948)	1:61:B:HIS:H	1:60:B:SER:HG	7	0.19
(2,1935)	1:61:A:HIS:H	1:57:A:ILE:HG23	4	0.19
(2,1924)	1:63:B:GLN:HG2	1:63:B:GLN:H	9	0.19
(2,1889)	1:49:A:TRP:H	1:48:A:ARG:HG3	2	0.19
(2,1884)	1:63:B:GLN:H	1:61:B:HIS:HB3	3	0.19
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE1	7	0.19
(2,1512)	1:39:B:LEU:HD21	1:39:B:LEU:HA	9	0.19
(2,1466)	1:54:B:GLU:HB2	1:54:B:GLU:H	4	0.19
(2,1191)	1:16:A:ALA:HB1	1:14:A:LYS:HA	3	0.19
(2,1190)	1:16:B:ALA:HB1	1:17:B:LEU:HA	1	0.19
(2,1189)	1:16:A:ALA:HB1	1:17:A:LEU:HA	1	0.19
(2,1124)	1:20:B:ALA:HB2	1:21:B:PHE:H	4	0.19
(2,1064)	1:27:B:LEU:HD21	1:43:B:GLU:HB3	10	0.19
(2,958)	1:54:B:GLU:HG2	1:54:B:GLU:HA	7	0.19
(2,818)	1:62:B:PRO:HD2	1:60:B:SER:HG	2	0.19
(2,590)	1:47:B:GLU:HA	1:46:B:ILE:HB	1	0.19
(2,589)	1:47:A:GLU:HA	1:46:A:ILE:HB	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,449)	1:9:A:PHE:HD1	1:10:A:SER:H	1	0.19
(2,444)	1:16:B:ALA:HB3	1:16:A:ALA:H	8	0.19
(2,443)	1:16:A:ALA:HB3	1:16:B:ALA:H	8	0.19
(2,438)	1:20:B:ALA:HB3	1:20:A:ALA:H	3	0.19
(2,365)	1:14:A:LYS:H	1:39:A:LEU:HD12	6	0.19
(2,318)	1:59:B:TRP:HB2	1:55:B:GLN:H	7	0.19
(2,311)	1:17:A:LEU:H	1:14:A:LYS:HB3	1	0.19
(2,223)	1:45:A:GLN:HG3	1:41:A:LEU:HA	1	0.19
(2,150)	1:33:B:ARG:HG3	1:34:B:TYR:HA	1	0.19
(2,149)	1:33:A:ARG:HG3	1:34:A:TYR:HA	1	0.19
(2,114)	1:57:B:ILE:HB	1:58:B:GLY:H	6	0.19
(2,101)	1:19:A:LEU:HB3	1:16:B:ALA:HA	6	0.19
(2,100)	1:51:B:ARG:HD3	1:55:B:GLN:HG3	7	0.19
(2,99)	1:51:A:ARG:HD3	1:55:A:GLN:HG3	7	0.19
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	1	0.19
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	9	0.19
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	1	0.19
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	7	0.19
(2,20)	1:5:B:PRO:HA	1:6:B:ARG:HG3	6	0.19
(2,19)	1:5:A:PRO:HA	1:6:A:ARG:HG3	6	0.19
(1,84)	1:54:B:GLU:N	1:50:B:PHE:O	5	0.19
(1,41)	1:54:A:GLU:H	1:50:A:PHE:O	1	0.19
(3,178)	1:49:B:TRP:H	1:45:B:GLN:H	10	0.18
(3,56)	1:57:B:ILE:HB	1:58:B:GLY:HA2	3	0.18
(3,55)	1:57:A:ILE:HB	1:58:A:GLY:HA2	3	0.18
(2,2430)	1:57:B:ILE:H	1:56:B:GLN:HB3	6	0.18
(2,2420)	1:51:B:ARG:H	1:54:B:GLU:HG3	9	0.18
(2,2396)	1:42:B:ASN:H	1:45:B:GLN:HE22	10	0.18
(2,2301)	1:36:A:SER:H	1:34:A:TYR:HB2	1	0.18
(2,2260)	1:6:B:ARG:H	1:6:B:ARG:HD3	6	0.18
(2,2259)	1:6:A:ARG:H	1:6:A:ARG:HD3	6	0.18
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	9	0.18
(2,2090)	1:28:B:THR:H	1:27:B:LEU:HD21	7	0.18
(2,2089)	1:28:A:THR:H	1:27:A:LEU:HD21	7	0.18
(2,1898)	1:59:B:TRP:H	1:55:B:GLN:H	6	0.18
(2,1897)	1:59:A:TRP:H	1:55:A:GLN:H	6	0.18
(2,1883)	1:63:A:GLN:H	1:61:A:HIS:HB3	3	0.18
(2,1854)	1:16:B:ALA:H	1:15:B:LYS:HB3	7	0.18
(2,1779)	1:66:A:LYS:HB3	1:66:A:LYS:H	7	0.18
(2,1762)	1:36:B:SER:H	1:36:B:SER:HG	5	0.18
(2,1735)	1:64:A:PHE:H	1:64:A:PHE:HD1	5	0.18
(2,1694)	1:7:B:THR:HB	1:41:B:LEU:HG	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD13	1	0.18
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD11	8	0.18
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD13	1	0.18
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD11	8	0.18
(2,1604)	1:53:B:LYS:HB3	1:21:B:PHE:HZ	7	0.18
(2,1513)	1:9:A:PHE:HA	1:17:A:LEU:HD23	9	0.18
(2,1512)	1:39:B:LEU:HD22	1:39:B:LEU:HA	2	0.18
(2,1511)	1:39:A:LEU:HD22	1:39:A:LEU:HA	2	0.18
(2,1473)	1:58:A:GLY:HA3	1:57:A:ILE:HB	7	0.18
(2,1465)	1:54:A:GLU:HB2	1:54:A:GLU:H	4	0.18
(2,1340)	1:27:B:LEU:HD23	1:46:B:ILE:H	5	0.18
(2,1268)	1:10:B:SER:HB2	1:12:B:GLU:H	1	0.18
(2,1268)	1:10:B:SER:HB2	1:12:B:GLU:H	3	0.18
(2,1267)	1:10:A:SER:HB2	1:12:A:GLU:H	1	0.18
(2,1250)	1:27:B:LEU:HA	1:32:B:ARG:H	7	0.18
(2,1209)	1:49:A:TRP:HB3	1:17:A:LEU:HD13	5	0.18
(2,957)	1:54:A:GLU:HG2	1:54:A:GLU:HA	9	0.18
(2,944)	1:54:B:GLU:HG2	1:21:B:PHE:HZ	10	0.18
(2,943)	1:54:A:GLU:HG2	1:21:A:PHE:HZ	10	0.18
(2,896)	1:42:B:ASN:HB3	1:44:B:GLU:HB3	2	0.18
(2,757)	1:7:A:THR:HA	1:8:A:GLU:H	7	0.18
(2,704)	1:64:B:PHE:HA	1:64:B:PHE:HD2	1	0.18
(2,703)	1:64:A:PHE:HA	1:64:A:PHE:HD2	1	0.18
(2,652)	1:64:B:PHE:HA	1:64:B:PHE:HB3	4	0.18
(2,651)	1:64:A:PHE:HA	1:64:A:PHE:HB3	4	0.18
(2,590)	1:47:B:GLU:HA	1:46:B:ILE:HB	4	0.18
(2,590)	1:47:B:GLU:HA	1:46:B:ILE:HB	7	0.18
(2,589)	1:47:A:GLU:HA	1:46:A:ILE:HB	4	0.18
(2,589)	1:47:A:GLU:HA	1:46:A:ILE:HB	7	0.18
(2,548)	1:57:B:ILE:HA	1:57:B:ILE:HG13	5	0.18
(2,547)	1:57:A:ILE:HA	1:57:A:ILE:HG13	5	0.18
(2,450)	1:9:B:PHE:HD1	1:10:B:SER:H	1	0.18
(2,440)	1:20:B:ALA:HB3	1:20:A:ALA:HB3	3	0.18
(2,439)	1:20:A:ALA:HB3	1:20:B:ALA:HB3	3	0.18
(2,312)	1:17:B:LEU:H	1:14:B:LYS:HB3	1	0.18
(2,310)	1:42:B:ASN:H	1:45:B:GLN:HA	6	0.18
(2,303)	1:59:A:TRP:H	1:60:A:SER:HB3	6	0.18
(2,274)	1:44:B:GLU:HA	1:48:B:ARG:HD3	2	0.18
(2,273)	1:44:A:GLU:HA	1:48:A:ARG:HD3	9	0.18
(2,203)	1:28:A:THR:HB	1:24:A:ASP:HB3	3	0.18
(2,182)	1:16:B:ALA:HB3	1:15:A:LYS:HB3	9	0.18
(2,102)	1:19:B:LEU:HB3	1:16:A:ALA:HA	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,100)	1:51:B:ARG:HD3	1:55:B:GLN:HG3	4	0.18
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	2	0.18
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	5	0.18
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	2	0.18
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	5	0.18
(2,16)	1:36:B:SER:HB3	1:46:B:ILE:HD13	8	0.18
(2,15)	1:36:A:SER:HB3	1:46:A:ILE:HD13	8	0.18
(2,10)	1:16:B:ALA:HB3	1:15:A:LYS:HD3	9	0.18
(2,3)	1:9:A:PHE:HD2	1:48:A:ARG:HD3	9	0.18
(1,84)	1:54:B:GLU:N	1:50:B:PHE:O	8	0.18
(1,83)	1:54:B:GLU:H	1:50:B:PHE:O	1	0.18
(1,80)	1:16:B:ALA:N	1:12:B:GLU:O	2	0.18
(1,42)	1:54:A:GLU:N	1:50:A:PHE:O	8	0.18
(1,38)	1:16:A:ALA:N	1:12:A:GLU:O	2	0.18
(1,32)	1:33:A:ARG:N	1:29:A:PRO:O	7	0.18
(3,76)	1:57:B:ILE:HG12	1:61:B:HIS:HB2	8	0.17
(3,75)	1:57:A:ILE:HG12	1:61:A:HIS:HB2	8	0.17
(3,18)	1:60:B:SER:HA	1:58:B:GLY:HA3	6	0.17
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	6	0.17
(3,12)	1:28:B:THR:HA	1:32:B:ARG:HB2	7	0.17
(2,2438)	1:53:B:LYS:H	1:21:B:PHE:HE1	3	0.17
(2,2302)	1:36:B:SER:H	1:34:B:TYR:HB2	1	0.17
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD13	8	0.17
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD13	8	0.17
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	7	0.17
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	7	0.17
(2,2106)	1:54:B:GLU:HB3	1:54:B:GLU:H	1	0.17
(2,2105)	1:54:A:GLU:HB3	1:54:A:GLU:H	1	0.17
(2,2094)	1:54:B:GLU:H	1:53:B:LYS:HG3	8	0.17
(2,2093)	1:54:A:GLU:H	1:53:A:LYS:HG3	8	0.17
(2,2081)	1:14:A:LYS:H	1:9:A:PHE:HB2	10	0.17
(2,1959)	1:34:A:TYR:H	1:33:A:ARG:HG3	3	0.17
(2,1947)	1:61:A:HIS:H	1:60:A:SER:HG	7	0.17
(2,1890)	1:49:B:TRP:H	1:48:B:ARG:HG3	2	0.17
(2,1825)	1:11:A:GLU:H	1:12:A:GLU:HB3	9	0.17
(2,1802)	1:65:B:GLU:H	1:64:B:PHE:HD1	7	0.17
(2,1780)	1:66:B:LYS:HB3	1:66:B:LYS:H	7	0.17
(2,1736)	1:64:B:PHE:H	1:64:B:PHE:HD1	5	0.17
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD11	5	0.17
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD11	9	0.17
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD11	10	0.17
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD11	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1608)	1:16:B:ALA:HB3	1:35:B:LEU:HD23	8	0.17
(2,1607)	1:16:A:ALA:HB3	1:35:A:LEU:HD23	8	0.17
(2,1597)	1:54:A:GLU:HB2	1:21:A:PHE:HE2	6	0.17
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD23	10	0.17
(2,1512)	1:39:B:LEU:HD22	1:39:B:LEU:HA	5	0.17
(2,1511)	1:39:A:LEU:HD22	1:39:A:LEU:HA	5	0.17
(2,1510)	1:65:B:GLU:HG2	1:65:B:GLU:HA	3	0.17
(2,1474)	1:58:B:GLY:HA3	1:57:B:ILE:HB	7	0.17
(2,1448)	1:53:B:LYS:HB2	1:21:B:PHE:HE1	7	0.17
(2,1267)	1:10:A:SER:HB2	1:12:A:GLU:H	3	0.17
(2,1192)	1:16:B:ALA:HB1	1:14:B:LYS:HA	3	0.17
(2,1165)	1:46:A:ILE:HD13	1:36:A:SER:H	6	0.17
(2,1110)	1:41:B:LEU:HD12	1:41:B:LEU:HD23	4	0.17
(2,1109)	1:41:A:LEU:HD12	1:41:A:LEU:HD23	4	0.17
(2,963)	1:55:A:GLN:HG2	1:55:A:GLN:H	2	0.17
(2,895)	1:42:A:ASN:HB3	1:44:A:GLU:HB3	2	0.17
(2,758)	1:7:B:THR:HA	1:8:B:GLU:H	7	0.17
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	2	0.17
(2,584)	1:32:B:ARG:HA	1:27:B:LEU:HD13	3	0.17
(2,574)	1:32:B:ARG:HA	1:27:B:LEU:HD21	5	0.17
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	1	0.17
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	1	0.17
(2,478)	1:19:B:LEU:HD21	1:19:A:LEU:HA	8	0.17
(2,374)	1:56:B:GLN:H	1:57:B:ILE:HG13	7	0.17
(2,365)	1:14:A:LYS:H	1:17:A:LEU:HB2	3	0.17
(2,361)	1:55:A:GLN:HB3	1:58:A:GLY:H	4	0.17
(2,309)	1:42:A:ASN:H	1:45:A:GLN:HA	6	0.17
(2,304)	1:59:B:TRP:H	1:60:B:SER:HB3	6	0.17
(2,285)	1:50:A:PHE:H	1:9:A:PHE:HE2	7	0.17
(2,273)	1:44:A:GLU:HA	1:48:A:ARG:HD3	2	0.17
(2,240)	1:59:B:TRP:HB2	1:57:B:ILE:HG12	4	0.17
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	7	0.17
(2,80)	1:62:B:PRO:HD3	1:62:B:PRO:HB2	10	0.17
(2,79)	1:62:A:PRO:HD3	1:62:A:PRO:HB2	10	0.17
(2,68)	1:25:B:ARG:HA	1:19:A:LEU:HD23	6	0.17
(2,67)	1:25:A:ARG:HA	1:19:B:LEU:HD23	6	0.17
(3,191)	1:44:A:GLU:H	1:36:A:SER:HB2	5	0.16
(3,53)	1:9:A:PHE:HB2	1:39:A:LEU:HG	10	0.16
(3,21)	1:3:A:LYS:HA	1:2:A:GLU:HG3	10	0.16
(3,17)	1:60:A:SER:HA	1:58:A:GLY:HA3	4	0.16
(3,11)	1:28:A:THR:HA	1:32:A:ARG:HB2	7	0.16
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	2	0.16
(2,1889)	1:49:A:TRP:H	1:48:A:ARG:HG3	4	0.16
(2,1826)	1:11:B:GLU:H	1:12:B:GLU:HB3	9	0.16
(2,1689)	1:9:A:PHE:HB3	1:14:A:LYS:HG3	5	0.16
(2,1678)	1:30:B:GLU:HA	1:33:B:ARG:HD3	9	0.16
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD12	4	0.16
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD13	2	0.16
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD12	4	0.16
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD11	9	0.16
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD11	10	0.16
(2,1553)	1:27:A:LEU:HB3	1:50:A:PHE:HB2	2	0.16
(2,1521)	1:13:A:GLN:HA	1:17:A:LEU:HD23	10	0.16
(2,1509)	1:65:A:GLU:HG2	1:65:A:GLU:HA	3	0.16
(2,1166)	1:46:B:ILE:HD13	1:36:B:SER:H	6	0.16
(2,1079)	1:13:A:GLN:HB2	1:13:A:GLN:HG2	8	0.16
(2,1026)	1:52:B:ARG:HD2	1:52:B:ARG:HG3	2	0.16
(2,1026)	1:52:B:ARG:HD2	1:52:B:ARG:HG3	8	0.16
(2,1025)	1:52:A:ARG:HD2	1:52:A:ARG:HG3	2	0.16
(2,1025)	1:52:A:ARG:HD2	1:52:A:ARG:HG3	8	0.16
(2,957)	1:54:A:GLU:HG2	1:54:A:GLU:HA	7	0.16
(2,906)	1:18:B:ASP:HB2	1:19:B:LEU:H	3	0.16
(2,817)	1:62:A:PRO:HD2	1:60:A:SER:HG	2	0.16
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	8	0.16
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	8	0.16
(2,548)	1:57:B:ILE:HA	1:57:B:ILE:HG13	1	0.16
(2,548)	1:57:B:ILE:HA	1:57:B:ILE:HG13	2	0.16
(2,548)	1:57:B:ILE:HA	1:57:B:ILE:HG13	10	0.16
(2,547)	1:57:A:ILE:HA	1:57:A:ILE:HG13	1	0.16
(2,547)	1:57:A:ILE:HA	1:57:A:ILE:HG13	10	0.16
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	2	0.16
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	3	0.16
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	7	0.16
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	10	0.16
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	2	0.16
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	3	0.16
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	7	0.16
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	10	0.16
(2,477)	1:19:A:LEU:HD21	1:19:B:LEU:HA	8	0.16
(2,403)	1:9:A:PHE:HD2	1:8:A:GLU:HB3	1	0.16
(2,320)	1:9:B:PHE:H	1:45:B:GLN:HB2	10	0.16
(2,274)	1:44:B:GLU:HA	1:48:B:ARG:HD3	9	0.16
(2,273)	1:44:A:GLU:HA	1:48:A:ARG:HD3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	4	0.16
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	4	0.16
(2,110)	1:3:B:LYS:HE2	1:4:B:ARG:HA	3	0.16
(2,67)	1:65:A:GLU:HA	1:53:A:LYS:HD2	5	0.16
(2,20)	1:5:B:PRO:HA	1:4:B:ARG:HG3	4	0.16
(2,4)	1:9:B:PHE:HD2	1:48:B:ARG:HD3	9	0.16
(1,51)	1:35:B:LEU:H	1:31:B:TRP:O	3	0.16
(1,48)	1:20:B:ALA:H	1:16:B:ALA:O	1	0.16
(1,6)	1:20:A:ALA:H	1:16:A:ALA:O	1	0.16
(3,172)	1:17:B:LEU:H	1:14:B:LYS:HG3	5	0.15
(3,171)	1:17:A:LEU:H	1:14:A:LYS:HG3	5	0.15
(3,148)	1:8:B:GLU:H	1:42:B:ASN:H	9	0.15
(3,116)	1:3:B:LYS:HG3	1:1:B:MET:HA	1	0.15
(3,115)	1:3:A:LYS:HG3	1:1:A:MET:HA	1	0.15
(3,22)	1:3:B:LYS:HA	1:2:B:GLU:HG3	10	0.15
(2,2347)	1:16:A:ALA:H	1:17:A:LEU:HD21	1	0.15
(2,2277)	1:9:A:PHE:H	1:41:A:LEU:HA	3	0.15
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD12	7	0.15
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD12	7	0.15
(2,2150)	1:52:B:ARG:HB3	1:56:B:GLN:H	7	0.15
(2,2128)	1:55:B:GLN:H	1:53:B:LYS:HB2	1	0.15
(2,2127)	1:55:A:GLN:H	1:53:A:LYS:HB2	1	0.15
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG22	5	0.15
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG22	5	0.15
(2,2053)	1:47:A:GLU:H	1:44:A:GLU:H	4	0.15
(2,1966)	1:13:B:GLN:HB3	1:13:B:GLN:H	7	0.15
(2,1690)	1:9:B:PHE:HB3	1:14:B:LYS:HG3	5	0.15
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD13	2	0.15
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD12	3	0.15
(2,1642)	1:39:B:LEU:HB3	1:39:B:LEU:HD11	6	0.15
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD12	3	0.15
(2,1641)	1:39:A:LEU:HB3	1:39:A:LEU:HD11	6	0.15
(2,1603)	1:53:A:LYS:HB3	1:21:A:PHE:HZ	7	0.15
(2,1598)	1:54:B:GLU:HB2	1:21:B:PHE:HE2	6	0.15
(2,1554)	1:27:B:LEU:HB3	1:50:B:PHE:HB2	2	0.15
(2,1553)	1:27:A:LEU:HB3	1:50:A:PHE:HB2	4	0.15
(2,1548)	1:27:B:LEU:HB3	1:50:B:PHE:HD1	4	0.15
(2,1522)	1:13:B:GLN:HA	1:17:B:LEU:HD23	3	0.15
(2,1512)	1:39:B:LEU:HD21	1:39:B:LEU:HA	3	0.15
(2,1447)	1:53:A:LYS:HB2	1:21:A:PHE:HE1	7	0.15
(2,1394)	1:46:B:ILE:HD11	1:36:B:SER:HG	1	0.15
(2,1393)	1:46:A:ILE:HD11	1:36:A:SER:HG	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1216)	1:50:B:PHE:HB2	1:27:B:LEU:HD12	1	0.15
(2,1215)	1:50:A:PHE:HB2	1:27:A:LEU:HD12	1	0.15
(2,1195)	1:16:A:ALA:HB2	1:13:A:GLN:HG2	4	0.15
(2,1137)	1:17:A:LEU:HA	1:20:A:ALA:HB1	7	0.15
(2,1110)	1:41:B:LEU:HD11	1:41:B:LEU:HD22	1	0.15
(2,1110)	1:41:B:LEU:HD13	1:41:B:LEU:HD21	9	0.15
(2,1109)	1:41:A:LEU:HD11	1:41:A:LEU:HD22	1	0.15
(2,1088)	1:15:B:LYS:HG3	1:15:B:LYS:HE3	3	0.15
(2,1087)	1:15:A:LYS:HG3	1:15:A:LYS:HE3	3	0.15
(2,1080)	1:13:B:GLN:HB2	1:13:B:GLN:HG2	3	0.15
(2,1080)	1:13:B:GLN:HB2	1:13:B:GLN:HG2	8	0.15
(2,1080)	1:13:B:GLN:HB2	1:13:B:GLN:HG2	10	0.15
(2,1079)	1:13:A:GLN:HB2	1:13:A:GLN:HG2	3	0.15
(2,1079)	1:13:A:GLN:HB2	1:13:A:GLN:HG2	10	0.15
(2,1026)	1:52:B:ARG:HD2	1:52:B:ARG:HG3	5	0.15
(2,1025)	1:52:A:ARG:HD2	1:52:A:ARG:HG3	5	0.15
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	6	0.15
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	5	0.15
(2,958)	1:54:B:GLU:HG2	1:54:B:GLU:HA	9	0.15
(2,946)	1:54:B:GLU:HG3	1:21:B:PHE:HZ	1	0.15
(2,945)	1:54:A:GLU:HG3	1:21:A:PHE:HZ	1	0.15
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	6	0.15
(2,738)	1:60:B:SER:HB3	1:60:B:SER:H	9	0.15
(2,737)	1:60:A:SER:HB3	1:60:A:SER:H	9	0.15
(2,703)	1:64:A:PHE:HA	1:64:A:PHE:HD1	3	0.15
(2,590)	1:47:B:GLU:HA	1:46:B:ILE:HB	8	0.15
(2,589)	1:47:A:GLU:HA	1:46:A:ILE:HB	8	0.15
(2,548)	1:57:B:ILE:HA	1:57:B:ILE:HG13	7	0.15
(2,547)	1:57:A:ILE:HA	1:57:A:ILE:HG13	2	0.15
(2,547)	1:57:A:ILE:HA	1:57:A:ILE:HG13	7	0.15
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	8	0.15
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	9	0.15
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	4	0.15
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	8	0.15
(2,487)	1:50:A:PHE:HE1	1:50:A:PHE:HB3	9	0.15
(2,437)	1:20:A:ALA:HB3	1:20:B:ALA:H	3	0.15
(2,404)	1:9:B:PHE:HD2	1:8:B:GLU:HB3	1	0.15
(2,273)	1:44:A:GLU:HA	1:48:A:ARG:HD3	10	0.15
(2,268)	1:15:B:LYS:HG3	1:19:B:LEU:HD22	2	0.15
(2,170)	1:12:B:GLU:HA	1:13:B:GLN:H	6	0.15
(2,169)	1:12:A:GLU:HA	1:13:A:GLN:H	6	0.15
(2,109)	1:3:A:LYS:HE2	1:4:A:ARG:HA	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	4	0.15
(3,147)	1:8:A:GLU:H	1:42:A:ASN:H	9	0.14
(3,118)	1:39:B:LEU:HG	1:9:B:PHE:H	2	0.14
(3,96)	1:59:B:TRP:HB2	1:55:B:GLN:H	4	0.14
(3,74)	1:39:B:LEU:HG	1:15:A:LYS:HE3	2	0.14
(2,2441)	1:14:A:LYS:H	1:17:A:LEU:HD23	10	0.14
(2,2370)	1:31:B:TRP:H	1:34:B:TYR:HD1	3	0.14
(2,2326)	1:7:B:THR:H	1:4:B:ARG:HD3	1	0.14
(2,2294)	1:60:B:SER:H	1:57:B:ILE:HG23	10	0.14
(2,2293)	1:60:A:SER:H	1:57:A:ILE:HG23	10	0.14
(2,2246)	1:66:B:LYS:H	1:64:B:PHE:H	3	0.14
(2,2234)	1:40:B:GLY:H	1:39:B:LEU:HD13	6	0.14
(2,2233)	1:40:A:GLY:H	1:39:A:LEU:HD13	6	0.14
(2,2079)	1:48:A:ARG:H	1:49:A:TRP:HB2	9	0.14
(2,2074)	1:55:B:GLN:H	1:53:B:LYS:HA	9	0.14
(2,1965)	1:13:A:GLN:HB3	1:13:A:GLN:H	7	0.14
(2,1952)	1:49:B:TRP:H	1:52:B:ARG:H	7	0.14
(2,1950)	1:61:B:HIS:H	1:60:B:SER:H	8	0.14
(2,1949)	1:61:A:HIS:H	1:60:A:SER:H	8	0.14
(2,1936)	1:61:B:HIS:H	1:57:B:ILE:HG23	4	0.14
(2,1781)	1:66:A:LYS:H	1:65:A:GLU:HG2	7	0.14
(2,1742)	1:49:B:TRP:HD1	1:49:B:TRP:H	4	0.14
(2,1678)	1:30:B:GLU:HA	1:33:B:ARG:HD3	1	0.14
(2,1677)	1:30:A:GLU:HA	1:33:A:ARG:HD3	9	0.14
(2,1512)	1:39:B:LEU:HD22	1:39:B:LEU:HA	6	0.14
(2,1512)	1:39:B:LEU:HD23	1:39:B:LEU:HA	8	0.14
(2,1511)	1:39:A:LEU:HD21	1:39:A:LEU:HA	3	0.14
(2,1511)	1:39:A:LEU:HD22	1:39:A:LEU:HA	6	0.14
(2,1511)	1:39:A:LEU:HD23	1:39:A:LEU:HA	8	0.14
(2,1510)	1:65:B:GLU:HG2	1:65:B:GLU:HA	1	0.14
(2,1509)	1:65:A:GLU:HG2	1:65:A:GLU:HA	1	0.14
(2,1368)	1:13:B:GLN:HB3	1:9:B:PHE:HD1	10	0.14
(2,1340)	1:27:B:LEU:HD22	1:46:B:ILE:H	9	0.14
(2,1313)	1:39:A:LEU:HD23	1:40:A:GLY:HA3	2	0.14
(2,1117)	1:7:A:THR:HG23	1:7:A:THR:H	5	0.14
(2,1110)	1:41:B:LEU:HD11	1:41:B:LEU:HD22	2	0.14
(2,1110)	1:41:B:LEU:HD11	1:41:B:LEU:HD22	3	0.14
(2,1109)	1:41:A:LEU:HD11	1:41:A:LEU:HD22	2	0.14
(2,1109)	1:41:A:LEU:HD13	1:41:A:LEU:HD21	9	0.14
(2,1088)	1:15:B:LYS:HG3	1:15:B:LYS:HE3	4	0.14
(2,1087)	1:15:A:LYS:HG3	1:15:A:LYS:HE3	4	0.14
(2,974)	1:56:B:GLN:HG3	1:56:B:GLN:HA	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,973)	1:56:A:GLN:HG3	1:56:A:GLN:HA	6	0.14
(2,958)	1:54:B:GLU:HG2	1:54:B:GLU:HA	4	0.14
(2,958)	1:54:B:GLU:HG2	1:54:B:GLU:HA	10	0.14
(2,957)	1:54:A:GLU:HG2	1:54:A:GLU:HA	4	0.14
(2,957)	1:54:A:GLU:HG2	1:54:A:GLU:HA	10	0.14
(2,952)	1:45:B:GLN:HG3	1:45:B:GLN:H	5	0.14
(2,777)	1:9:A:PHE:HA	1:4:A:ARG:HB2	6	0.14
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	5	0.14
(2,755)	1:43:A:GLU:HA	1:36:A:SER:HB2	6	0.14
(2,724)	1:10:B:SER:HB2	1:11:B:GLU:H	3	0.14
(2,723)	1:10:A:SER:HB2	1:11:A:GLU:H	3	0.14
(2,714)	1:3:B:LYS:HA	1:4:B:ARG:H	4	0.14
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	8	0.14
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	8	0.14
(2,600)	1:50:B:PHE:HA	1:53:B:LYS:HB3	10	0.14
(2,599)	1:50:A:PHE:HA	1:53:A:LYS:HB3	10	0.14
(2,590)	1:47:B:GLU:HA	1:46:B:ILE:HB	3	0.14
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	2	0.14
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	3	0.14
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	2	0.14
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	3	0.14
(2,488)	1:50:B:PHE:HE1	1:50:B:PHE:HB3	4	0.14
(2,478)	1:19:B:LEU:HD21	1:19:A:LEU:HA	1	0.14
(2,477)	1:19:A:LEU:HD21	1:19:B:LEU:HA	1	0.14
(2,373)	1:56:A:GLN:H	1:57:A:ILE:HG13	7	0.14
(2,344)	1:36:B:SER:H	1:37:B:GLN:HB2	3	0.14
(2,336)	1:15:B:LYS:H	1:15:B:LYS:HD3	7	0.14
(2,318)	1:59:B:TRP:HB2	1:55:B:GLN:H	4	0.14
(2,204)	1:28:B:THR:HB	1:24:B:ASP:HB3	3	0.14
(2,186)	1:17:B:LEU:HD21	1:50:B:PHE:HA	7	0.14
(2,119)	1:47:A:GLU:HG2	1:27:A:LEU:HD23	5	0.14
(2,116)	1:45:B:GLN:HG3	1:45:B:GLN:HE22	2	0.14
(2,115)	1:45:A:GLN:HG3	1:45:A:GLN:HE22	2	0.14
(2,99)	1:51:A:ARG:HD3	1:55:A:GLN:HG3	4	0.14
(2,88)	1:48:B:ARG:HD3	1:45:B:GLN:HE21	8	0.14
(2,87)	1:48:A:ARG:HD3	1:45:A:GLN:HE21	8	0.14
(2,85)	1:38:A:ARG:HD3	1:64:B:PHE:HA	6	0.14
(2,68)	1:65:B:GLU:HA	1:53:B:LYS:HD2	5	0.14
(2,14)	1:36:B:SER:HB2	1:45:B:GLN:HB2	8	0.14
(2,13)	1:36:A:SER:HB2	1:45:A:GLN:HB2	8	0.14
(1,36)	1:17:A:LEU:N	1:13:A:GLN:O	10	0.14
(3,120)	1:9:B:PHE:HB3	1:45:B:GLN:HA	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,117)	1:39:A:LEU:HG	1:9:A:PHE:H	2	0.13
(3,73)	1:39:A:LEU:HG	1:15:B:LYS:HE3	2	0.13
(3,63)	1:8:A:GLU:HG3	1:45:A:GLN:HE22	10	0.13
(2,2369)	1:31:A:TRP:H	1:34:A:TYR:HD1	3	0.13
(2,2325)	1:7:A:THR:H	1:4:A:ARG:HD3	1	0.13
(2,2322)	1:6:B:ARG:H	1:5:B:PRO:HB3	2	0.13
(2,2321)	1:6:A:ARG:H	1:5:A:PRO:HB3	2	0.13
(2,2245)	1:66:A:LYS:H	1:64:A:PHE:H	3	0.13
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	10	0.13
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	10	0.13
(2,2073)	1:55:A:GLN:H	1:53:A:LYS:HA	9	0.13
(2,2053)	1:47:A:GLU:H	1:44:A:GLU:H	10	0.13
(2,1862)	1:53:B:LYS:H	1:55:B:GLN:H	5	0.13
(2,1861)	1:53:A:LYS:H	1:55:A:GLN:H	5	0.13
(2,1761)	1:36:A:SER:H	1:36:A:SER:HG	5	0.13
(2,1761)	1:36:A:SER:H	1:36:A:SER:HG	7	0.13
(2,1693)	1:7:A:THR:HB	1:41:A:LEU:HG	3	0.13
(2,1677)	1:30:A:GLU:HA	1:33:A:ARG:HD3	1	0.13
(2,1608)	1:16:B:ALA:HB3	1:35:B:LEU:HD23	4	0.13
(2,1573)	1:27:A:LEU:HD13	1:46:A:ILE:H	4	0.13
(2,1509)	1:65:A:GLU:HG2	1:65:A:GLU:HA	7	0.13
(2,1339)	1:27:A:LEU:HD22	1:46:A:ILE:H	9	0.13
(2,1314)	1:39:B:LEU:HD23	1:40:B:GLY:HA3	2	0.13
(2,1196)	1:16:B:ALA:HB2	1:13:B:GLN:HG2	10	0.13
(2,1148)	1:16:B:ALA:HB3	1:19:A:LEU:HD23	8	0.13
(2,1138)	1:17:B:LEU:HA	1:20:B:ALA:HB1	7	0.13
(2,1118)	1:7:B:THR:HG23	1:7:B:THR:H	5	0.13
(2,1110)	1:41:B:LEU:HD11	1:41:B:LEU:HD23	5	0.13
(2,1110)	1:41:B:LEU:HD13	1:41:B:LEU:HD21	7	0.13
(2,1110)	1:41:B:LEU:HD12	1:41:B:LEU:HD23	8	0.13
(2,1110)	1:41:B:LEU:HD13	1:41:B:LEU:HD21	10	0.13
(2,1109)	1:41:A:LEU:HD11	1:41:A:LEU:HD22	3	0.13
(2,1109)	1:41:A:LEU:HD11	1:41:A:LEU:HD23	5	0.13
(2,1109)	1:41:A:LEU:HD13	1:41:A:LEU:HD21	7	0.13
(2,1109)	1:41:A:LEU:HD12	1:41:A:LEU:HD23	8	0.13
(2,1109)	1:41:A:LEU:HD13	1:41:A:LEU:HD21	10	0.13
(2,1063)	1:27:A:LEU:HD21	1:43:A:GLU:HB3	7	0.13
(2,958)	1:54:B:GLU:HG2	1:54:B:GLU:HA	2	0.13
(2,957)	1:54:A:GLU:HG2	1:54:A:GLU:HA	2	0.13
(2,951)	1:45:A:GLN:HG3	1:45:A:GLN:H	5	0.13
(2,943)	1:54:A:GLU:HG2	1:21:A:PHE:HZ	2	0.13
(2,896)	1:42:B:ASN:HB3	1:44:B:GLU:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,714)	1:3:B:LYS:HA	1:4:B:ARG:H	9	0.13
(2,713)	1:3:A:LYS:HA	1:4:A:ARG:H	4	0.13
(2,704)	1:64:B:PHE:HA	1:64:B:PHE:HD1	3	0.13
(2,608)	1:52:B:ARG:HA	1:52:B:ARG:HG3	5	0.13
(2,607)	1:52:A:ARG:HA	1:52:A:ARG:HG3	5	0.13
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	8	0.13
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	10	0.13
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	8	0.13
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	10	0.13
(2,472)	1:19:B:LEU:HD23	1:19:A:LEU:HG	2	0.13
(2,343)	1:36:A:SER:H	1:37:A:GLN:HB2	3	0.13
(2,335)	1:15:A:LYS:H	1:15:A:LYS:HD3	7	0.13
(2,312)	1:17:B:LEU:H	1:14:B:LYS:HB3	3	0.13
(2,274)	1:44:B:GLU:HA	1:48:B:ARG:HD3	10	0.13
(2,224)	1:45:B:GLN:HG3	1:41:B:LEU:HA	6	0.13
(2,223)	1:45:A:GLN:HG3	1:41:A:LEU:HA	6	0.13
(2,188)	1:17:B:LEU:HD23	1:13:B:GLN:HB3	3	0.13
(2,186)	1:17:B:LEU:HD21	1:50:B:PHE:HA	10	0.13
(2,181)	1:16:A:ALA:HB3	1:15:B:LYS:HB3	9	0.13
(2,76)	1:25:B:ARG:HA	1:20:B:ALA:HA	4	0.13
(2,10)	1:16:B:ALA:HB1	1:15:A:LYS:HD3	4	0.13
(3,95)	1:59:A:TRP:HB2	1:55:A:GLN:H	4	0.12
(3,64)	1:8:B:GLU:HG3	1:45:B:GLN:HE22	9	0.12
(3,63)	1:8:A:GLU:HG3	1:45:A:GLN:HE22	9	0.12
(3,56)	1:57:B:ILE:HB	1:58:B:GLY:HA2	6	0.12
(3,55)	1:57:A:ILE:HB	1:58:A:GLY:HA2	6	0.12
(3,54)	1:9:B:PHE:HB2	1:39:B:LEU:HG	10	0.12
(3,42)	1:61:B:HIS:HA	1:60:B:SER:HG	2	0.12
(2,2348)	1:16:B:ALA:H	1:17:B:LEU:HD21	1	0.12
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	3	0.12
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	4	0.12
(2,2220)	1:57:B:ILE:HA	1:58:B:GLY:H	5	0.12
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	3	0.12
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	4	0.12
(2,2219)	1:57:A:ILE:HA	1:58:A:GLY:H	5	0.12
(2,2096)	1:9:B:PHE:H	1:7:B:THR:HG23	9	0.12
(2,2095)	1:9:A:PHE:H	1:7:A:THR:HG23	9	0.12
(2,1951)	1:49:A:TRP:H	1:52:A:ARG:H	7	0.12
(2,1868)	1:43:B:GLU:H	1:42:B:ASN:HB2	2	0.12
(2,1867)	1:43:A:GLU:H	1:42:A:ASN:HB2	2	0.12
(2,1853)	1:16:A:ALA:H	1:15:A:LYS:HB3	7	0.12
(2,1786)	1:66:B:LYS:H	1:64:B:PHE:HB3	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1762)	1:36:B:SER:H	1:36:B:SER:HG	7	0.12
(2,1692)	1:7:B:THR:HB	1:42:B:ASN:HB2	2	0.12
(2,1685)	1:9:A:PHE:HA	1:45:A:GLN:HB2	10	0.12
(2,1575)	1:27:A:LEU:HD13	1:51:A:ARG:H	4	0.12
(2,1466)	1:54:B:GLU:HB2	1:54:B:GLU:H	7	0.12
(2,1465)	1:54:A:GLU:HB2	1:54:A:GLU:H	7	0.12
(2,1416)	1:46:B:ILE:HG22	1:32:B:ARG:H	1	0.12
(2,1415)	1:46:A:ILE:HG22	1:32:A:ARG:H	1	0.12
(2,1350)	1:42:B:ASN:HA	1:42:B:ASN:HD21	5	0.12
(2,1349)	1:42:A:ASN:HA	1:42:A:ASN:HD21	5	0.12
(2,1332)	1:27:B:LEU:HD23	1:50:B:PHE:H	6	0.12
(2,1331)	1:27:A:LEU:HD23	1:50:A:PHE:H	6	0.12
(2,1147)	1:16:A:ALA:HB3	1:19:B:LEU:HD23	8	0.12
(2,1064)	1:27:B:LEU:HD21	1:43:B:GLU:HB3	7	0.12
(2,957)	1:54:A:GLU:HG2	1:54:A:GLU:HA	3	0.12
(2,944)	1:54:B:GLU:HG2	1:21:B:PHE:HZ	6	0.12
(2,896)	1:42:B:ASN:HB3	1:44:B:GLU:HB3	1	0.12
(2,895)	1:42:A:ASN:HB3	1:44:A:GLU:HB3	1	0.12
(2,895)	1:42:A:ASN:HB3	1:44:A:GLU:HB3	7	0.12
(2,816)	1:61:B:HIS:HA	1:62:B:PRO:HD2	2	0.12
(2,815)	1:61:A:HIS:HA	1:62:A:PRO:HD2	2	0.12
(2,778)	1:9:B:PHE:HA	1:4:B:ARG:HB2	6	0.12
(2,756)	1:43:B:GLU:HA	1:36:B:SER:HB2	4	0.12
(2,724)	1:10:B:SER:HB2	1:11:B:GLU:H	7	0.12
(2,713)	1:3:A:LYS:HA	1:4:A:ARG:H	9	0.12
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	6	0.12
(2,590)	1:47:B:GLU:HA	1:46:B:ILE:HB	6	0.12
(2,589)	1:47:A:GLU:HA	1:46:A:ILE:HB	3	0.12
(2,589)	1:47:A:GLU:HA	1:46:A:ILE:HB	6	0.12
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	7	0.12
(2,515)	1:62:A:PRO:HA	1:62:A:PRO:HB2	7	0.12
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	1	0.12
(2,471)	1:19:A:LEU:HD23	1:19:B:LEU:HG	2	0.12
(2,328)	1:51:B:ARG:H	1:27:B:LEU:HD23	8	0.12
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD23	8	0.12
(2,317)	1:59:A:TRP:HB2	1:55:A:GLN:H	4	0.12
(2,267)	1:15:A:LYS:HG3	1:19:A:LEU:HD22	2	0.12
(2,239)	1:59:A:TRP:HB2	1:57:A:ILE:HG12	4	0.12
(2,161)	1:39:A:LEU:HG	1:13:A:GLN:H	3	0.12
(2,86)	1:38:B:ARG:HD3	1:64:A:PHE:HA	6	0.12
(2,75)	1:25:A:ARG:HA	1:20:A:ALA:HA	7	0.12
(1,8)	1:34:A:TYR:H	1:30:A:GLU:O	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2420)	1:51:B:ARG:H	1:54:B:GLU:HG3	2	0.11
(2,2278)	1:9:B:PHE:H	1:41:B:LEU:HA	3	0.11
(2,2235)	1:40:A:GLY:H	1:41:A:LEU:HD21	5	0.11
(2,2174)	1:17:B:LEU:HG	1:17:B:LEU:H	8	0.11
(2,2173)	1:17:A:LEU:HG	1:17:A:LEU:H	8	0.11
(2,2164)	1:14:B:LYS:H	1:14:B:LYS:HB3	3	0.11
(2,2163)	1:14:A:LYS:H	1:14:A:LYS:HB3	3	0.11
(2,2080)	1:48:B:ARG:H	1:49:B:TRP:HB2	9	0.11
(2,2054)	1:47:B:GLU:H	1:44:B:GLU:H	10	0.11
(2,1902)	1:59:B:TRP:H	1:62:B:PRO:HD2	4	0.11
(2,1806)	1:65:B:GLU:H	1:64:B:PHE:HB2	4	0.11
(2,1785)	1:66:A:LYS:H	1:64:A:PHE:HB3	3	0.11
(2,1691)	1:7:A:THR:HB	1:42:A:ASN:HB2	2	0.11
(2,1658)	1:28:B:THR:HA	1:31:B:TRP:HB2	10	0.11
(2,1657)	1:28:A:THR:HA	1:31:A:TRP:HB2	10	0.11
(2,1510)	1:65:B:GLU:HG2	1:65:B:GLU:HA	10	0.11
(2,1509)	1:65:A:GLU:HG2	1:65:A:GLU:HA	10	0.11
(2,1496)	1:61:B:HIS:HA	1:54:B:GLU:HB2	9	0.11
(2,1415)	1:46:A:ILE:HG23	1:32:A:ARG:H	4	0.11
(2,1192)	1:16:B:ALA:HB1	1:14:B:LYS:HA	6	0.11
(2,1191)	1:16:A:ALA:HB1	1:14:A:LYS:HA	6	0.11
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG22	2	0.11
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG23	3	0.11
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG22	4	0.11
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG23	8	0.11
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG22	9	0.11
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG22	10	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG22	2	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG23	3	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG21	4	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG23	7	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG23	8	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG22	9	0.11
(2,1113)	1:7:A:THR:HB	1:7:A:THR:HG22	10	0.11
(2,1107)	1:39:A:LEU:HD21	1:17:A:LEU:HG	7	0.11
(2,1047)	1:57:A:ILE:HG13	1:57:A:ILE:H	9	0.11
(2,958)	1:54:B:GLU:HG2	1:54:B:GLU:HA	3	0.11
(2,944)	1:54:B:GLU:HG2	1:21:B:PHE:HZ	2	0.11
(2,790)	1:16:B:ALA:HA	1:15:B:LYS:HB3	2	0.11
(2,724)	1:10:B:SER:HB2	1:11:B:GLU:H	4	0.11
(2,723)	1:10:A:SER:HB2	1:11:A:GLU:H	7	0.11
(2,642)	1:48:B:ARG:HA	1:48:B:ARG:HD3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	3	0.11
(2,641)	1:48:A:ARG:HA	1:48:A:ARG:HD3	6	0.11
(2,590)	1:47:B:GLU:HA	1:46:B:ILE:HB	9	0.11
(2,589)	1:47:A:GLU:HA	1:46:A:ILE:HB	9	0.11
(2,584)	1:32:B:ARG:HA	1:27:B:LEU:HD11	6	0.11
(2,583)	1:32:A:ARG:HA	1:27:A:LEU:HD11	6	0.11
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	1	0.11
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	10	0.11
(2,515)	1:62:A:PRO:HA	1:62:A:PRO:HB2	1	0.11
(2,515)	1:62:A:PRO:HA	1:62:A:PRO:HB2	10	0.11
(2,514)	1:5:B:PRO:HA	1:5:B:PRO:HB2	6	0.11
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	1	0.11
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	4	0.11
(2,513)	1:5:A:PRO:HA	1:5:A:PRO:HB2	6	0.11
(2,327)	1:51:A:ARG:H	1:27:A:LEU:HD21	3	0.11
(2,309)	1:42:A:ASN:H	1:45:A:GLN:HA	3	0.11
(2,304)	1:59:B:TRP:H	1:60:B:SER:HB3	4	0.11
(2,304)	1:59:B:TRP:H	1:60:B:SER:HB3	7	0.11
(2,303)	1:59:A:TRP:H	1:60:A:SER:HB3	7	0.11
(2,200)	1:20:B:ALA:HB3	1:17:B:LEU:HB3	1	0.11
(2,185)	1:17:A:LEU:HD21	1:50:A:PHE:HA	7	0.11
(2,185)	1:17:A:LEU:HD21	1:50:A:PHE:HA	10	0.11
(2,67)	1:65:A:GLU:HA	1:19:A:LEU:HD21	9	0.11
(2,64)	1:24:B:ASP:HA	1:23:B:PHE:HA	7	0.11
(2,63)	1:24:A:ASP:HA	1:23:A:PHE:HA	7	0.11
(2,12)	1:36:B:SER:HB3	1:45:B:GLN:HB2	4	0.11
(1,65)	1:15:B:LYS:N	1:11:B:GLU:O	6	0.11
(1,50)	1:34:B:TYR:H	1:30:B:GLU:O	8	0.11
(1,19)	1:55:A:GLN:H	1:51:A:ARG:O	6	0.11
(3,232)	1:60:B:SER:H	1:57:B:ILE:HA	1	0.1
(3,231)	1:60:A:SER:H	1:57:A:ILE:HA	1	0.1
(3,78)	1:37:B:GLN:HB3	1:34:B:TYR:HB2	7	0.1
(3,41)	1:61:A:HIS:HA	1:60:A:SER:HG	2	0.1
(2,1952)	1:49:B:TRP:H	1:52:B:ARG:H	1	0.1
(2,1951)	1:49:A:TRP:H	1:52:A:ARG:H	1	0.1
(2,1923)	1:63:A:GLN:HG2	1:63:A:GLN:H	10	0.1
(2,1856)	1:16:B:ALA:H	1:17:B:LEU:HB2	8	0.1
(2,1855)	1:16:A:ALA:H	1:17:A:LEU:HB2	8	0.1
(2,1853)	1:16:A:ALA:H	1:15:A:LYS:HB3	9	0.1
(2,1816)	1:4:B:ARG:H	1:10:B:SER:HB3	2	0.1
(2,1815)	1:4:A:ARG:H	1:10:A:SER:HB3	2	0.1
(2,1511)	1:39:A:LEU:HD22	1:39:A:LEU:HA	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1445)	1:53:A:LYS:HB2	1:21:A:PHE:HZ	3	0.1
(2,1350)	1:42:B:ASN:HA	1:42:B:ASN:HD21	8	0.1
(2,1349)	1:42:A:ASN:HA	1:42:A:ASN:HD21	8	0.1
(2,1208)	1:17:B:LEU:HD21	1:18:B:ASP:H	4	0.1
(2,1195)	1:16:A:ALA:HB2	1:13:A:GLN:HG2	10	0.1
(2,1193)	1:16:A:ALA:HB1	1:13:A:GLN:HB3	6	0.1
(2,1114)	1:7:B:THR:HB	1:7:B:THR:HG23	7	0.1
(2,1109)	1:41:A:LEU:HD11	1:41:A:LEU:HD23	6	0.1
(2,1108)	1:39:B:LEU:HD21	1:17:B:LEU:HG	7	0.1
(2,943)	1:54:A:GLU:HG2	1:21:A:PHE:HZ	6	0.1
(2,789)	1:16:A:ALA:HA	1:15:A:LYS:HB3	2	0.1
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	2	0.1
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	5	0.1
(2,516)	1:62:B:PRO:HA	1:62:B:PRO:HB2	9	0.1
(2,515)	1:62:A:PRO:HA	1:62:A:PRO:HB2	2	0.1
(2,515)	1:62:A:PRO:HA	1:62:A:PRO:HB2	5	0.1
(2,421)	1:49:A:TRP:HD1	1:49:A:TRP:HA	6	0.1
(2,322)	1:54:B:GLU:H	1:52:B:ARG:HB2	10	0.1
(2,321)	1:54:A:GLU:H	1:52:A:ARG:HB2	10	0.1
(2,294)	1:53:B:LYS:H	1:54:B:GLU:HB3	9	0.1
(2,49)	1:49:A:TRP:HA	1:9:A:PHE:HE2	2	0.1

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

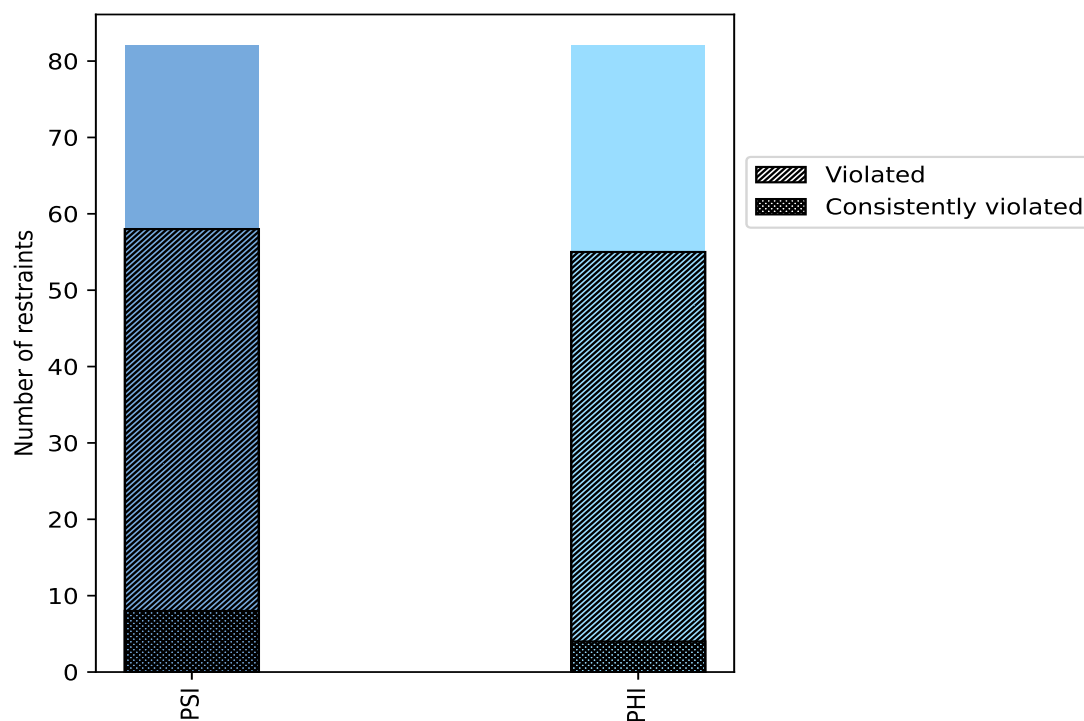
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	82	50.0	58	70.7	35.4	8	9.8	4.9
PHI	82	50.0	55	67.1	33.5	4	4.9	2.4
Total	164	100.0	113	68.9	68.9	12	7.3	7.3

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

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



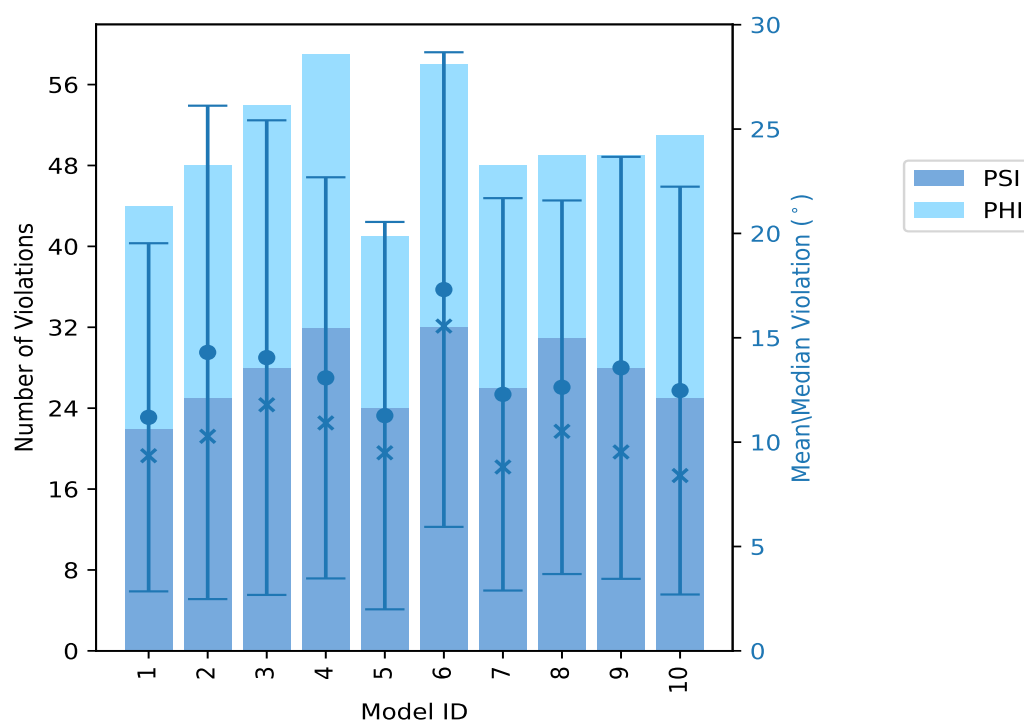
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	22	22	44	11.19	37.98	8.34	9.35
2	25	23	48	14.3	45.97	11.82	10.28
3	28	26	54	14.05	44.23	11.37	11.79
4	32	27	59	13.08	36.23	9.61	10.92
5	24	17	41	11.27	40.51	9.28	9.49
6	32	26	58	17.31	39.41	11.37	15.56
7	26	22	48	12.29	36.68	9.4	8.81
8	31	18	49	12.63	33.92	8.95	10.52
9	28	21	49	13.56	41.67	10.11	9.53
10	25	26	51	12.47	35.4	9.77	8.4

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

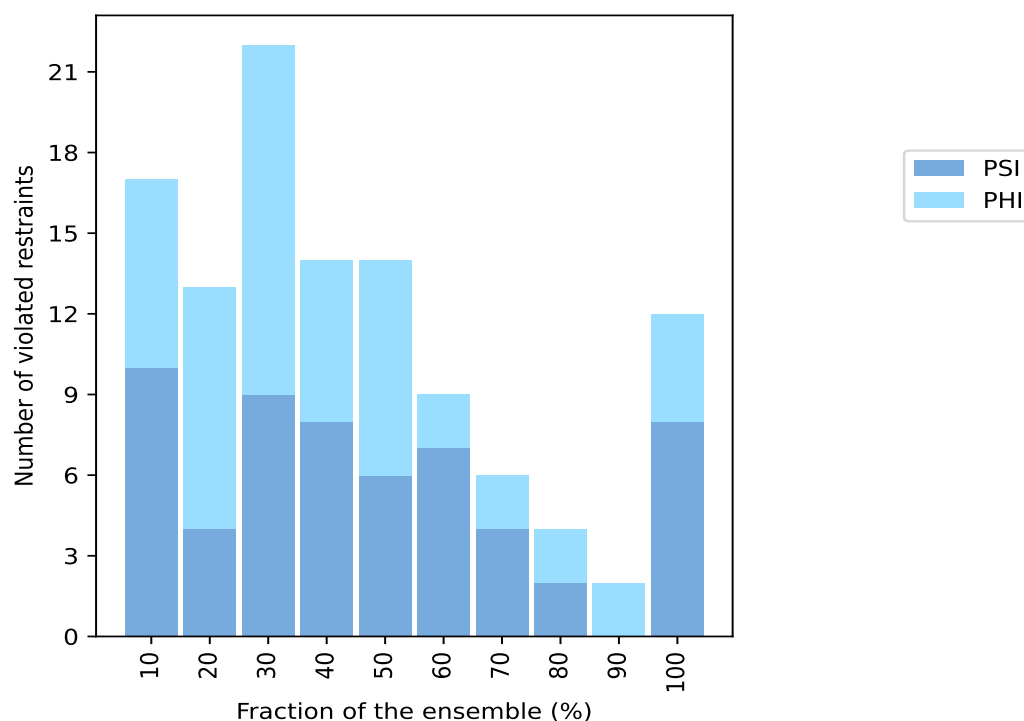
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PSI	PHI	Total	Count ¹	%
10	7	17	1	10.0
4	9	13	2	20.0
9	13	22	3	30.0
8	6	14	4	40.0
6	8	14	5	50.0
7	2	9	6	60.0
4	2	6	7	70.0
2	2	4	8	80.0
0	2	2	9	90.0
8	4	12	10	100.0

¹ Number of models with violations

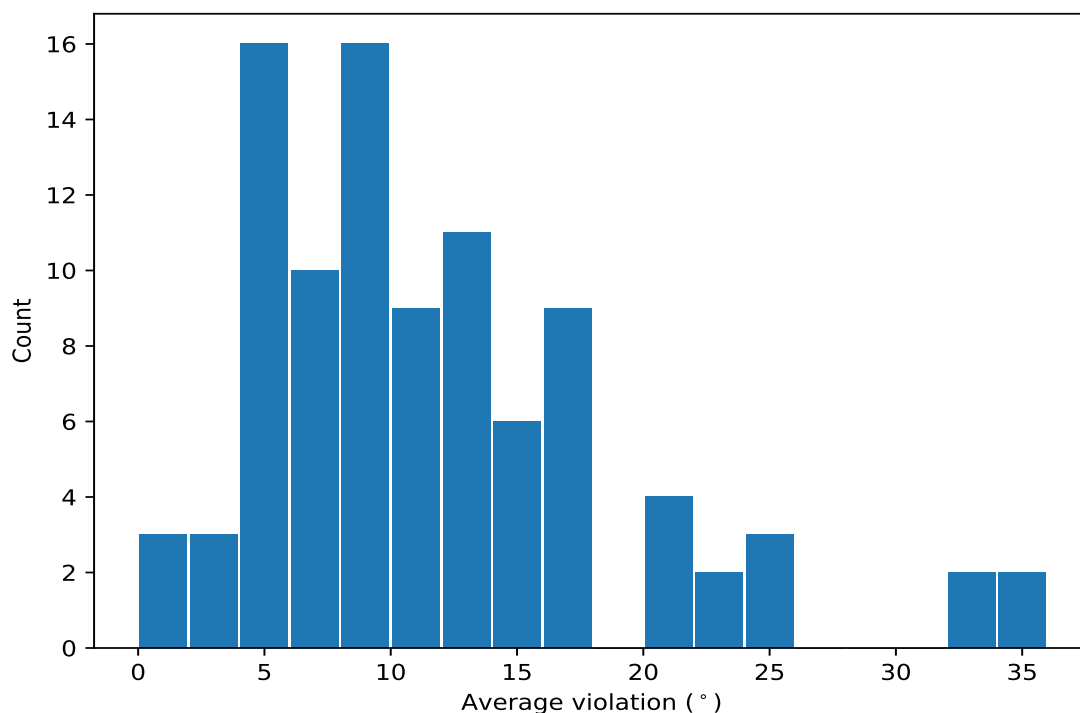
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	10	35.16	3.38	34.66
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	10	34.94	3.33	34.08
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	10	24.52	5.08	26.04
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	10	24.37	5.01	25.72
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	10	24.05	5.66	25.51
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	10	23.76	5.65	24.34
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	10	21.9	11.71	21.66
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	10	21.36	11.8	21.99
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	10	13.24	1.56	13.16
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	10	13.07	1.6	12.95
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	10	4.28	1.95	3.87
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	10	4.26	1.93	3.9
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	9	17.86	10.59	14.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	9	17.65	10.77	13.96
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	8	20.45	10.01	18.49
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	8	20.02	9.91	18.98
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	8	7.64	4.91	6.0
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	8	7.62	4.92	5.99
(1,49)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:ASP:N	7	14.83	7.05	13.43
(1,131)	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	1:18:B:ASP:N	7	12.1	4.56	11.18
(1,52)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:PHE:N	7	8.95	3.82	7.46
(1,134)	1:20:B:ALA:N	1:20:B:ALA:CA	1:20:B:ALA:C	1:21:B:PHE:N	7	8.93	3.88	7.51
(1,30)	1:45:A:GLN:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	7	1.96	0.55	2.03
(1,112)	1:45:B:GLN:C	1:46:B:ILE:N	1:46:B:ILE:CA	1:46:B:ILE:C	7	1.89	0.42	1.97
(1,51)	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	1:20:A:ALA:N	6	16.79	11.26	12.69
(1,133)	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	1:20:B:ALA:N	6	15.97	8.73	13.26
(1,141)	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	1:34:B:TYR:N	6	15.09	2.62	14.18
(1,59)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:TYR:N	6	14.9	3.09	13.75
(1,78)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:GLU:N	6	13.38	3.56	12.27
(1,160)	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	1:54:B:GLU:N	6	13.02	3.43	12.04
(1,6)	1:14:A:LYS:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	6	9.67	6.08	9.63
(1,88)	1:14:B:LYS:C	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	6	9.28	6.22	9.2
(1,147)	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	1:41:B:LEU:N	6	5.09	2.71	4.69
(1,39)	1:54:A:GLU:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	5	17.61	10.63	19.47
(1,121)	1:54:B:GLU:C	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	5	16.2	9.67	16.85
(1,44)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:GLN:N	5	15.35	8.8	17.26
(1,159)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:LYS:N	5	12.14	4.19	10.97
(1,1)	1:9:A:PHE:C	1:10:A:SER:N	1:10:A:SER:CA	1:10:A:SER:C	5	12.12	10.88	4.05
(1,83)	1:9:B:PHE:C	1:10:B:SER:N	1:10:B:SER:CA	1:10:B:SER:C	5	12.01	10.78	4.22
(1,77)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:LYS:N	5	11.75	4.07	10.55
(1,79)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:GLN:N	5	8.76	6.1	5.15
(1,161)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:GLN:N	5	8.25	5.65	4.58
(1,65)	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	1:41:A:LEU:N	5	5.72	2.37	5.31
(1,19)	1:33:A:ARG:C	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	5	4.75	2.07	3.83
(1,101)	1:33:B:ARG:C	1:34:B:TYR:N	1:34:B:TYR:CA	1:34:B:TYR:C	5	4.17	1.83	3.88
(1,114)	1:47:B:GLU:C	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	5	4.12	0.79	3.88
(1,32)	1:47:A:GLU:C	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	5	3.65	0.52	3.84
(1,53)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:LEU:N	4	33.9	6.09	31.45
(1,135)	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	1:27:B:LEU:N	4	33.24	5.03	31.41
(1,126)	1:12:B:GLU:N	1:12:B:GLU:CA	1:12:B:GLU:C	1:13:B:GLN:N	4	17.72	7.98	20.3
(1,46)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:LYS:N	4	17.33	9.24	18.23
(1,128)	1:14:B:LYS:N	1:14:B:LYS:CA	1:14:B:LYS:C	1:15:B:LYS:N	4	16.8	9.43	17.4
(1,47)	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	1:16:A:ALA:N	4	16.58	14.3	14.48
(1,12)	1:25:A:ARG:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	4	11.33	3.61	11.04
(1,132)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:LEU:N	4	10.14	3.69	9.7
(1,41)	1:56:A:GLN:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	4	9.89	2.96	10.98
(1,94)	1:25:B:ARG:C	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	4	9.88	4.92	10.21
(1,123)	1:56:B:GLN:C	1:57:B:ILE:N	1:57:B:ILE:CA	1:57:B:ILE:C	4	9.64	3.41	11.03
(1,125)	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	1:12:B:GLU:N	4	6.42	1.65	6.42
(1,21)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	4	5.86	2.88	5.28
(1,103)	1:35:B:LEU:C	1:36:B:SER:N	1:36:B:SER:CA	1:36:B:SER:C	4	5.82	2.7	5.35
(1,129)	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	1:16:B:ALA:N	3	22.19	11.41	22.83
(1,9)	1:17:A:LEU:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	3	13.01	8.21	8.75
(1,84)	1:10:B:SER:C	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	3	12.11	2.17	13.26

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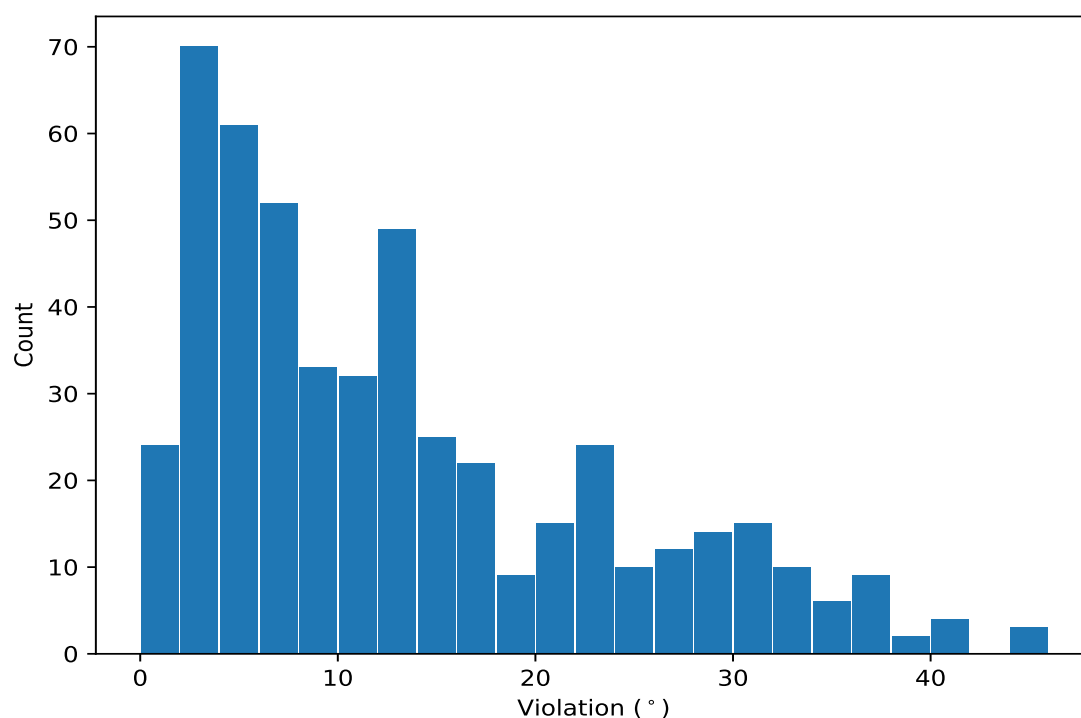
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,8)	1:16:A:ALA:C	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	3	12.1	11.01	8.1
(1,50)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LEU:N	3	11.91	3.09	11.66
(1,2)	1:10:A:SER:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	3	11.48	3.34	13.3
(1,90)	1:16:B:ALA:C	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	3	11.03	8.89	7.95
(1,92)	1:18:B:ASP:C	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	3	10.84	10.74	5.45
(1,151)	1:44:B:GLU:N	1:44:B:GLU:CA	1:44:B:GLU:C	1:45:B:GLN:N	3	10.17	5.8	13.25
(1,102)	1:34:B:TYR:C	1:35:B:LEU:N	1:35:B:LEU:CA	1:35:B:LEU:C	3	9.87	9.65	3.86
(1,20)	1:34:A:TYR:C	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	3	9.43	9.18	3.86
(1,37)	1:52:A:ARG:C	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	3	8.52	8.34	3.69
(1,119)	1:52:B:ARG:C	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	3	8.52	8.33	3.61
(1,158)	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	1:52:B:ARG:N	3	7.94	6.24	3.99
(1,76)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:ARG:N	3	7.93	6.28	4.03
(1,43)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:GLU:N	3	7.34	1.08	7.65
(1,5)	1:13:A:GLN:C	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	3	7.17	3.47	5.26
(1,154)	1:47:B:GLU:N	1:47:B:GLU:CA	1:47:B:GLU:C	1:48:B:ARG:N	3	6.86	0.57	6.95
(1,72)	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	1:48:A:ARG:N	3	5.75	3.15	7.53
(1,22)	1:36:A:SER:C	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	3	4.51	2.63	4.2
(1,104)	1:36:B:SER:C	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	3	4.18	2.37	4.12
(1,155)	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	1:49:B:TRP:N	3	1.51	0.37	1.52
(1,69)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:GLN:N	2	14.27	1.0	14.27
(1,85)	1:11:B:GLU:C	1:12:B:GLU:N	1:12:B:GLU:CA	1:12:B:GLU:C	2	11.44	4.24	11.44
(1,164)	1:57:B:ILE:N	1:57:B:ILE:CA	1:57:B:ILE:C	1:58:B:GLY:N	2	9.45	6.86	9.45
(1,82)	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	1:58:A:GLY:N	2	9.32	6.79	9.32
(1,87)	1:13:B:GLN:C	1:14:B:LYS:N	1:14:B:LYS:CA	1:14:B:LYS:C	2	8.7	4.34	8.7
(1,99)	1:31:B:TRP:C	1:32:B:ARG:N	1:32:B:ARG:CA	1:32:B:ARG:C	2	7.1	2.16	7.1
(1,100)	1:32:B:ARG:C	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	2	6.94	0.31	6.94
(1,29)	1:44:A:GLU:C	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	2	5.93	1.88	5.93
(1,111)	1:44:B:GLU:C	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	2	5.93	2.04	5.93
(1,10)	1:18:A:ASP:C	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	2	4.58	0.96	4.58
(1,18)	1:32:A:ARG:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	2	4.28	2.8	4.28
(1,17)	1:31:A:TRP:C	1:32:A:ARG:N	1:32:A:ARG:CA	1:32:A:ARG:C	2	3.72	1.2	3.72
(1,73)	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	1:49:A:TRP:N	2	2.52	0.1	2.52

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 (°)
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	2	45.97
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	2	45.56
(1,53)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:LEU:N	3	44.23
(1,135)	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	1:27:B:LEU:N	3	41.68
(1,51)	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	1:20:A:ALA:N	9	41.67
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	5	40.51
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	5	40.34
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	6	39.41
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	6	39.36
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	1	37.98
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	1	37.75
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	7	36.68
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	3	36.57
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	3	36.45
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	3	36.44
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	4	36.23
(1,47)	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	1:16:A:ALA:N	6	36.19
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	7	36.13
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	4	35.9
(1,129)	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	1:16:B:ALA:N	6	35.84
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	10	35.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,133)	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	1:20:B:ALA:N	9	35.02
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	3	34.72
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	10	34.21
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	4	33.95
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	8	33.92
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	9	33.91
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	4	33.85
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	8	33.8
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	9	33.59
(1,39)	1:54:A:GLU:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	2	33.38
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	10	32.74
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	6	32.65
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	6	32.54
(1,135)	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	1:27:B:LEU:N	2	31.95
(1,53)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:LEU:N	2	31.94
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	7	31.32
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	6	31.25
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	6	31.21
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	6	31.1
(1,53)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:LEU:N	8	30.96
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	6	30.93
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	10	30.89
(1,135)	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	1:27:B:LEU:N	8	30.87
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	3	30.83
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	7	30.71
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	3	30.56
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	10	30.26
(1,121)	1:54:B:GLU:C	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	2	30.14
(1,146)	1:39:B:LEU:N	1:39:B:LEU:CA	1:39:B:LEU:C	1:40:B:GLY:N	2	29.57
(1,64)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLY:N	2	29.33
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	8	28.91
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	8	28.86
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	6	28.81
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	5	28.71
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	5	28.57
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	6	28.55
(1,135)	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	1:27:B:LEU:N	6	28.48
(1,53)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:LEU:N	6	28.48
(1,128)	1:14:B:LYS:N	1:14:B:LYS:CA	1:14:B:LYS:C	1:15:B:LYS:N	6	28.46
(1,46)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:LYS:N	6	28.4
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	10	28.31
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	10	28.31
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	7	27.86
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	7	27.66
(1,1)	1:9:A:PHE:C	1:10:A:SER:N	1:10:A:SER:CA	1:10:A:SER:C	2	27.51
(1,83)	1:9:B:PHE:C	1:10:B:SER:N	1:10:B:SER:CA	1:10:B:SER:C	2	27.41
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	2	27.19
(1,8)	1:16:A:ALA:C	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	9	27.13
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	10	26.63
(1,48)	1:16:A:ALA:N	1:16:A:ALA:CA	1:16:A:ALA:C	1:17:A:LEU:N	9	26.33
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	4	26.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	4	26.03
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	9	26.03
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	9	26.01
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	10	25.99
(1,92)	1:18:B:ASP:C	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	9	25.84
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	10	25.41
(1,126)	1:12:B:GLU:N	1:12:B:GLU:CA	1:12:B:GLU:C	1:13:B:GLN:N	6	25.4
(1,49)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:ASP:N	4	25.39
(1,44)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:GLN:N	6	25.16
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	2	24.69
(1,9)	1:17:A:LEU:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	4	24.49
(1,47)	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	1:16:A:ALA:N	3	24.13
(1,44)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:GLN:N	4	24.13
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	4	23.99
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	1	23.97
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	1	23.85
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	4	23.82
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	6	23.59
(1,102)	1:34:B:TYR:C	1:35:B:LEU:N	1:35:B:LEU:CA	1:35:B:LEU:C	3	23.49
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	6	23.47
(1,46)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:LYS:N	4	23.3
(1,126)	1:12:B:GLU:N	1:12:B:GLU:CA	1:12:B:GLU:C	1:13:B:GLN:N	4	23.26
(1,90)	1:16:B:ALA:C	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	9	23.12
(1,1)	1:9:A:PHE:C	1:10:A:SER:N	1:10:A:SER:CA	1:10:A:SER:C	6	23.11
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	7	22.95
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	7	22.95
(1,129)	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	1:16:B:ALA:N	3	22.83
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	9	22.76
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	3	22.74
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	3	22.73
(1,83)	1:9:B:PHE:C	1:10:B:SER:N	1:10:B:SER:CA	1:10:B:SER:C	6	22.67
(1,128)	1:14:B:LYS:N	1:14:B:LYS:CA	1:14:B:LYS:C	1:15:B:LYS:N	4	22.62
(1,49)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:ASP:N	9	22.46
(1,130)	1:16:B:ALA:N	1:16:B:ALA:CA	1:16:B:ALA:C	1:17:B:LEU:N	9	22.42
(1,20)	1:34:A:TYR:C	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	3	22.38
(1,39)	1:54:A:GLU:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	6	22.1
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	9	22.07
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	1	21.92
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	1	21.88
(1,59)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:TYR:N	4	21.62
(1,121)	1:54:B:GLU:C	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	6	21.58
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	8	21.47
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	8	21.4
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1	21.04
(1,88)	1:14:B:LYS:C	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	6	20.62
(1,6)	1:14:A:LYS:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	6	20.55
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	8	20.49
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	8	20.46
(1,141)	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	1:34:B:TYR:N	4	20.41
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1	20.37
(1,37)	1:52:A:ARG:C	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	7	20.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,119)	1:52:B:ARG:C	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	7	20.24
(1,78)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:GLU:N	2	19.84
(1,159)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:LYS:N	7	19.77
(1,131)	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	1:18:B:ASP:N	10	19.52
(1,39)	1:54:A:GLU:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	7	19.47
(1,49)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:ASP:N	10	19.32
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	5	19.23
(1,160)	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	1:54:B:GLU:N	2	19.13
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	5	19.1
(1,77)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:LYS:N	7	19.01
(1,79)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:GLN:N	2	17.95
(1,126)	1:12:B:GLU:N	1:12:B:GLU:CA	1:12:B:GLU:C	1:13:B:GLN:N	3	17.33
(1,44)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:GLN:N	3	17.26
(1,131)	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	1:18:B:ASP:N	4	17.17
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	8	17.05
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	8	17.03
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	8	17.01
(1,121)	1:54:B:GLU:C	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	7	16.85
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	8	16.81
(1,76)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:ARG:N	8	16.78
(1,3)	1:11:A:GLU:C	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	4	16.77
(1,158)	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	1:52:B:ARG:N	8	16.75
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	4	16.48
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	4	16.45
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	2	16.39
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	2	16.38
(1,161)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:GLN:N	2	16.36
(1,164)	1:57:B:ILE:N	1:57:B:ILE:CA	1:57:B:ILE:C	1:58:B:GLY:N	6	16.31
(1,12)	1:25:A:ARG:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	9	16.21
(1,134)	1:20:B:ALA:N	1:20:B:ALA:CA	1:20:B:ALA:C	1:21:B:PHE:N	10	16.19
(1,52)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:PHE:N	10	16.12
(1,82)	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	1:58:A:GLY:N	6	16.11
(1,141)	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	1:34:B:TYR:N	9	15.97
(1,50)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LEU:N	8	15.81
(1,78)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:GLU:N	6	15.75
(1,94)	1:25:B:ARG:C	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	9	15.67
(1,85)	1:11:B:GLU:C	1:12:B:GLU:N	1:12:B:GLU:CA	1:12:B:GLU:C	4	15.67
(1,132)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:LEU:N	8	15.66
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	4	15.59
(1,160)	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	1:54:B:GLU:N	6	15.37
(1,69)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:GLN:N	2	15.27
(1,151)	1:44:B:GLU:N	1:44:B:GLU:CA	1:44:B:GLU:C	1:45:B:GLN:N	2	15.22
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	8	14.77
(1,133)	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	1:20:B:ALA:N	3	14.75
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	8	14.72
(1,59)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:TYR:N	9	14.67
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	7	14.57
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	10	14.53
(1,141)	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	1:34:B:TYR:N	5	14.47
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	7	14.43
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	10	14.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:10:A:SER:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	2	14.34
(1,51)	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	1:20:A:ALA:N	5	14.29
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	5	14.18
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	3	14.13
(1,133)	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	1:20:B:ALA:N	5	14.09
(1,59)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:TYR:N	5	14.05
(1,84)	1:10:B:SER:C	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	2	13.99
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	4	13.99
(1,79)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:GLN:N	6	13.97
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	3	13.96
(1,141)	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	1:34:B:TYR:N	10	13.88
(1,78)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:GLU:N	5	13.69
(1,161)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:GLN:N	6	13.64
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	9	13.64
(1,131)	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	1:18:B:ASP:N	6	13.63
(1,160)	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	1:54:B:GLU:N	5	13.57
(1,141)	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	1:34:B:TYR:N	6	13.55
(1,80)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLN:N	3	13.49
(1,94)	1:25:B:ARG:C	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	10	13.47
(1,162)	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	1:56:B:GLN:N	3	13.46
(1,59)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:TYR:N	6	13.45
(1,49)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:ASP:N	6	13.43
(1,51)	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	1:20:A:ALA:N	3	13.39
(1,59)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:TYR:N	10	13.36
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	4	13.32
(1,2)	1:10:A:SER:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	5	13.3
(1,69)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:GLN:N	10	13.28
(1,84)	1:10:B:SER:C	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	5	13.26
(1,151)	1:44:B:GLU:N	1:44:B:GLU:CA	1:44:B:GLU:C	1:45:B:GLN:N	10	13.25
(1,12)	1:25:A:ARG:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	10	13.25
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	4	13.16
(1,46)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:LYS:N	7	13.16
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	9	13.11
(1,87)	1:13:B:GLN:C	1:14:B:LYS:N	1:14:B:LYS:CA	1:14:B:LYS:C	3	13.04
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	3	13.0
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	5	12.84
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	3	12.79
(1,106)	1:39:B:LEU:C	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	2	12.76
(1,159)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:LYS:N	1	12.71
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1	12.71
(1,77)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:LYS:N	1	12.65
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1	12.59
(1,24)	1:39:A:LEU:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	2	12.59
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	5	12.53
(1,41)	1:56:A:GLN:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	1	12.5
(1,123)	1:56:B:GLN:C	1:57:B:ILE:N	1:57:B:ILE:CA	1:57:B:ILE:C	1	12.48
(1,133)	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	1:20:B:ALA:N	4	12.44
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	1	12.39
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	1	12.37
(1,141)	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	1:34:B:TYR:N	1	12.27
(1,59)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:TYR:N	1	12.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,123)	1:56:B:GLN:C	1:57:B:ILE:N	1:57:B:ILE:CA	1:57:B:ILE:C	6	12.25
(1,41)	1:56:A:GLN:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	6	12.21
(1,128)	1:14:B:LYS:N	1:14:B:LYS:CA	1:14:B:LYS:C	1:15:B:LYS:N	7	12.18
(1,5)	1:13:A:GLN:C	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	3	12.05
(1,51)	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	1:20:A:ALA:N	4	11.99
(1,6)	1:14:A:LYS:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	7	11.95
(1,6)	1:14:A:LYS:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	3	11.92
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	5	11.82
(1,134)	1:20:B:ALA:N	1:20:B:ALA:CA	1:20:B:ALA:C	1:21:B:PHE:N	8	11.66
(1,50)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LEU:N	3	11.66
(1,52)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:PHE:N	8	11.62
(1,88)	1:14:B:LYS:C	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	7	11.54
(1,39)	1:54:A:GLU:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	4	11.47
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	9	11.34
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	5	11.25
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	9	11.24
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	5	11.2
(1,131)	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	1:18:B:ASP:N	9	11.18
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	6	11.15
(1,88)	1:14:B:LYS:C	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	3	11.14
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	6	11.0
(1,159)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:LYS:N	4	10.97
(1,152)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ILE:N	8	10.93
(1,70)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ILE:N	8	10.93
(1,121)	1:54:B:GLU:C	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	4	10.92
(1,78)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:GLU:N	4	10.86
(1,15)	1:29:A:PRO:C	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1	10.74
(1,132)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:LEU:N	3	10.71
(1,97)	1:29:B:PRO:C	1:30:B:GLU:N	1:30:B:GLU:CA	1:30:B:GLU:C	1	10.71
(1,77)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:LYS:N	4	10.55
(1,160)	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	1:54:B:GLU:N	8	10.52
(1,78)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:GLU:N	8	10.49
(1,134)	1:20:B:ALA:N	1:20:B:ALA:CA	1:20:B:ALA:C	1:21:B:PHE:N	3	10.26
(1,65)	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	1:41:A:LEU:N	1	10.08
(1,52)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:PHE:N	3	10.06
(1,147)	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	1:41:B:LEU:N	1	10.0
(1,159)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:LYS:N	3	9.85
(1,160)	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	1:54:B:GLU:N	4	9.83
(1,133)	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	1:20:B:ALA:N	6	9.82
(1,123)	1:56:B:GLN:C	1:57:B:ILE:N	1:57:B:ILE:CA	1:57:B:ILE:C	4	9.81
(1,21)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	9	9.8
(1,41)	1:56:A:GLN:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	4	9.75
(1,51)	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	1:20:A:ALA:N	6	9.73
(1,160)	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	1:54:B:GLU:N	7	9.7
(1,133)	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	1:20:B:ALA:N	8	9.69
(1,51)	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	1:20:A:ALA:N	8	9.68
(1,78)	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1:54:A:GLU:N	7	9.67
(1,77)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:LYS:N	3	9.65
(1,103)	1:35:B:LEU:C	1:36:B:SER:N	1:36:B:SER:CA	1:36:B:SER:C	9	9.53
(1,49)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:ASP:N	5	9.49
(1,131)	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	1:18:B:ASP:N	5	9.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	9	9.42
(1,99)	1:31:B:TRP:C	1:32:B:ARG:N	1:32:B:ARG:CA	1:32:B:ARG:C	5	9.26
(1,84)	1:10:B:SER:C	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	10	9.07
(1,120)	1:53:B:LYS:C	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	10	9.04
(1,38)	1:53:A:LYS:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	10	9.0
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	7	8.99
(1,12)	1:25:A:ARG:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	7	8.82
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	7	8.8
(1,9)	1:17:A:LEU:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	9	8.75
(1,132)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:LEU:N	1	8.7
(1,43)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:GLU:N	8	8.48
(1,125)	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	1:12:B:GLU:N	8	8.46
(1,72)	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	1:48:A:ARG:N	10	8.4
(1,19)	1:33:A:ARG:C	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	3	8.4
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	5	8.29
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	5	8.28
(1,50)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LEU:N	1	8.25
(1,8)	1:16:A:ALA:C	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	10	8.1
(1,111)	1:44:B:GLU:C	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	2	7.97
(1,90)	1:16:B:ALA:C	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	10	7.95
(1,129)	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	1:16:B:ALA:N	7	7.91
(1,22)	1:36:A:SER:C	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	1	7.87
(1,11)	1:19:A:LEU:C	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	9	7.82
(1,29)	1:44:A:GLU:C	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	2	7.81
(1,43)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:GLU:N	4	7.65
(1,125)	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	1:12:B:GLU:N	4	7.55
(1,72)	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	1:48:A:ARG:N	1	7.53
(1,154)	1:47:B:GLU:N	1:47:B:GLU:CA	1:47:B:GLU:C	1:48:B:ARG:N	1	7.51
(1,134)	1:20:B:ALA:N	1:20:B:ALA:CA	1:20:B:ALA:C	1:21:B:PHE:N	7	7.51
(1,52)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:PHE:N	7	7.46
(1,21)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	1	7.43
(1,52)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:PHE:N	1	7.42
(1,159)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:LYS:N	9	7.38
(1,127)	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	1:14:B:LYS:N	2	7.35
(1,6)	1:14:A:LYS:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	10	7.34
(1,103)	1:35:B:LEU:C	1:36:B:SER:N	1:36:B:SER:CA	1:36:B:SER:C	1	7.27
(1,100)	1:32:B:ARG:C	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	9	7.26
(1,88)	1:14:B:LYS:C	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	10	7.26
(1,134)	1:20:B:ALA:N	1:20:B:ALA:CA	1:20:B:ALA:C	1:21:B:PHE:N	1	7.2
(1,85)	1:11:B:GLU:C	1:12:B:GLU:N	1:12:B:GLU:CA	1:12:B:GLU:C	10	7.2
(1,104)	1:36:B:SER:C	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	1	7.11
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	7	7.11
(1,49)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:ASP:N	8	7.08
(1,18)	1:32:A:ARG:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	9	7.08
(1,131)	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	1:18:B:ASP:N	8	7.07
(1,12)	1:25:A:ARG:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	4	7.04
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	7	7.01
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	9	6.99
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	9	6.96
(1,154)	1:47:B:GLU:N	1:47:B:GLU:CA	1:47:B:GLU:C	1:48:B:ARG:N	10	6.95
(1,94)	1:25:B:ARG:C	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	7	6.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,77)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:LYS:N	9	6.89
(1,45)	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	1:14:A:LYS:N	2	6.87
(1,101)	1:33:B:ARG:C	1:34:B:TYR:N	1:34:B:TYR:CA	1:34:B:TYR:C	3	6.86
(1,2)	1:10:A:SER:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	10	6.8
(1,52)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:PHE:N	9	6.78
(1,131)	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	1:18:B:ASP:N	2	6.72
(1,49)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:ASP:N	2	6.64
(1,100)	1:32:B:ARG:C	1:33:B:ARG:N	1:33:B:ARG:CA	1:33:B:ARG:C	4	6.63
(1,147)	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	1:41:B:LEU:N	7	6.53
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	5	6.53
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	9	6.52
(1,134)	1:20:B:ALA:N	1:20:B:ALA:CA	1:20:B:ALA:C	1:21:B:PHE:N	9	6.45
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	3	6.45
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	3	6.43
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	9	6.17
(1,154)	1:47:B:GLU:N	1:47:B:GLU:CA	1:47:B:GLU:C	1:48:B:ARG:N	4	6.13
(1,91)	1:17:B:LEU:C	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	10	6.12
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	5	6.03
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	5	6.01
(1,65)	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	1:41:A:LEU:N	7	5.99
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	9	5.97
(1,43)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:GLU:N	9	5.9
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	5	5.83
(1,75)	1:50:A:PHE:N	1:50:A:PHE:CA	1:50:A:PHE:C	1:51:A:ARG:N	7	5.83
(1,157)	1:50:B:PHE:N	1:50:B:PHE:CA	1:50:B:PHE:C	1:51:B:ARG:N	7	5.8
(1,9)	1:17:A:LEU:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	10	5.79
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	4	5.7
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	4	5.6
(1,137)	1:29:B:PRO:N	1:29:B:PRO:CA	1:29:B:PRO:C	1:30:B:GLU:N	1	5.59
(1,10)	1:18:A:ASP:C	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	8	5.55
(1,147)	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	1:41:B:LEU:N	6	5.5
(1,132)	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	1:19:B:LEU:N	9	5.5
(1,55)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:GLU:N	1	5.46
(1,92)	1:18:B:ASP:C	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	8	5.45
(1,19)	1:33:A:ARG:C	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	8	5.44
(1,101)	1:33:B:ARG:C	1:34:B:TYR:N	1:34:B:TYR:CA	1:34:B:TYR:C	8	5.42
(1,114)	1:47:B:GLU:C	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	4	5.39
(1,65)	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	1:41:A:LEU:N	6	5.31
(1,125)	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	1:12:B:GLU:N	10	5.3
(1,44)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:GLN:N	10	5.3
(1,5)	1:13:A:GLN:C	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	10	5.26
(1,79)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:GLN:N	4	5.15
(1,41)	1:56:A:GLN:C	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	2	5.11
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	10	5.09
(1,163)	1:56:B:GLN:N	1:56:B:GLN:CA	1:56:B:GLN:C	1:57:B:ILE:N	2	4.93
(1,99)	1:31:B:TRP:C	1:32:B:ARG:N	1:32:B:ARG:CA	1:32:B:ARG:C	8	4.93
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1	4.92
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	1	4.91
(1,17)	1:31:A:TRP:C	1:32:A:ARG:N	1:32:A:ARG:CA	1:32:A:ARG:C	8	4.91
(1,44)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:GLN:N	7	4.89
(1,126)	1:12:B:GLU:N	1:12:B:GLU:CA	1:12:B:GLU:C	1:13:B:GLN:N	7	4.88

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:12:B:GLU:C	1:13:B:GLN:N	1:13:B:GLN:CA	1:13:B:GLN:C	2	4.87
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	10	4.85
(1,47)	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	1:16:A:ALA:N	7	4.84
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	2	4.71
(1,4)	1:12:A:GLU:C	1:13:A:GLN:N	1:13:A:GLN:CA	1:13:A:GLN:C	2	4.69
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	2	4.67
(1,79)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:GLN:N	10	4.67
(1,117)	1:50:B:PHE:C	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	2	4.64
(1,161)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:GLN:N	10	4.58
(1,114)	1:47:B:GLU:C	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	7	4.55
(1,161)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:GLN:N	4	4.53
(1,46)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:LYS:N	3	4.45
(1,125)	1:11:B:GLU:N	1:11:B:GLU:CA	1:11:B:GLU:C	1:12:B:GLU:N	9	4.37
(1,87)	1:13:B:GLN:C	1:14:B:LYS:N	1:14:B:LYS:CA	1:14:B:LYS:C	6	4.35
(1,35)	1:50:A:PHE:C	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	2	4.31
(1,32)	1:47:A:GLU:C	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	7	4.3
(1,6)	1:14:A:LYS:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	4	4.23
(1,83)	1:9:B:PHE:C	1:10:B:SER:N	1:10:B:SER:CA	1:10:B:SER:C	8	4.22
(1,5)	1:13:A:GLN:C	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	6	4.21
(1,22)	1:36:A:SER:C	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	6	4.2
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	7	4.17
(1,104)	1:36:B:SER:C	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	6	4.12
(1,83)	1:9:B:PHE:C	1:10:B:SER:N	1:10:B:SER:CA	1:10:B:SER:C	9	4.08
(1,32)	1:47:A:GLU:C	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	10	4.05
(1,29)	1:44:A:GLU:C	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	10	4.05
(1,1)	1:9:A:PHE:C	1:10:A:SER:N	1:10:A:SER:CA	1:10:A:SER:C	8	4.05
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	7	4.04
(1,123)	1:56:B:GLN:C	1:57:B:ILE:N	1:57:B:ILE:CA	1:57:B:ILE:C	2	4.03
(1,76)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:ARG:N	5	4.03
(1,158)	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	1:52:B:ARG:N	5	3.99
(1,128)	1:14:B:LYS:N	1:14:B:LYS:CA	1:14:B:LYS:C	1:15:B:LYS:N	3	3.96
(1,7)	1:15:A:LYS:C	1:16:A:ALA:N	1:16:A:ALA:CA	1:16:A:ALA:C	6	3.91
(1,111)	1:44:B:GLU:C	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	10	3.89
(1,147)	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	1:41:B:LEU:N	8	3.88
(1,114)	1:47:B:GLU:C	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	1	3.88
(1,101)	1:33:B:ARG:C	1:34:B:TYR:N	1:34:B:TYR:CA	1:34:B:TYR:C	2	3.88
(1,102)	1:34:B:TYR:C	1:35:B:LEU:N	1:35:B:LEU:CA	1:35:B:LEU:C	8	3.86
(1,20)	1:34:A:TYR:C	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	8	3.86
(1,32)	1:47:A:GLU:C	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	1	3.84
(1,19)	1:33:A:ARG:C	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	2	3.83
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	8	3.76
(1,65)	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	1:41:A:LEU:N	8	3.75
(1,114)	1:47:B:GLU:C	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	10	3.71
(1,1)	1:9:A:PHE:C	1:10:A:SER:N	1:10:A:SER:CA	1:10:A:SER:C	9	3.7
(1,81)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:ILE:N	2	3.69
(1,37)	1:52:A:ARG:C	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	3	3.69
(1,19)	1:33:A:ARG:C	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	4	3.69
(1,89)	1:15:B:LYS:C	1:16:B:ALA:N	1:16:B:ALA:CA	1:16:B:ALA:C	6	3.68
(1,10)	1:18:A:ASP:C	1:19:A:LEU:N	1:19:A:LEU:CA	1:19:A:LEU:C	3	3.62
(1,119)	1:52:B:ARG:C	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	3	3.61
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	8	3.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,65)	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	1:41:A:LEU:N	4	3.49
(1,103)	1:35:B:LEU:C	1:36:B:SER:N	1:36:B:SER:CA	1:36:B:SER:C	7	3.43
(1,94)	1:25:B:ARG:C	1:26:B:ARG:N	1:26:B:ARG:CA	1:26:B:ARG:C	4	3.41
(1,61)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:SER:N	3	3.39
(1,143)	1:35:B:LEU:N	1:35:B:LEU:CA	1:35:B:LEU:C	1:36:B:SER:N	3	3.32
(1,134)	1:20:B:ALA:N	1:20:B:ALA:CA	1:20:B:ALA:C	1:21:B:PHE:N	5	3.24
(1,52)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:PHE:N	5	3.2
(1,101)	1:33:B:ARG:C	1:34:B:TYR:N	1:34:B:TYR:CA	1:34:B:TYR:C	4	3.16
(1,21)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	7	3.14
(1,88)	1:14:B:LYS:C	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	4	3.13
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	3	3.11
(1,158)	1:51:B:ARG:N	1:51:B:ARG:CA	1:51:B:ARG:C	1:52:B:ARG:N	2	3.09
(1,114)	1:47:B:GLU:C	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	3	3.07
(1,32)	1:47:A:GLU:C	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	2	3.07
(1,21)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	6	3.07
(1,103)	1:35:B:LEU:C	1:36:B:SER:N	1:36:B:SER:CA	1:36:B:SER:C	6	3.06
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	3	3.03
(1,32)	1:47:A:GLU:C	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	3	3.0
(1,76)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:ARG:N	2	2.97
(1,30)	1:45:A:GLN:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	5	2.9
(1,147)	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	1:41:B:LEU:N	4	2.88
(1,73)	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	1:49:A:TRP:N	9	2.62
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	1	2.62
(1,164)	1:57:B:ILE:N	1:57:B:ILE:CA	1:57:B:ILE:C	1:58:B:GLY:N	8	2.59
(1,82)	1:57:A:ILE:N	1:57:A:ILE:CA	1:57:A:ILE:C	1:58:A:GLY:N	8	2.53
(1,17)	1:31:A:TRP:C	1:32:A:ARG:N	1:32:A:ARG:CA	1:32:A:ARG:C	5	2.52
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	1	2.51
(1,112)	1:45:B:GLN:C	1:46:B:ILE:N	1:46:B:ILE:CA	1:46:B:ILE:C	5	2.49
(1,73)	1:48:A:ARG:N	1:48:A:ARG:CA	1:48:A:ARG:C	1:49:A:TRP:N	5	2.42
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	4	2.4
(1,19)	1:33:A:ARG:C	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	7	2.37
(1,102)	1:34:B:TYR:C	1:35:B:LEU:N	1:35:B:LEU:CA	1:35:B:LEU:C	6	2.27
(1,1)	1:9:A:PHE:C	1:10:A:SER:N	1:10:A:SER:CA	1:10:A:SER:C	4	2.23
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	4	2.22
(1,30)	1:45:A:GLN:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	3	2.22
(1,112)	1:45:B:GLN:C	1:46:B:ILE:N	1:46:B:ILE:CA	1:46:B:ILE:C	3	2.19
(1,30)	1:45:A:GLN:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	2	2.19
(1,112)	1:45:B:GLN:C	1:46:B:ILE:N	1:46:B:ILE:CA	1:46:B:ILE:C	7	2.15
(1,161)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:GLN:N	9	2.14
(1,66)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ASN:N	6	2.09
(1,79)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:GLN:N	9	2.08
(1,20)	1:34:A:TYR:C	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	6	2.06
(1,6)	1:14:A:LYS:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	5	2.05
(1,151)	1:44:B:GLU:N	1:44:B:GLU:CA	1:44:B:GLU:C	1:45:B:GLN:N	4	2.04
(1,148)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:C	1:42:B:ASN:N	6	2.04
(1,30)	1:45:A:GLN:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	7	2.03
(1,90)	1:16:B:ALA:C	1:17:B:LEU:N	1:17:B:LEU:CA	1:17:B:LEU:C	4	2.01
(1,88)	1:14:B:LYS:C	1:15:B:LYS:N	1:15:B:LYS:CA	1:15:B:LYS:C	5	2.01
(1,112)	1:45:B:GLN:C	1:46:B:ILE:N	1:46:B:ILE:CA	1:46:B:ILE:C	2	1.97
(1,155)	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	1:49:B:TRP:N	5	1.96
(1,30)	1:45:A:GLN:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1	1.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:45:B:GLN:C	1:46:B:ILE:N	1:46:B:ILE:CA	1:46:B:ILE:C	1	1.83
(1,147)	1:40:B:GLY:N	1:40:B:GLY:CA	1:40:B:GLY:C	1:41:B:LEU:N	10	1.73
(1,119)	1:52:B:ARG:C	1:53:B:LYS:N	1:53:B:LYS:CA	1:53:B:LYS:C	1	1.7
(1,83)	1:9:B:PHE:C	1:10:B:SER:N	1:10:B:SER:CA	1:10:B:SER:C	4	1.67
(1,39)	1:54:A:GLU:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	10	1.65
(1,37)	1:52:A:ARG:C	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	1	1.62
(1,101)	1:33:B:ARG:C	1:34:B:TYR:N	1:34:B:TYR:CA	1:34:B:TYR:C	7	1.55
(1,155)	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	1:49:B:TRP:N	9	1.52
(1,121)	1:54:B:GLU:C	1:55:B:GLN:N	1:55:B:GLN:CA	1:55:B:GLN:C	10	1.51
(1,18)	1:32:A:ARG:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	4	1.48
(1,22)	1:36:A:SER:C	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	3	1.45
(1,72)	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	1:48:A:ARG:N	2	1.33
(1,30)	1:45:A:GLN:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	6	1.32
(1,112)	1:45:B:GLN:C	1:46:B:ILE:N	1:46:B:ILE:CA	1:46:B:ILE:C	6	1.31
(1,104)	1:36:B:SER:C	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	3	1.3
(1,112)	1:45:B:GLN:C	1:46:B:ILE:N	1:46:B:ILE:CA	1:46:B:ILE:C	10	1.27
(1,92)	1:18:B:ASP:C	1:19:B:LEU:N	1:19:B:LEU:CA	1:19:B:LEU:C	3	1.24
(1,47)	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	1:16:A:ALA:N	9	1.15
(1,30)	1:45:A:GLN:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	10	1.13
(1,8)	1:16:A:ALA:C	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	5	1.06
(1,155)	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	1:49:B:TRP:N	8	1.05