



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:55 AM UTC

PDB ID : 5I8N / pdb_00005i8n
BMRB ID : 30017
Title : Solution Structure of human calcium-binding S100A9 (C3S) protein
Authors : Chang, C.-C.; Chin, Y.
Deposited on : 2016-02-19

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

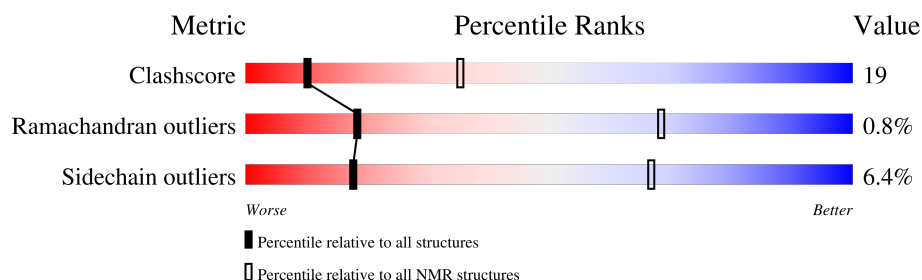
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 40%.

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	114	
1	B	114	

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:92, B:5-B:92 (176)	0.70	4

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3678 atoms, of which 1822 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A9.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1839	579	911	163	180	6	
1	B	114	Total	C	H	N	O	S	0
			1839	579	911	163	180	6	

There are 2 discrepancies between the modelled and reference sequences:

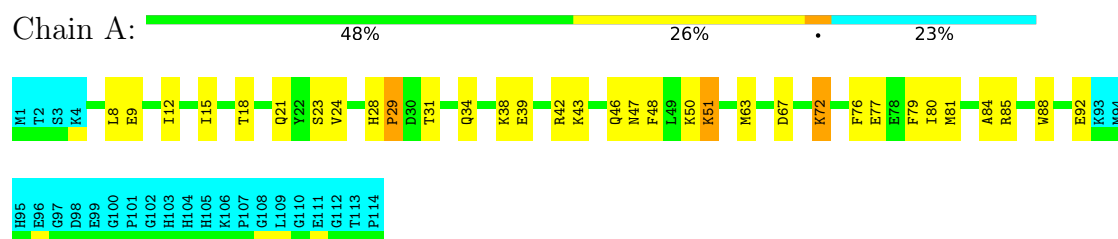
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	CYS	engineered mutation	UNP P06702
B	3	SER	CYS	engineered mutation	UNP P06702

4 Residue-property plots [i](#)

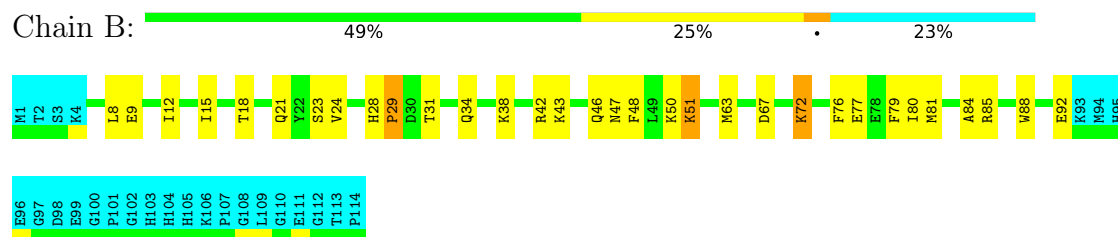
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Protein S100-A9



• Molecule 1: Protein S100-A9

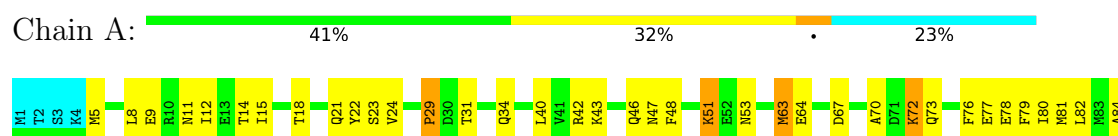


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Protein S100-A9





• Molecule 1: Protein S100-A9

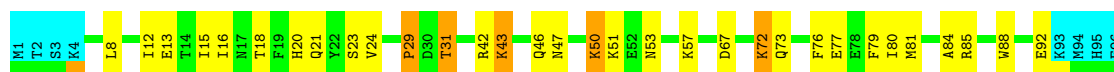


4.2.2 Score per residue for model 2

• Molecule 1: Protein S100-A9

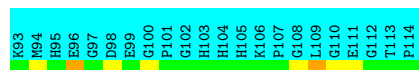


• Molecule 1: Protein S100-A9

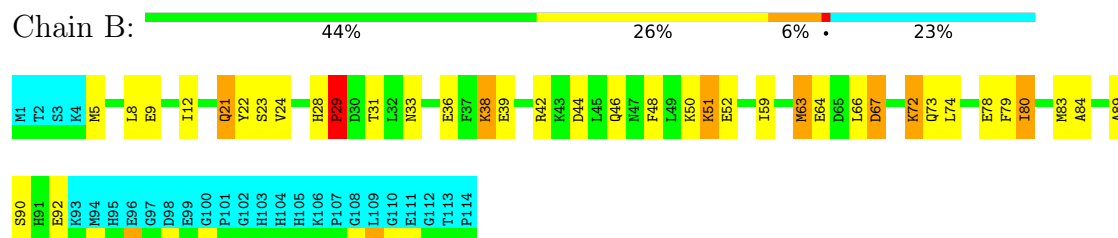


4.2.3 Score per residue for model 3

• Molecule 1: Protein S100-A9

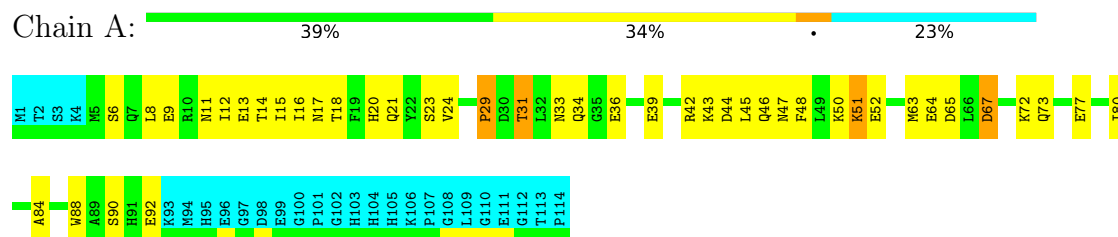


• Molecule 1: Protein S100-A9

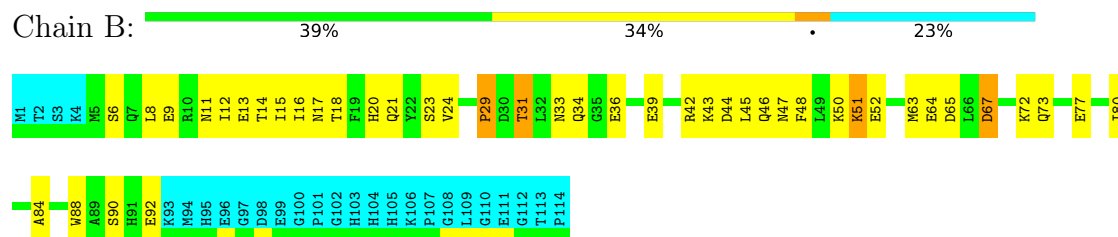


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Protein S100-A9

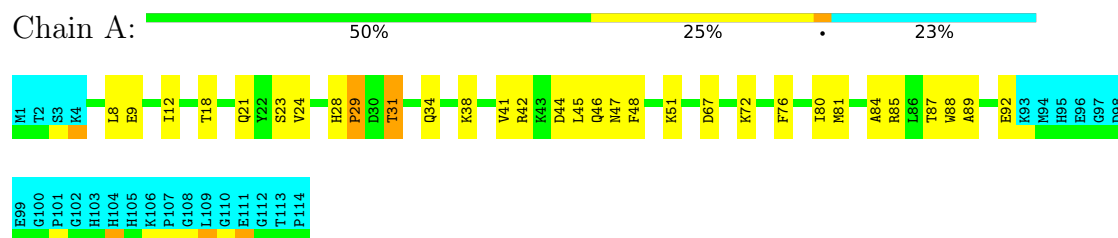


- Molecule 1: Protein S100-A9

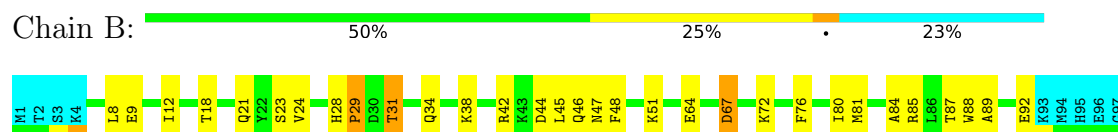


4.2.5 Score per residue for model 5

- Molecule 1: Protein S100-A9



- Molecule 1: Protein S100-A9

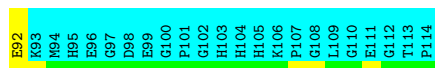




4.2.6 Score per residue for model 6

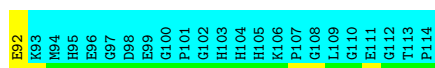
- Molecule 1: Protein S100-A9

Chain A: 45% 30% 23%



- Molecule 1: Protein S100-A9

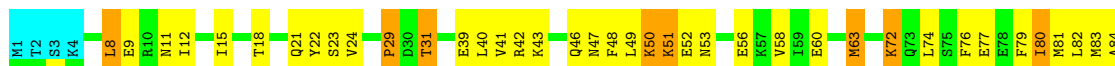
Chain B: 45% 30% 23%



4.2.7 Score per residue for model 7

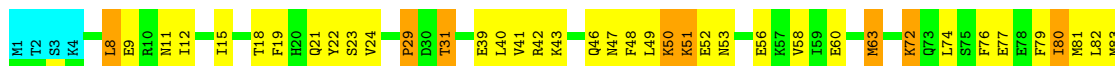
- Molecule 1: Protein S100-A9

Chain A: 40% 30% 7% 23%



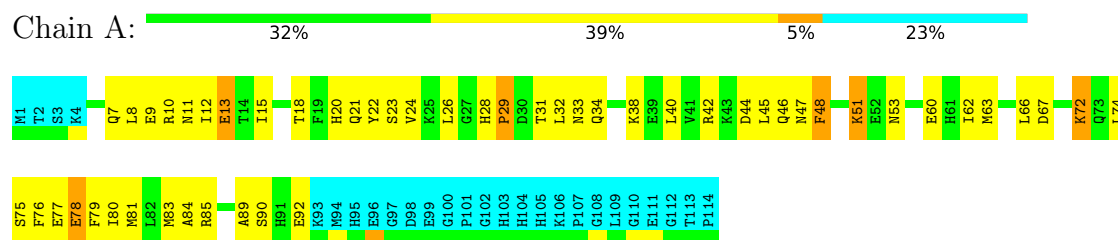
- Molecule 1: Protein S100-A9

Chain B: 40% 30% 7% 23%

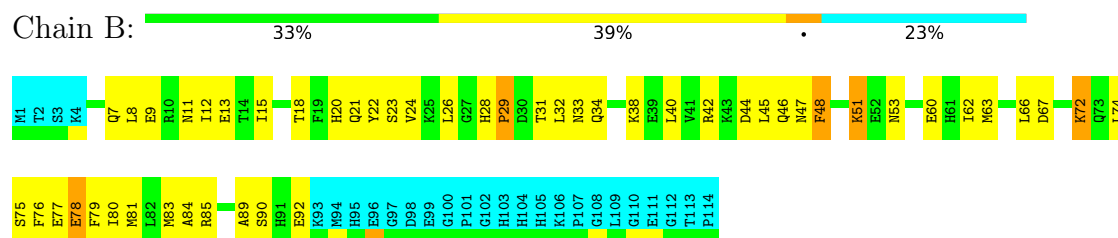


4.2.8 Score per residue for model 8

• Molecule 1: Protein S100-A9

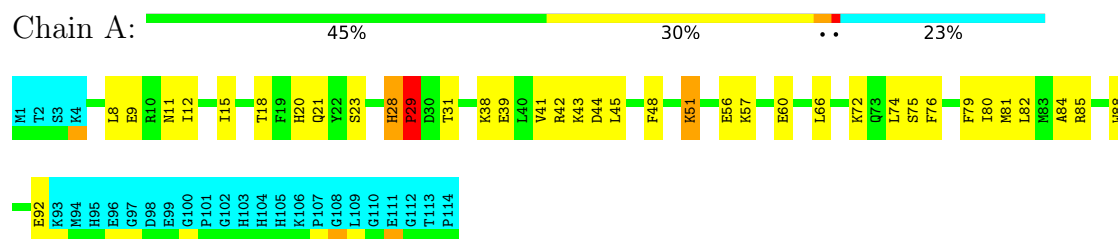


• Molecule 1: Protein S100-A9

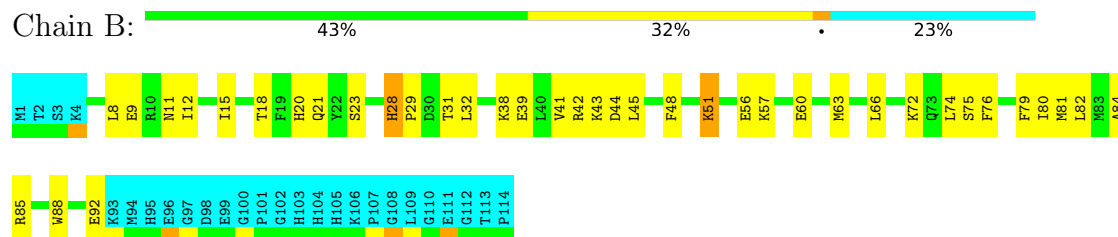


4.2.9 Score per residue for model 9

• Molecule 1: Protein S100-A9



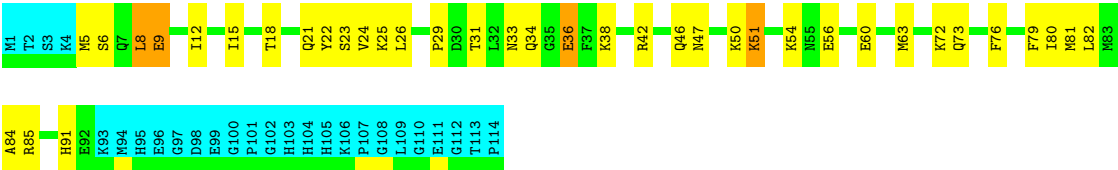
• Molecule 1: Protein S100-A9



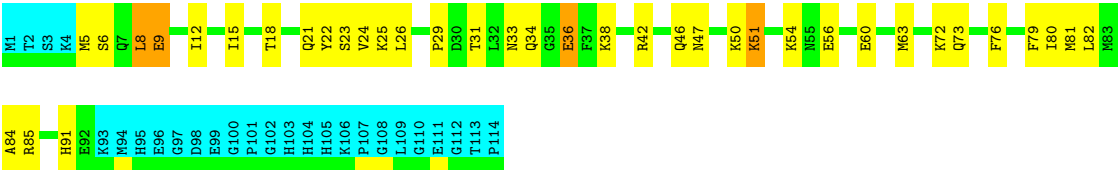
4.2.10 Score per residue for model 10

• Molecule 1: Protein S100-A9





● Molecule 1: Protein S100-A9



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 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
CNS	structure calculation	1.1
CNS	refinement	1.1

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	1201
Number of shifts mapped to atoms	1201
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

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	0.50±0.04	0±1/749 (0.0± 0.1%)	0.81±0.03	0±0/1006 (0.0± 0.0%)
1	B	0.50±0.02	0±0/749 (0.0± 0.0%)	0.81±0.03	0±0/1006 (0.0± 0.0%)
All	All	0.50	2/14980 (0.0%)	0.81	4/20120 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.7
1	B	0.0±0.0	0.8±0.7
All	All	0	16

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	29	PRO	C-N	-5.85	1.25	1.33	9	1
1	A	29	PRO	CA-C	-5.16	1.45	1.52	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	29	PRO	CA-C-O	-5.93	116.92	121.31	3	2
1	B	29	PRO	CA-C-O	-5.87	116.97	121.31	3	2

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	29	PRO	Peptide	6
1	A	29	PRO	Peptide	5
1	A	28	HIS	Peptide	3
1	B	28	HIS	Peptide	2

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	736	729	725	34±10
1	B	736	729	725	34±10
All	All	14720	14580	14500	560

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:GLN:HA	1:B:63:MET:SD	0.85	2.11	4	4
1:A:34:GLN:HA	1:A:63:MET:SD	0.85	2.11	4	4
1:A:80:ILE:HD13	1:B:84:ALA:HB2	0.77	1.55	8	1
1:A:84:ALA:HB2	1:B:80:ILE:HD13	0.77	1.56	8	1
1:A:81:MET:HA	1:B:80:ILE:HD12	0.75	1.58	8	1
1:A:80:ILE:HD12	1:B:81:MET:HA	0.75	1.58	8	1
1:A:8:LEU:HA	1:A:11:ASN:ND2	0.72	2.00	7	1
1:B:8:LEU:HA	1:B:11:ASN:ND2	0.72	2.00	7	1
1:B:77:GLU:O	1:B:80:ILE:HG12	0.71	1.85	8	1
1:A:77:GLU:O	1:A:80:ILE:HG12	0.71	1.85	8	1
1:A:23:SER:HB2	1:A:29:PRO:O	0.70	1.87	5	5
1:B:72:LYS:N	1:B:72:LYS:HE3	0.70	2.02	7	5
1:B:23:SER:HB2	1:B:29:PRO:O	0.70	1.87	5	5
1:A:72:LYS:N	1:A:72:LYS:HE3	0.69	2.02	7	5
1:B:76:PHE:HA	1:B:79:PHE:CE1	0.69	2.23	6	2
1:A:76:PHE:HA	1:A:79:PHE:CE1	0.68	2.23	6	2
1:A:80:ILE:HG21	1:B:84:ALA:HB2	0.67	1.66	2	9
1:A:84:ALA:HB2	1:B:80:ILE:HG21	0.67	1.66	10	9
1:B:18:THR:O	1:B:21:GLN:HG2	0.65	1.92	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:76:PHE:O	1:B:80:ILE:HG23	0.65	1.92	7	2
1:A:18:THR:O	1:A:21:GLN:HG2	0.64	1.92	6	9
1:A:28:HIS:N	1:A:29:PRO:HD3	0.63	2.09	6	1
1:A:76:PHE:O	1:A:80:ILE:HG23	0.63	1.92	7	2
1:A:9:GLU:CD	1:B:48:PHE:HB2	0.62	2.19	4	3
1:A:15:ILE:HG13	1:B:11:ASN:ND2	0.62	2.07	8	1
1:B:28:HIS:N	1:B:29:PRO:HD3	0.62	2.09	6	1
1:A:11:ASN:ND2	1:B:15:ILE:HG13	0.62	2.08	8	1
1:A:15:ILE:HA	1:B:8:LEU:CD2	0.62	2.24	1	2
1:A:31:THR:OG1	1:A:73:GLN:HB3	0.62	1.95	1	3
1:A:80:ILE:HD12	1:B:84:ALA:HB2	0.62	1.70	7	1
1:A:48:PHE:HB2	1:B:9:GLU:CD	0.62	2.20	4	3
1:B:31:THR:OG1	1:B:73:GLN:HB3	0.61	1.95	1	3
1:A:84:ALA:HB2	1:B:80:ILE:HD12	0.61	1.71	7	1
1:A:20:HIS:HA	1:A:23:SER:OG	0.61	1.96	4	3
1:A:48:PHE:HB2	1:B:9:GLU:OE2	0.61	1.96	8	1
1:B:20:HIS:HA	1:B:23:SER:OG	0.61	1.96	4	3
1:B:51:LYS:HD2	1:B:52:GLU:N	0.61	2.10	4	2
1:A:45:LEU:HA	1:B:9:GLU:OE1	0.61	1.96	5	1
1:B:46:GLN:O	1:B:50:LYS:HE3	0.60	1.95	7	1
1:A:42:ARG:HA	1:A:53:ASN:ND2	0.60	2.11	8	2
1:B:74:LEU:HB3	1:B:78:GLU:OE1	0.60	1.96	3	1
1:A:51:LYS:HD2	1:A:52:GLU:N	0.60	2.10	4	2
1:A:46:GLN:O	1:A:50:LYS:HE3	0.60	1.96	7	1
1:B:5:MET:HA	1:B:9:GLU:OE1	0.60	1.96	6	1
1:A:34:GLN:O	1:A:38:LYS:HD3	0.60	1.97	8	1
1:A:76:PHE:HA	1:A:79:PHE:CE2	0.60	2.32	2	2
1:A:8:LEU:CD2	1:B:15:ILE:HA	0.60	2.26	1	2
1:A:9:GLU:OE2	1:B:48:PHE:HB2	0.60	1.96	8	1
1:B:76:PHE:HA	1:B:79:PHE:CE2	0.59	2.32	10	2
1:A:74:LEU:HB3	1:A:78:GLU:OE1	0.59	1.96	3	1
1:B:42:ARG:HA	1:B:53:ASN:ND2	0.59	2.12	8	2
1:A:17:ASN:HA	1:A:20:HIS:CE1	0.59	2.32	4	1
1:B:34:GLN:O	1:B:38:LYS:HD3	0.59	1.97	8	1
1:A:9:GLU:OE1	1:B:45:LEU:HA	0.59	1.96	5	1
1:A:76:PHE:O	1:A:80:ILE:HB	0.59	1.98	9	3
1:B:17:ASN:HA	1:B:20:HIS:CE1	0.59	2.33	4	1
1:B:39:GLU:O	1:B:43:LYS:HG2	0.59	1.98	6	3
1:A:5:MET:HA	1:A:9:GLU:OE1	0.58	1.97	6	1
1:A:39:GLU:O	1:A:43:LYS:HG2	0.58	1.99	6	3
1:A:80:ILE:CD1	1:B:84:ALA:HB2	0.58	2.28	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:76:PHE:O	1:B:80:ILE:HB	0.58	1.99	9	3
1:A:88:TRP:O	1:A:92:GLU:HG2	0.58	1.99	4	6
1:B:8:LEU:O	1:B:12:ILE:HG13	0.58	1.99	4	10
1:B:88:TRP:O	1:B:92:GLU:HG2	0.58	1.99	4	5
1:A:84:ALA:HB2	1:B:80:ILE:CD1	0.58	2.28	7	1
1:A:8:LEU:O	1:A:12:ILE:HG13	0.57	1.99	4	10
1:B:47:ASN:O	1:B:50:LYS:HD2	0.57	2.00	2	1
1:A:48:PHE:HB2	1:B:9:GLU:OE1	0.57	2.00	5	1
1:B:42:ARG:O	1:B:46:GLN:HB3	0.56	2.00	10	9
1:A:44:ASP:CG	1:B:8:LEU:HB3	0.56	2.25	4	1
1:A:9:GLU:OE1	1:B:48:PHE:HB2	0.56	2.00	5	1
1:A:84:ALA:HB2	1:B:80:ILE:CG2	0.56	2.31	3	5
1:A:76:PHE:HA	1:A:79:PHE:CZ	0.56	2.35	2	3
1:A:66:LEU:HB3	1:A:78:GLU:CG	0.56	2.31	3	1
1:A:18:THR:HB	1:B:8:LEU:HD21	0.56	1.77	1	1
1:A:42:ARG:O	1:A:46:GLN:HB3	0.56	2.01	10	8
1:A:8:LEU:HB3	1:B:44:ASP:CG	0.56	2.26	4	1
1:B:76:PHE:HA	1:B:79:PHE:CZ	0.56	2.35	2	3
1:B:66:LEU:HB3	1:B:78:GLU:CG	0.56	2.31	3	1
1:A:47:ASN:O	1:A:50:LYS:HD2	0.55	2.00	2	1
1:A:38:LYS:O	1:A:42:ARG:HB2	0.55	2.02	9	1
1:B:38:LYS:O	1:B:42:ARG:HB2	0.55	2.02	9	1
1:A:44:ASP:O	1:B:9:GLU:HG3	0.55	2.02	3	2
1:A:80:ILE:CG2	1:B:84:ALA:HB2	0.54	2.31	3	5
1:B:28:HIS:H	1:B:29:PRO:CD	0.54	2.15	9	1
1:A:15:ILE:HD12	1:B:15:ILE:HD12	0.54	1.80	4	4
1:A:9:GLU:OE2	1:B:45:LEU:HA	0.53	2.02	4	2
1:A:28:HIS:H	1:A:29:PRO:CD	0.53	2.16	9	1
1:A:20:HIS:O	1:A:24:VAL:HB	0.53	2.04	4	1
1:A:8:LEU:HD21	1:B:18:THR:HB	0.53	1.78	1	1
1:A:50:LYS:HG2	1:A:51:LYS:N	0.53	2.18	2	1
1:A:66:LEU:HB3	1:A:78:GLU:HG2	0.53	1.79	3	1
1:B:66:LEU:HB3	1:B:78:GLU:HG2	0.53	1.80	3	1
1:B:78:GLU:O	1:B:81:MET:HG2	0.53	2.04	1	1
1:B:50:LYS:HG2	1:B:51:LYS:N	0.53	2.18	2	1
1:A:9:GLU:HG3	1:B:44:ASP:O	0.53	2.04	3	2
1:A:81:MET:O	1:A:85:ARG:HG3	0.52	2.03	1	7
1:A:45:LEU:HA	1:B:9:GLU:OE2	0.52	2.03	8	2
1:A:47:ASN:ND2	1:B:5:MET:HA	0.52	2.19	1	2
1:B:79:PHE:O	1:B:82:LEU:HB3	0.52	2.04	1	4
1:A:23:SER:OG	1:A:32:LEU:HG	0.52	2.05	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:GLU:O	1:A:81:MET:HG2	0.52	2.03	1	1
1:B:81:MET:O	1:B:85:ARG:HG3	0.52	2.03	1	7
1:B:28:HIS:N	1:B:29:PRO:CD	0.52	2.72	6	2
1:A:24:VAL:HA	1:A:29:PRO:HB3	0.52	1.81	8	6
1:A:79:PHE:O	1:A:82:LEU:HB3	0.52	2.04	1	4
1:B:20:HIS:O	1:B:24:VAL:HB	0.52	2.04	4	1
1:B:89:ALA:O	1:B:92:GLU:HG3	0.52	2.05	8	2
1:A:28:HIS:N	1:A:29:PRO:CD	0.52	2.72	6	2
1:B:23:SER:OG	1:B:32:LEU:HG	0.52	2.05	8	1
1:B:24:VAL:HA	1:B:29:PRO:HB3	0.51	1.81	8	6
1:B:74:LEU:HB3	1:B:78:GLU:CD	0.51	2.30	8	1
1:A:11:ASN:OD1	1:B:15:ILE:HG13	0.51	2.05	9	1
1:A:74:LEU:HB3	1:A:78:GLU:CD	0.51	2.30	8	1
1:A:89:ALA:O	1:A:92:GLU:HG3	0.51	2.06	8	2
1:A:15:ILE:HG13	1:B:11:ASN:OD1	0.51	2.06	9	1
1:A:80:ILE:HG12	1:B:80:ILE:HG12	0.51	1.83	7	1
1:A:81:MET:SD	1:A:85:ARG:HD2	0.50	2.46	8	1
1:B:38:LYS:O	1:B:42:ARG:HG3	0.50	2.06	3	2
1:A:80:ILE:O	1:A:83:MET:HB2	0.50	2.07	7	1
1:B:81:MET:SD	1:B:85:ARG:HD2	0.50	2.46	8	1
1:A:77:GLU:O	1:A:80:ILE:HG22	0.50	2.07	1	4
1:A:15:ILE:HA	1:B:8:LEU:CD1	0.49	2.37	2	1
1:B:51:LYS:N	1:B:51:LYS:HD2	0.49	2.22	1	1
1:A:80:ILE:HD13	1:B:84:ALA:CB	0.49	2.35	8	1
1:A:80:ILE:HG23	1:B:80:ILE:HG23	0.49	1.84	9	3
1:A:5:MET:HA	1:B:47:ASN:ND2	0.49	2.21	10	2
1:B:80:ILE:O	1:B:83:MET:HB2	0.49	2.07	7	1
1:A:84:ALA:CB	1:B:80:ILE:HD13	0.49	2.36	8	1
1:B:77:GLU:O	1:B:80:ILE:HG22	0.49	2.08	1	4
1:A:38:LYS:O	1:A:42:ARG:HG3	0.49	2.07	3	2
1:A:15:ILE:HG13	1:B:11:ASN:HD22	0.49	1.68	8	1
1:B:26:LEU:HD11	1:B:33:ASN:ND2	0.49	2.22	8	2
1:A:51:LYS:N	1:A:51:LYS:HD2	0.49	2.23	1	1
1:B:24:VAL:CA	1:B:29:PRO:HB3	0.49	2.38	8	5
1:A:31:THR:CB	1:A:73:GLN:HB3	0.49	2.37	3	1
1:B:31:THR:HG22	1:B:75:SER:CA	0.49	2.38	9	1
1:B:9:GLU:H	1:B:9:GLU:CD	0.49	2.16	10	1
1:A:24:VAL:CA	1:A:29:PRO:HB3	0.49	2.38	8	5
1:A:11:ASN:OD1	1:B:15:ILE:HG12	0.49	2.07	7	1
1:A:9:GLU:H	1:A:9:GLU:CD	0.49	2.16	10	1
1:B:31:THR:CB	1:B:73:GLN:HB3	0.49	2.37	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:31:THR:HG21	1:B:73:GLN:OE1	0.49	2.08	4	1
1:B:75:SER:HB3	1:B:78:GLU:OE1	0.49	2.08	6	1
1:A:8:LEU:CD1	1:B:15:ILE:HA	0.48	2.38	2	1
1:A:46:GLN:HA	1:A:53:ASN:ND2	0.48	2.23	7	1
1:A:26:LEU:HD11	1:A:33:ASN:ND2	0.48	2.23	8	2
1:A:75:SER:HB3	1:A:78:GLU:OE1	0.48	2.08	6	1
1:B:20:HIS:CD2	1:B:29:PRO:HG3	0.48	2.44	8	1
1:A:15:ILE:HG12	1:B:11:ASN:OD1	0.48	2.08	7	1
1:A:31:THR:HG22	1:A:75:SER:CA	0.48	2.39	9	1
1:A:11:ASN:HD22	1:B:15:ILE:HG13	0.48	1.69	8	1
1:A:6:SER:HB2	1:A:9:GLU:OE1	0.48	2.09	10	1
1:A:11:ASN:HA	1:B:11:ASN:ND2	0.47	2.23	1	1
1:A:56:GLU:O	1:A:60:GLU:HG2	0.47	2.09	10	3
1:B:21:GLN:HG3	1:B:22:TYR:N	0.47	2.24	3	1
1:A:64:GLU:HA	1:A:67:ASP:CB	0.47	2.39	6	3
1:B:56:GLU:O	1:B:60:GLU:HG2	0.47	2.09	10	3
1:A:81:MET:CA	1:B:80:ILE:HD12	0.47	2.36	8	1
1:B:25:LYS:HD2	1:B:36:GLU:CG	0.47	2.40	10	1
1:A:31:THR:HG21	1:A:73:GLN:OE1	0.47	2.09	4	1
1:B:46:GLN:O	1:B:50:LYS:HA	0.47	2.10	6	2
1:B:46:GLN:HA	1:B:53:ASN:ND2	0.47	2.23	7	1
1:A:20:HIS:CD2	1:A:29:PRO:HG3	0.47	2.43	8	1
1:A:80:ILE:HG13	1:B:80:ILE:HG13	0.47	1.87	9	1
1:A:90:SER:OG	1:B:16:ILE:HD13	0.47	2.10	4	1
1:A:21:GLN:HG3	1:A:22:TYR:N	0.47	2.24	3	1
1:A:16:ILE:HD13	1:B:90:SER:OG	0.47	2.10	4	1
1:A:81:MET:HA	1:B:80:ILE:CD1	0.47	2.37	8	1
1:A:11:ASN:ND2	1:B:11:ASN:HA	0.47	2.24	1	1
1:A:11:ASN:ND2	1:B:14:THR:HB	0.47	2.25	1	2
1:A:80:ILE:HD13	1:A:81:MET:N	0.47	2.25	7	1
1:A:14:THR:HB	1:B:11:ASN:ND2	0.47	2.25	1	2
1:A:80:ILE:HD12	1:B:81:MET:CA	0.47	2.36	8	1
1:A:46:GLN:O	1:A:50:LYS:HA	0.46	2.10	10	2
1:B:80:ILE:HD13	1:B:81:MET:N	0.46	2.25	7	1
1:B:59:ILE:O	1:B:63:MET:HB2	0.46	2.10	3	1
1:B:74:LEU:HB3	1:B:78:GLU:OE2	0.46	2.10	8	1
1:B:64:GLU:O	1:B:67:ASP:HB3	0.46	2.09	1	1
1:A:25:LYS:HD2	1:A:36:GLU:CG	0.46	2.40	10	1
1:B:33:ASN:HB3	1:B:36:GLU:OE2	0.46	2.11	3	1
1:B:6:SER:HB2	1:B:9:GLU:OE1	0.46	2.09	10	1
1:A:59:ILE:O	1:A:63:MET:HB2	0.46	2.10	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ASN:HB2	1:A:36:GLU:OE1	0.46	2.10	4	1
1:A:34:GLN:HA	1:A:63:MET:CG	0.46	2.40	1	1
1:B:64:GLU:HA	1:B:67:ASP:CB	0.46	2.40	6	3
1:A:74:LEU:HB3	1:A:78:GLU:OE2	0.46	2.10	8	1
1:B:66:LEU:CD1	1:B:82:LEU:HB2	0.46	2.40	9	1
1:A:79:PHE:O	1:A:83:MET:HG2	0.46	2.10	3	2
1:A:8:LEU:HD12	1:B:18:THR:HG21	0.46	1.88	7	1
1:B:34:GLN:HA	1:B:63:MET:CG	0.46	2.41	1	1
1:B:88:TRP:O	1:B:91:HIS:HB3	0.46	2.11	1	2
1:B:33:ASN:HB2	1:B:36:GLU:OE1	0.46	2.10	4	1
1:A:66:LEU:CD1	1:A:82:LEU:HB2	0.46	2.40	9	1
1:A:51:LYS:HD2	1:A:51:LYS:H	0.46	1.70	1	1
1:A:88:TRP:O	1:A:91:HIS:HB3	0.45	2.11	1	2
1:A:21:GLN:O	1:A:24:VAL:HG12	0.45	2.12	4	2
1:B:51:LYS:HD2	1:B:51:LYS:H	0.45	1.70	1	1
1:A:33:ASN:HB3	1:A:36:GLU:OE2	0.45	2.11	3	1
1:A:64:GLU:O	1:A:67:ASP:HB3	0.45	2.11	1	1
1:A:31:THR:HA	1:A:74:LEU:O	0.45	2.11	3	3
1:B:77:GLU:HA	1:B:80:ILE:HD12	0.45	1.88	7	1
1:A:80:ILE:CD1	1:B:81:MET:HA	0.45	2.37	8	1
1:A:76:PHE:CE1	1:B:88:TRP:HB2	0.45	2.47	9	1
1:B:28:HIS:H	1:B:29:PRO:HD2	0.45	1.70	9	1
1:B:31:THR:HA	1:B:74:LEU:O	0.45	2.12	3	3
1:B:21:GLN:O	1:B:24:VAL:HG12	0.45	2.12	4	2
1:A:43:LYS:HB2	1:A:43:LYS:NZ	0.45	2.27	2	1
1:A:88:TRP:HB2	1:B:76:PHE:CE1	0.45	2.47	9	1
1:A:51:LYS:HD3	1:A:51:LYS:H	0.45	1.71	2	4
1:B:63:MET:O	1:B:67:ASP:HB2	0.45	2.12	3	1
1:A:23:SER:O	1:A:29:PRO:HB2	0.45	2.12	6	1
1:A:48:PHE:HB2	1:B:9:GLU:HG3	0.45	1.88	7	1
1:A:75:SER:O	1:A:78:GLU:HB3	0.45	2.12	8	1
1:A:77:GLU:HA	1:A:80:ILE:HD12	0.44	1.88	7	1
1:A:63:MET:O	1:A:67:ASP:HB2	0.44	2.12	3	1
1:B:79:PHE:O	1:B:83:MET:HG2	0.44	2.11	3	2
1:B:22:TYR:O	1:B:36:GLU:HG2	0.44	2.12	10	1
1:B:43:LYS:HB2	1:B:43:LYS:NZ	0.44	2.27	2	1
1:A:64:GLU:HA	1:A:67:ASP:HB3	0.44	1.89	4	1
1:B:42:ARG:HA	1:B:53:ASN:HD21	0.44	1.72	8	1
1:B:75:SER:O	1:B:78:GLU:HB3	0.44	2.12	8	1
1:A:7:GLN:O	1:A:11:ASN:HB2	0.44	2.13	8	1
1:A:9:GLU:HG3	1:B:48:PHE:HB2	0.44	1.89	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LYS:HD2	1:A:52:GLU:H	0.44	1.73	7	1
1:A:63:MET:HE2	1:A:74:LEU:HG	0.44	1.90	3	2
1:A:42:ARG:HA	1:A:53:ASN:HD21	0.44	1.71	8	1
1:B:67:ASP:OD2	1:B:70:ALA:HA	0.44	2.13	1	1
1:B:51:LYS:HD2	1:B:52:GLU:H	0.44	1.73	7	1
1:B:63:MET:HE2	1:B:74:LEU:HG	0.44	1.90	3	2
1:A:22:TYR:O	1:A:36:GLU:HG2	0.44	2.12	10	1
1:B:64:GLU:HA	1:B:67:ASP:HB3	0.43	1.90	4	2
1:A:22:TYR:CD2	1:A:40:LEU:HD23	0.43	2.48	8	2
1:B:51:LYS:HD3	1:B:51:LYS:H	0.43	1.71	2	3
1:B:23:SER:O	1:B:29:PRO:HB2	0.43	2.12	6	1
1:B:26:LEU:HD11	1:B:33:ASN:HD22	0.43	1.72	10	1
1:A:67:ASP:OD2	1:A:70:ALA:HA	0.43	2.13	1	1
1:B:11:ASN:O	1:B:15:ILE:HG13	0.43	2.12	4	1
1:A:9:GLU:CD	1:B:47:ASN:HB3	0.43	2.38	6	1
1:B:5:MET:SD	1:B:5:MET:N	0.43	2.91	10	1
1:B:63:MET:HE2	1:B:74:LEU:CD2	0.43	2.44	3	1
1:B:41:VAL:HG13	1:B:49:LEU:HD12	0.43	1.89	7	1
1:A:5:MET:SD	1:A:5:MET:N	0.43	2.91	10	1
1:B:23:SER:HB3	1:B:31:THR:O	0.43	2.14	1	1
1:B:51:LYS:HZ1	1:B:52:GLU:CD	0.43	2.21	3	1
1:A:5:MET:HA	1:A:9:GLU:OE2	0.43	2.13	3	1
1:A:63:MET:HE2	1:A:74:LEU:CD2	0.43	2.44	3	1
1:B:5:MET:HA	1:B:9:GLU:OE2	0.43	2.13	3	1
1:A:80:ILE:HD13	1:A:81:MET:H	0.43	1.74	7	1
1:B:80:ILE:HD13	1:B:81:MET:H	0.43	1.74	7	1
1:A:23:SER:HB3	1:A:31:THR:O	0.43	2.14	1	1
1:A:18:THR:HG21	1:B:8:LEU:HD12	0.43	1.90	7	1
1:B:22:TYR:CE1	1:B:40:LEU:HD23	0.43	2.49	7	1
1:B:31:THR:HB	1:B:73:GLN:HB3	0.43	1.91	3	1
1:A:11:ASN:O	1:A:15:ILE:HG13	0.43	2.12	4	1
1:A:50:LYS:HG3	1:A:51:LYS:N	0.43	2.29	4	1
1:B:22:TYR:CD2	1:B:40:LEU:HD23	0.43	2.48	8	2
1:A:47:ASN:HB3	1:B:9:GLU:CD	0.43	2.39	6	1
1:B:17:ASN:HA	1:B:20:HIS:NE2	0.43	2.29	4	1
1:A:22:TYR:CE1	1:A:40:LEU:HD23	0.43	2.49	7	1
1:A:41:VAL:HG13	1:A:49:LEU:HD12	0.43	1.89	7	1
1:A:31:THR:HB	1:A:73:GLN:HB3	0.42	1.90	3	1
1:A:67:ASP:OD2	1:A:72:LYS:HE3	0.42	2.15	2	1
1:A:76:PHE:CB	1:B:87:THR:HG21	0.42	2.44	5	1
1:B:29:PRO:O	1:B:31:THR:N	0.42	2.52	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD11	1:A:33:ASN:HD22	0.42	1.72	10	1
1:A:5:MET:HG2	1:A:9:GLU:OE1	0.42	2.14	1	1
1:B:67:ASP:OD2	1:B:72:LYS:HE3	0.42	2.14	2	1
1:A:28:HIS:H	1:A:29:PRO:HD2	0.42	1.73	9	1
1:B:39:GLU:HG3	1:B:43:LYS:HZ2	0.42	1.74	7	1
1:B:7:GLN:O	1:B:11:ASN:HB2	0.42	2.13	8	1
1:B:32:LEU:O	1:B:63:MET:HE1	0.42	2.15	9	1
1:B:5:MET:HG2	1:B:9:GLU:OE1	0.42	2.14	1	1
1:A:44:ASP:OD2	1:B:6:SER:HB3	0.42	2.15	4	1
1:A:34:GLN:O	1:A:38:LYS:HG3	0.42	2.15	5	1
1:A:77:GLU:O	1:A:80:ILE:HD13	0.42	2.15	7	1
1:A:80:ILE:CG1	1:A:81:MET:N	0.42	2.82	8	1
1:B:80:ILE:CG1	1:B:81:MET:N	0.42	2.82	8	1
1:A:17:ASN:HA	1:A:20:HIS:NE2	0.42	2.29	4	1
1:B:63:MET:O	1:B:74:LEU:HD21	0.42	2.14	8	1
1:B:77:GLU:O	1:B:80:ILE:HD13	0.41	2.15	7	1
1:A:80:ILE:HB	1:B:80:ILE:O	0.41	2.15	8	1
1:B:34:GLN:O	1:B:38:LYS:HG3	0.41	2.14	5	1
1:A:45:LEU:HD23	1:B:9:GLU:OE1	0.41	2.15	8	1
1:A:63:MET:O	1:A:74:LEU:HD21	0.41	2.14	8	1
1:A:6:SER:HB3	1:B:44:ASP:OD2	0.41	2.15	4	1
1:B:63:MET:CE	1:B:74:LEU:HG	0.41	2.45	7	2
1:B:31:THR:HG22	1:B:75:SER:HA	0.41	1.92	9	1
1:A:29:PRO:O	1:A:31:THR:N	0.41	2.52	5	2
1:B:50:LYS:HG3	1:B:51:LYS:N	0.41	2.29	4	1
1:A:87:THR:HG21	1:B:76:PHE:CB	0.41	2.44	5	1
1:B:52:GLU:HG2	1:B:58:VAL:HG11	0.41	1.93	7	1
1:A:63:MET:CE	1:A:74:LEU:HG	0.41	2.46	8	2
1:A:10:ARG:O	1:A:13:GLU:HG3	0.41	2.15	8	1
1:A:5:MET:HG3	1:B:47:ASN:ND2	0.41	2.30	10	1
1:A:39:GLU:HG3	1:A:43:LYS:HZ2	0.41	1.76	7	1
1:A:9:GLU:OE1	1:B:45:LEU:HD23	0.41	2.16	8	1
1:A:16:ILE:O	1:A:20:HIS:HB2	0.41	2.16	2	1
1:A:41:VAL:HA	1:A:45:LEU:HB2	0.41	1.92	9	2
1:B:33:ASN:HB2	1:B:36:GLU:OE2	0.41	2.16	6	1
1:B:16:ILE:O	1:B:20:HIS:HB2	0.41	2.16	2	1
1:A:90:SER:OG	1:B:16:ILE:HG21	0.41	2.16	4	1
1:A:52:GLU:HG2	1:A:58:VAL:HG11	0.41	1.93	7	1
1:A:39:GLU:HG2	1:A:43:LYS:CE	0.41	2.46	2	1
1:A:16:ILE:HG21	1:B:90:SER:OG	0.41	2.16	4	1
1:B:23:SER:OG	1:B:29:PRO:HB2	0.41	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ASN:HB2	1:A:36:GLU:OE2	0.41	2.16	6	1
1:A:80:ILE:O	1:B:80:ILE:HB	0.41	2.15	8	1
1:B:85:ARG:HA	1:B:88:TRP:CD2	0.40	2.51	5	1
1:A:8:LEU:HB3	1:B:44:ASP:OD2	0.40	2.15	4	1
1:A:85:ARG:HA	1:A:88:TRP:CD2	0.40	2.51	5	1
1:A:38:LYS:CE	1:A:60:GLU:HG2	0.40	2.46	8	1
1:A:62:ILE:O	1:A:66:LEU:HB2	0.40	2.16	8	1
1:B:51:LYS:H	1:B:51:LYS:HD3	0.40	1.76	8	1
1:B:62:ILE:O	1:B:66:LEU:HB2	0.40	2.16	8	1
1:B:42:ARG:HG2	1:B:53:ASN:OD1	0.40	2.17	2	1
1:A:23:SER:OG	1:A:29:PRO:HB2	0.40	2.16	4	1
1:A:23:SER:HB3	1:A:29:PRO:O	0.40	2.16	8	1
1:A:31:THR:HG22	1:A:75:SER:HA	0.40	1.92	9	1
1:B:41:VAL:HA	1:B:45:LEU:HB2	0.40	1.92	9	1
1:B:19:PHE:CE1	1:B:79:PHE:HE2	0.40	2.35	7	1
1:B:38:LYS:CE	1:B:60:GLU:HG2	0.40	2.47	8	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	88/114 (77%)	85±1 (96±1%)	2±1 (3±1%)	1±1 (1±1%)	18	68
1	B	88/114 (77%)	85±1 (96±1%)	2±1 (3±1%)	1±1 (1±1%)	18	68
All	All	1760/2280 (77%)	1698 (96%)	48 (3%)	14 (1%)	18	68

All 6 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	67	ASP	4
1	B	67	ASP	4
1	A	28	HIS	2
1	B	28	HIS	2
1	A	5	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	B	5	MET	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	83/103 (81%)	78±1 (93±2%)	5±1 (7±2%)	17	66
1	B	83/103 (81%)	78±1 (94±2%)	5±1 (6±2%)	18	67
All	All	1660/2060 (81%)	1553 (94%)	107 (6%)	18	67

All 43 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	72	LYS	10
1	B	72	LYS	10
1	A	51	LYS	9
1	B	51	LYS	9
1	A	31	THR	4
1	B	31	THR	4
1	A	43	LYS	3
1	A	63	MET	3
1	B	43	LYS	3
1	B	63	MET	3
1	A	13	GLU	3
1	B	13	GLU	3
1	A	50	LYS	2
1	A	57	LYS	2
1	B	50	LYS	2
1	B	57	LYS	2
1	A	48	PHE	2
1	A	80	ILE	2
1	B	48	PHE	2
1	B	80	ILE	2
1	A	44	ASP	2
1	B	44	ASP	2
1	A	8	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	B	8	LEU	2
1	A	21	GLN	1
1	A	38	LYS	1
1	A	39	GLU	1
1	B	21	GLN	1
1	B	38	LYS	1
1	B	39	GLU	1
1	A	65	ASP	1
1	B	65	ASP	1
1	A	68	THR	1
1	B	68	THR	1
1	A	78	GLU	1
1	B	78	GLU	1
1	A	29	PRO	1
1	A	9	GLU	1
1	A	36	GLU	1
1	A	54	LYS	1
1	B	9	GLU	1
1	B	36	GLU	1
1	B	54	LYS	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 ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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 40% for the well-defined parts and 38% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *NMR-STAR31.str*

7.1.1 Bookkeeping

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

Total number of shifts	1201
Number of shifts mapped to atoms	1201
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	105	-0.39 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	98	0.01 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	104	-0.11 ± 0.10	None needed (< 0.5 ppm)
^{15}N	98	2.95 ± 0.33	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 40%, i.e. 1026 atoms were assigned a chemical shift out of a possible 2542. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	419/880 (48%)	166/354 (47%)	170/352 (48%)	83/174 (48%)
Sidechain	607/1456 (42%)	411/934 (44%)	196/464 (42%)	0/58 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/206 (0%)	0/102 (0%)	0/86 (0%)	0/18 (0%)
Overall	1026/2542 (40%)	577/1390 (42%)	366/902 (41%)	83/250 (33%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 1201 atoms were assigned a chemical shift out of a possible 3168. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	509/1140 (45%)	202/464 (44%)	209/456 (46%)	98/220 (45%)
Sidechain	692/1758 (39%)	466/1128 (41%)	226/566 (40%)	0/64 (0%)
Aromatic	0/270 (0%)	0/134 (0%)	0/102 (0%)	0/34 (0%)
Overall	1201/3168 (38%)	668/1726 (39%)	435/1124 (39%)	98/318 (31%)

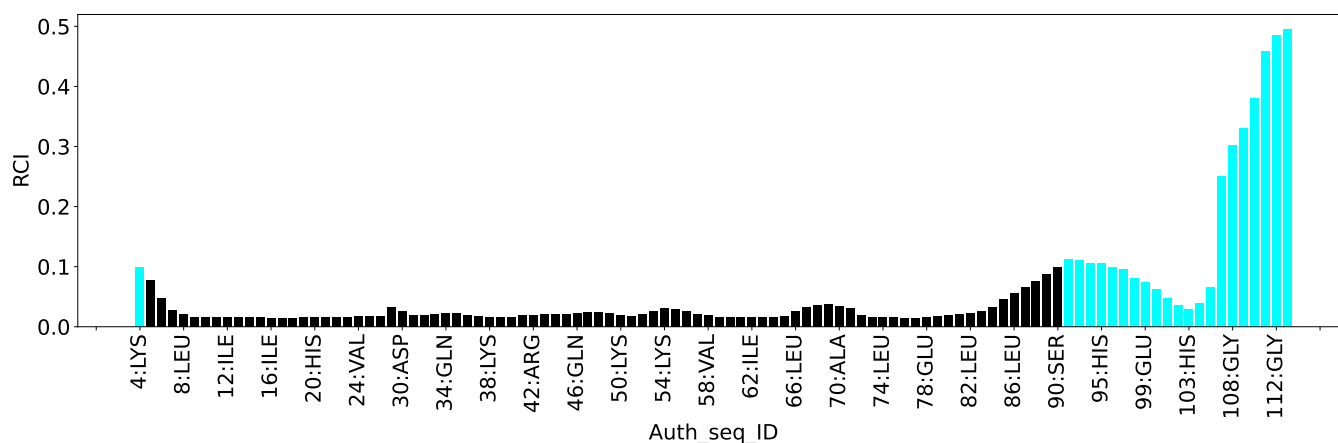
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3714
Intra-residue ($ i-j =0$)	660
Sequential ($ i-j =1$)	832
Medium range ($ i-j >1$ and $ i-j <5$)	1048
Long range ($ i-j \geq 5$)	790
Inter-chain	298
Hydrogen bond restraints	86
Disulfide bond restraints	0
Total dihedral-angle restraints	210
Number of unmapped restraints	0
Number of restraints per residue	17.2
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)	106.7	0.2
0.2-0.5 (Medium)	236.8	0.5
>0.5 (Large)	428.9	8.2

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)	51.9	10.0
10.0-20.0 (Medium)	4.8	20.0
>20.0 (Large)	4.5	158.81

9 Distance violation analysis ⓘ

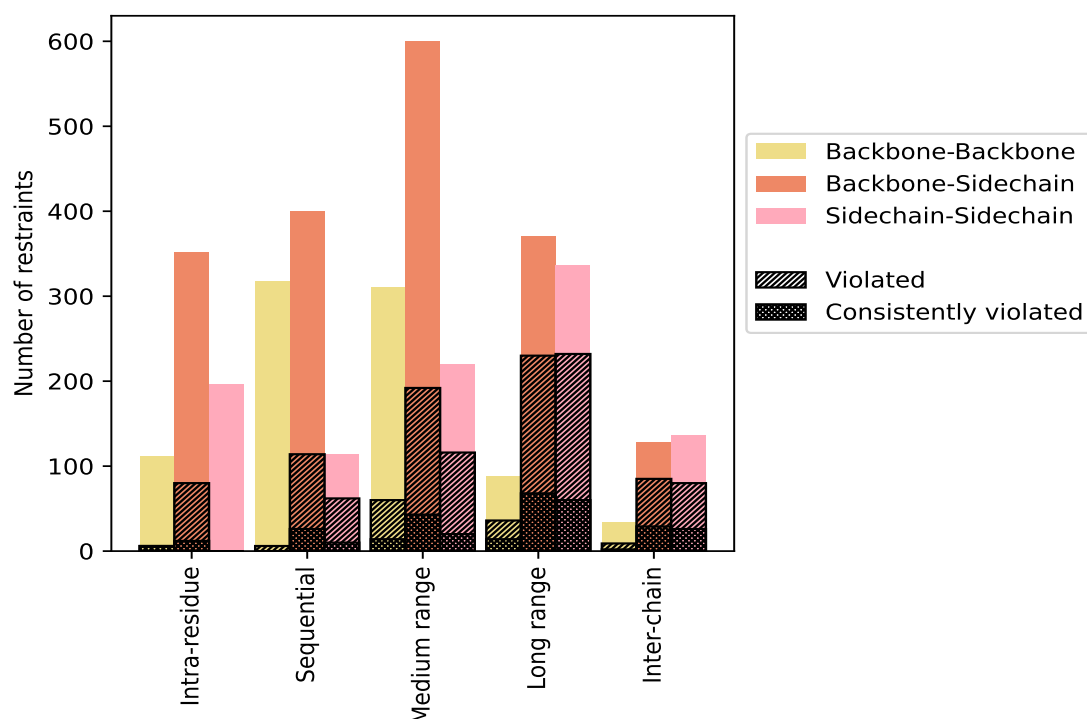
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	660	17.8	86	13.0	2.3	18	2.7	0.5
Backbone-Backbone	112	3.0	6	5.4	0.2	6	5.4	0.2
Backbone-Sidechain	352	9.5	80	22.7	2.2	12	3.4	0.3
Sidechain-Sidechain	196	5.3	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	832	22.4	182	21.9	4.9	36	4.3	1.0
Backbone-Backbone	318	8.6	6	1.9	0.2	0	0.0	0.0
Backbone-Sidechain	400	10.8	114	28.5	3.1	26	6.5	0.7
Sidechain-Sidechain	114	3.1	62	54.4	1.7	10	8.8	0.3
Medium range ($i-j >1$ & $i-j <5$)	1048	28.2	352	33.6	9.5	76	7.3	2.0
Backbone-Backbone	310	8.3	60	19.4	1.6	14	4.5	0.4
Backbone-Sidechain	518	13.9	176	34.0	4.7	42	8.1	1.1
Sidechain-Sidechain	220	5.9	116	52.7	3.1	20	9.1	0.5
Long range ($i-j \geq 5$)	790	21.3	495	62.7	13.3	142	18.0	3.8
Backbone-Backbone	88	2.4	36	40.9	1.0	14	15.9	0.4
Backbone-Sidechain	366	9.9	227	62.0	6.1	68	18.6	1.8
Sidechain-Sidechain	336	9.0	232	69.0	6.2	60	17.9	1.6
Inter-chain	298	8.0	174	58.4	4.7	57	19.1	1.5
Backbone-Backbone	34	0.9	9	26.5	0.2	2	5.9	0.1
Backbone-Sidechain	128	3.4	85	66.4	2.3	29	22.7	0.8
Sidechain-Sidechain	136	3.7	80	58.8	2.2	26	19.1	0.7
Hydrogen bond	86	2.3	19	22.1	0.5	1	1.2	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3714	100.0	1308	35.2	35.2	330	8.9	8.9
Backbone-Backbone	862	23.2	117	13.6	3.2	36	4.2	1.0
Backbone-Sidechain	1850	49.8	701	37.9	18.9	178	9.6	4.8
Sidechain-Sidechain	1002	27.0	490	48.9	13.2	116	11.6	3.1

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

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



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

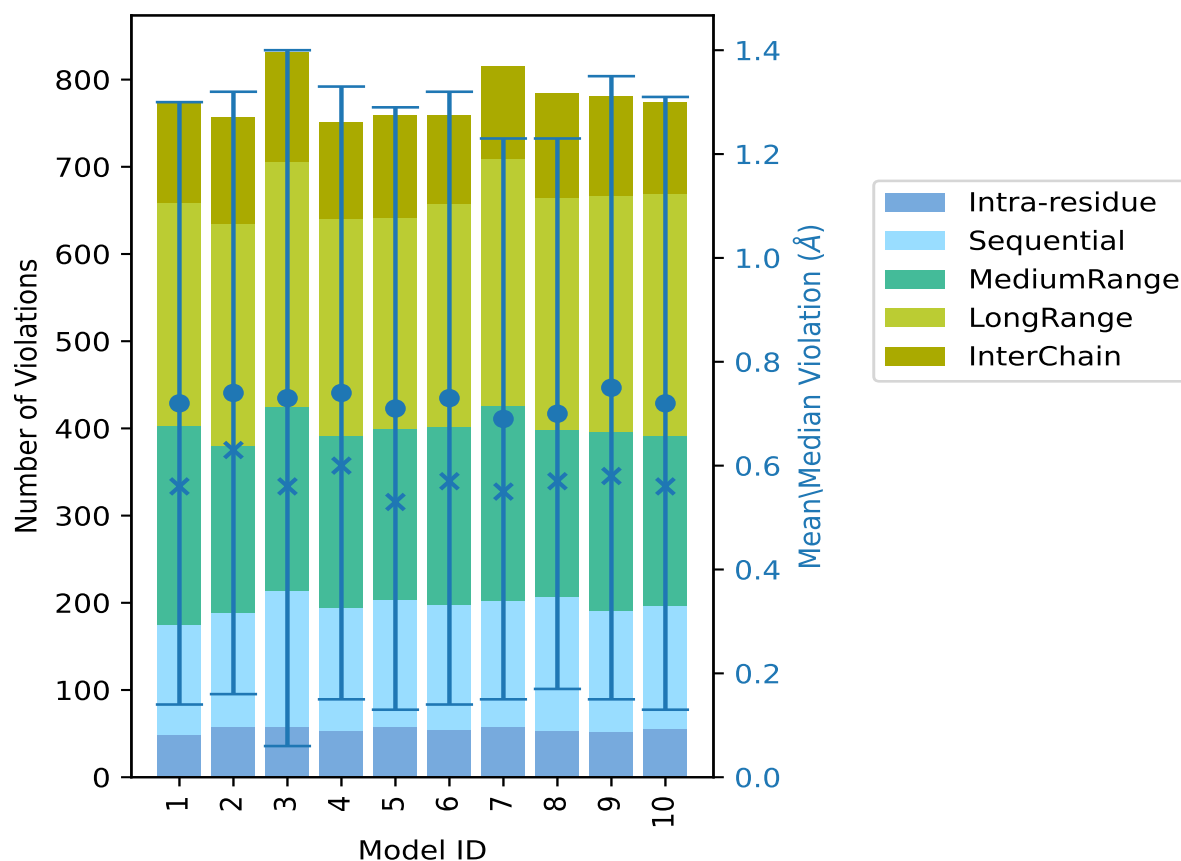
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	49	126	228	256	114	773	0.72	3.42	0.58	0.56
2	58	131	191	255	122	757	0.74	3.88	0.58	0.63
3	58	156	211	281	126	832	0.73	8.2	0.67	0.56
4	54	140	198	248	111	751	0.74	3.89	0.59	0.6
5	58	145	197	241	118	759	0.71	3.92	0.58	0.53
6	54	144	204	255	102	759	0.73	3.83	0.59	0.57
7	58	144	224	283	106	815	0.69	3.57	0.54	0.55
8	53	154	191	267	120	785	0.7	3.4	0.53	0.57
9	52	139	205	271	114	781	0.75	3.83	0.6	0.58
10	56	140	196	277	105	774	0.72	3.99	0.59	0.56

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, 2339(IR:574, SQ:650, MR:696, LR:295, IC:124) 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	%
14	20	45	79	30	188	1	10.0
15	16	35	44	12	122	2	20.0
8	16	34	33	12	103	3	30.0

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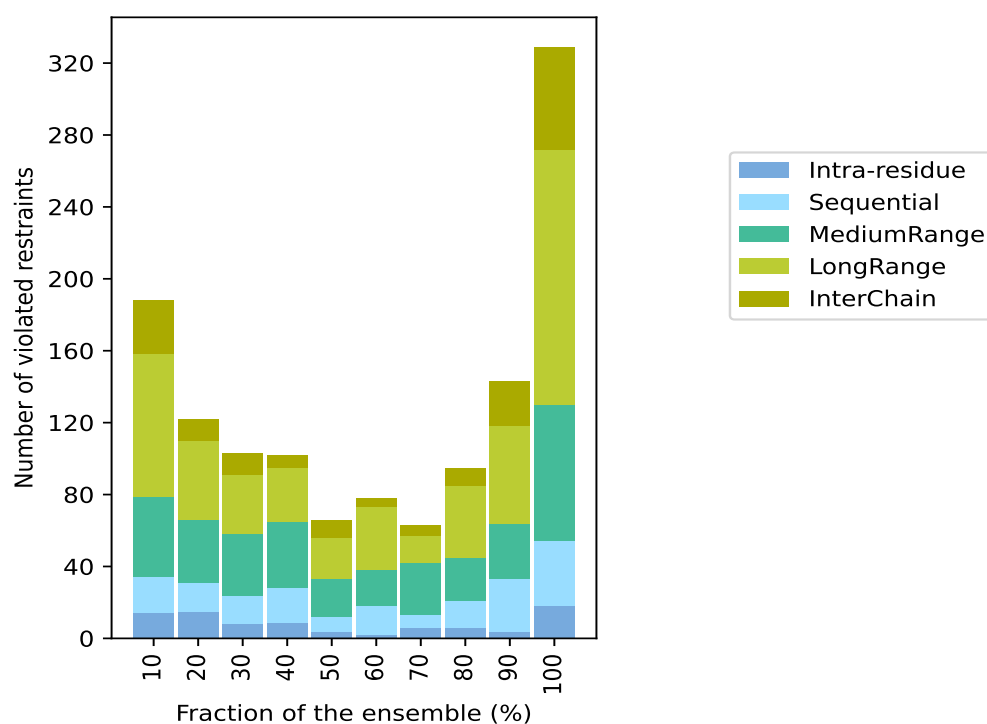
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
9	19	37	30	7	102	4	40.0
4	8	21	23	10	66	5	50.0
2	16	20	35	5	78	6	60.0
6	7	29	15	6	63	7	70.0
6	15	24	40	10	95	8	80.0
4	29	31	54	25	143	9	90.0
18	36	76	142	57	329	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](#)

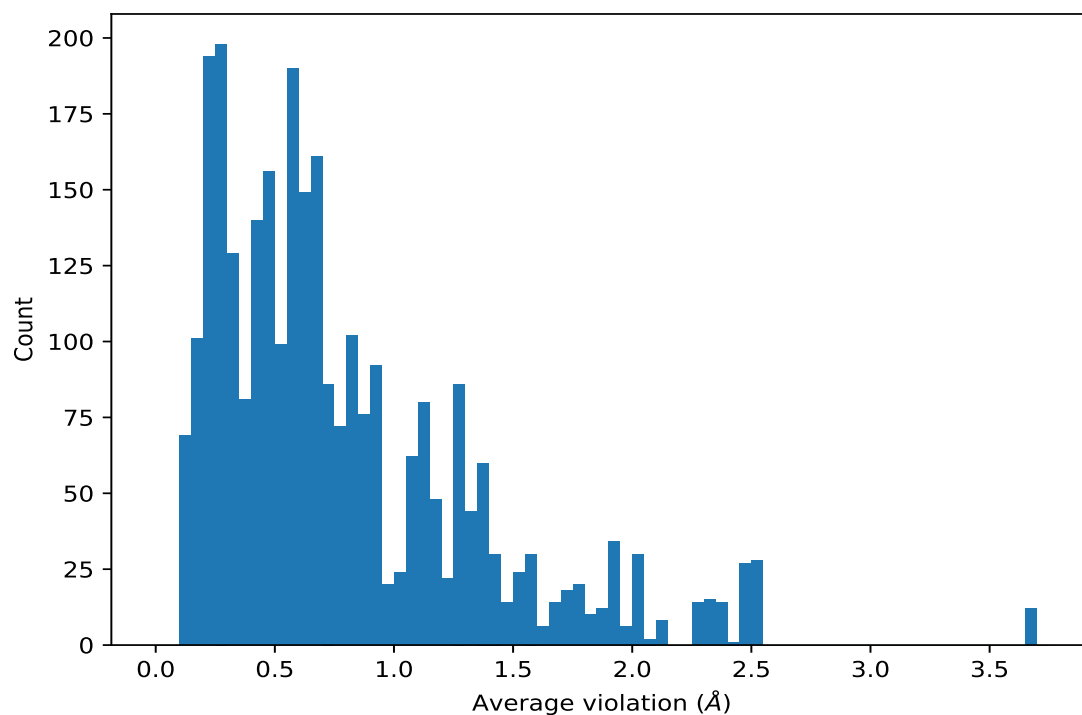


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,1202)	1:60:B:GLU:HB3	1:66:B:LEU:HD12	10	3.67	0.3	3.82
(1,1202)	1:34:B:GLN:HB2	1:32:B:LEU:HD11	10	3.67	0.3	3.82
(1,1202)	1:34:B:GLN:HB2	1:32:B:LEU:HD12	10	3.67	0.3	3.82
(1,1202)	1:34:B:GLN:HB3	1:32:B:LEU:HD23	10	3.67	0.3	3.82
(1,1202)	1:60:B:GLU:HB2	1:66:B:LEU:HD11	10	3.67	0.3	3.82
(1,1202)	1:34:B:GLN:HB3	1:32:B:LEU:HD21	10	3.67	0.3	3.82
(1,1201)	1:60:A:GLU:HB3	1:66:A:LEU:HD12	10	3.67	0.31	3.82
(1,1201)	1:34:A:GLN:HB2	1:32:A:LEU:HD11	10	3.67	0.31	3.82
(1,1201)	1:34:A:GLN:HB2	1:32:A:LEU:HD12	10	3.67	0.31	3.82
(1,1201)	1:34:A:GLN:HB3	1:32:A:LEU:HD23	10	3.67	0.31	3.82
(1,1201)	1:60:A:GLU:HB2	1:66:A:LEU:HD11	10	3.67	0.31	3.82
(1,1201)	1:34:A:GLN:HB3	1:32:A:LEU:HD21	10	3.67	0.31	3.82
(1,207)	1:13:A:GLU:HB3	1:8:B:LEU:HD23	10	2.51	0.32	2.53
(1,207)	1:13:A:GLU:HB3	1:8:B:LEU:HD12	10	2.51	0.32	2.53
(1,207)	1:13:A:GLU:HB2	1:87:B:THR:HG23	10	2.51	0.32	2.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,207)	1:13:A:GLU:HB2	1:8:A:LEU:HD13	10	2.51	0.32	2.53
(1,207)	1:13:A:GLU:HB2	1:8:A:LEU:HD12	10	2.51	0.32	2.53
(1,207)	1:13:A:GLU:HB3	1:87:B:THR:HG22	10	2.51	0.32	2.53
(1,207)	1:13:A:GLU:HB2	1:8:A:LEU:HD22	10	2.51	0.32	2.53
(1,208)	1:13:B:GLU:HB3	1:8:A:LEU:HD23	10	2.51	0.32	2.53
(1,208)	1:13:B:GLU:HB3	1:8:A:LEU:HD12	10	2.51	0.32	2.53
(1,208)	1:13:B:GLU:HB2	1:87:A:THR:HG23	10	2.51	0.32	2.53
(1,208)	1:13:B:GLU:HB2	1:8:B:LEU:HD13	10	2.51	0.32	2.53
(1,208)	1:13:B:GLU:HB2	1:8:B:LEU:HD12	10	2.51	0.32	2.53
(1,208)	1:13:B:GLU:HB3	1:87:A:THR:HG22	10	2.51	0.32	2.53
(1,208)	1:13:B:GLU:HB2	1:8:B:LEU:HD22	10	2.51	0.32	2.53
(1,914)	1:66:B:LEU:HD13	1:64:B:GLU:HG2	10	2.5	0.42	2.54
(1,914)	1:66:B:LEU:HD21	1:64:B:GLU:HG2	10	2.5	0.42	2.54
(1,914)	1:66:B:LEU:HD13	1:52:B:GLU:HG2	10	2.5	0.42	2.54
(1,914)	1:66:B:LEU:HD23	1:64:B:GLU:HG2	10	2.5	0.42	2.54
(1,914)	1:66:B:LEU:HD12	1:52:B:GLU:HG2	10	2.5	0.42	2.54
(1,914)	1:66:B:LEU:HD12	1:64:B:GLU:HG2	10	2.5	0.42	2.54
(1,914)	1:66:B:LEU:HD11	1:64:B:GLU:HG2	10	2.5	0.42	2.54
(1,913)	1:66:A:LEU:HD13	1:64:A:GLU:HG2	10	2.5	0.41	2.54
(1,913)	1:66:A:LEU:HD21	1:64:A:GLU:HG2	10	2.5	0.41	2.54
(1,913)	1:66:A:LEU:HD13	1:52:A:GLU:HG2	10	2.5	0.41	2.54
(1,913)	1:66:A:LEU:HD23	1:64:A:GLU:HG2	10	2.5	0.41	2.54
(1,913)	1:66:A:LEU:HD12	1:52:A:GLU:HG2	10	2.5	0.41	2.54
(1,913)	1:66:A:LEU:HD12	1:64:A:GLU:HG2	10	2.5	0.41	2.54
(1,913)	1:66:A:LEU:HD11	1:64:A:GLU:HG2	10	2.5	0.41	2.54
(1,1037)	1:70:A:ALA:HB1	1:74:A:LEU:HD22	10	2.48	0.23	2.46
(1,1037)	1:70:A:ALA:HB2	1:74:A:LEU:HD22	10	2.48	0.23	2.46
(1,1037)	1:70:A:ALA:HB3	1:74:A:LEU:HD23	10	2.48	0.23	2.46
(1,1037)	1:70:A:ALA:HB2	1:74:A:LEU:HD23	10	2.48	0.23	2.46
(1,1037)	1:70:A:ALA:HB3	1:74:A:LEU:HD22	10	2.48	0.23	2.46
(1,1037)	1:70:A:ALA:HB2	1:74:A:LEU:HD21	10	2.48	0.23	2.46
(1,1037)	1:70:A:ALA:HB1	1:74:A:LEU:HD21	10	2.48	0.23	2.46
(1,1038)	1:70:B:ALA:HB1	1:74:B:LEU:HD22	10	2.48	0.23	2.46
(1,1038)	1:70:B:ALA:HB2	1:74:B:LEU:HD22	10	2.48	0.23	2.46
(1,1038)	1:70:B:ALA:HB3	1:74:B:LEU:HD23	10	2.48	0.23	2.46
(1,1038)	1:70:B:ALA:HB2	1:74:B:LEU:HD23	10	2.48	0.23	2.46
(1,1038)	1:70:B:ALA:HB3	1:74:B:LEU:HD22	10	2.48	0.23	2.46
(1,1038)	1:70:B:ALA:HB2	1:74:B:LEU:HD21	10	2.48	0.23	2.46
(1,1038)	1:70:B:ALA:HB1	1:74:B:LEU:HD21	10	2.48	0.23	2.46
(1,402)	1:92:B:GLU:HB2	1:51:B:LYS:HE3	10	2.39	0.49	2.32
(1,402)	1:92:B:GLU:HB3	1:30:A:ASP:HB2	10	2.39	0.49	2.32
(1,402)	1:85:B:ARG:HB3	1:51:B:LYS:HE3	10	2.39	0.49	2.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,402)	1:42:B:ARG:HB3	1:4:A:LYS:HE2	10	2.39	0.49	2.32
(1,402)	1:85:B:ARG:HB2	1:51:B:LYS:HE3	10	2.39	0.49	2.32
(1,402)	1:38:B:LYS:HD2	1:57:B:LYS:HE3	10	2.39	0.49	2.32
(1,401)	1:92:A:GLU:HB2	1:51:A:LYS:HE3	10	2.38	0.49	2.3
(1,401)	1:92:A:GLU:HB3	1:30:B:ASP:HB2	10	2.38	0.49	2.3
(1,401)	1:85:A:ARG:HB3	1:51:A:LYS:HE3	10	2.38	0.49	2.3
(1,401)	1:42:A:ARG:HB3	1:4:B:LYS:HE2	10	2.38	0.49	2.3
(1,401)	1:85:A:ARG:HB2	1:51:A:LYS:HE3	10	2.38	0.49	2.3
(1,401)	1:38:A:LYS:HD2	1:57:A:LYS:HE3	10	2.38	0.49	2.3
(1,340)	1:66:B:LEU:HD23	1:76:B:PHE:HA	10	2.31	0.42	2.28
(1,340)	1:66:B:LEU:HD11	1:76:B:PHE:HA	10	2.31	0.42	2.28
(1,340)	1:41:B:VAL:HG13	1:6:A:SER:HB3	10	2.31	0.42	2.28
(1,340)	1:66:B:LEU:HD12	1:76:B:PHE:HA	10	2.31	0.42	2.28
(1,340)	1:66:B:LEU:HD13	1:76:B:PHE:HA	10	2.31	0.42	2.28
(1,340)	1:66:B:LEU:HD21	1:76:B:PHE:HA	10	2.31	0.42	2.28
(1,340)	1:66:B:LEU:HD22	1:76:B:PHE:HA	10	2.31	0.42	2.28
(1,339)	1:66:A:LEU:HD23	1:76:A:PHE:HA	10	2.31	0.41	2.28
(1,339)	1:41:A:VAL:HG12	1:6:B:SER:HB3	10	2.31	0.41	2.28
(1,339)	1:41:A:VAL:HG13	1:6:B:SER:HB3	10	2.31	0.41	2.28
(1,339)	1:66:A:LEU:HD12	1:76:A:PHE:HA	10	2.31	0.41	2.28
(1,339)	1:66:A:LEU:HD13	1:76:A:PHE:HA	10	2.31	0.41	2.28
(1,339)	1:66:A:LEU:HD21	1:76:A:PHE:HA	10	2.31	0.41	2.28
(1,339)	1:66:A:LEU:HD22	1:76:A:PHE:HA	10	2.31	0.41	2.28
(1,339)	1:66:A:LEU:HD11	1:76:A:PHE:HA	10	2.31	0.41	2.28
(1,107)	1:34:A:GLN:HG2	1:59:A:ILE:HD12	10	2.28	0.24	2.26
(1,107)	1:7:A:GLN:HG3	1:12:A:ILE:HD13	10	2.28	0.24	2.26
(1,107)	1:34:A:GLN:HG3	1:59:A:ILE:HD11	10	2.28	0.24	2.26
(1,107)	1:7:A:GLN:HG2	1:12:A:ILE:HD11	10	2.28	0.24	2.26
(1,107)	1:7:A:GLN:HG2	1:12:A:ILE:HD13	10	2.28	0.24	2.26
(1,107)	1:34:A:GLN:HG2	1:59:A:ILE:HD13	10	2.28	0.24	2.26
(1,107)	1:34:A:GLN:HG2	1:59:A:ILE:HD11	10	2.28	0.24	2.26
(1,108)	1:34:B:GLN:HG2	1:59:B:ILE:HD12	10	2.28	0.24	2.25
(1,108)	1:7:B:GLN:HG3	1:12:B:ILE:HD13	10	2.28	0.24	2.25
(1,108)	1:34:B:GLN:HG3	1:59:B:ILE:HD11	10	2.28	0.24	2.25
(1,108)	1:7:B:GLN:HG2	1:12:B:ILE:HD11	10	2.28	0.24	2.25
(1,108)	1:7:B:GLN:HG2	1:12:B:ILE:HD13	10	2.28	0.24	2.25
(1,108)	1:34:B:GLN:HG2	1:59:B:ILE:HD13	10	2.28	0.24	2.25
(1,108)	1:34:B:GLN:HG2	1:59:B:ILE:HD11	10	2.28	0.24	2.25
(1,220)	1:12:B:ILE:HG21	1:19:B:PHE:HB2	10	2.11	0.22	2.0
(1,220)	1:12:B:ILE:HG22	1:19:B:PHE:HB2	10	2.11	0.22	2.0
(1,220)	1:12:B:ILE:HG22	1:19:B:PHE:HB3	10	2.11	0.22	2.0
(1,220)	1:12:B:ILE:HG23	1:19:B:PHE:HB3	10	2.11	0.22	2.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,219)	1:12:A:ILE:HG21	1:19:A:PHE:HB2	10	2.11	0.22	2.0
(1,219)	1:12:A:ILE:HG22	1:19:A:PHE:HB2	10	2.11	0.22	2.0
(1,219)	1:12:A:ILE:HG22	1:19:A:PHE:HB3	10	2.11	0.22	2.0
(1,219)	1:12:A:ILE:HG23	1:19:A:PHE:HB3	10	2.11	0.22	2.0
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG23	10	2.02	0.19	2.02
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG22	10	2.02	0.19	2.02
(1,1385)	1:18:A:THR:H	1:12:A:ILE:HG23	10	2.02	0.19	2.02
(1,1385)	1:18:A:THR:H	1:12:A:ILE:HG21	10	2.02	0.19	2.02
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG23	10	2.02	0.19	2.0
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG22	10	2.02	0.19	2.0
(1,1386)	1:18:B:THR:H	1:12:B:ILE:HG23	10	2.02	0.19	2.0
(1,1386)	1:18:B:THR:H	1:12:B:ILE:HG21	10	2.02	0.19	2.0
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD23	10	2.01	0.3	1.96
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD22	10	2.01	0.3	1.96
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD12	10	2.01	0.3	1.96
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD21	10	2.01	0.3	1.96
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD23	10	2.01	0.3	1.96
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD22	10	2.01	0.3	1.96
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD12	10	2.01	0.3	1.96
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD21	10	2.01	0.3	1.96
(1,231)	1:12:A:ILE:HG23	1:80:A:ILE:HG22	10	2.0	0.77	2.28
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG21	10	2.0	0.77	2.28
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG23	10	2.0	0.77	2.28
(1,231)	1:12:A:ILE:HG22	1:80:A:ILE:HG21	10	2.0	0.77	2.28
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG22	10	2.0	0.77	2.28
(1,231)	1:12:A:ILE:HG22	1:80:A:ILE:HG23	10	2.0	0.77	2.28
(1,231)	1:12:A:ILE:HG23	1:80:A:ILE:HG21	10	2.0	0.77	2.28
(1,232)	1:12:B:ILE:HG23	1:80:B:ILE:HG22	10	2.0	0.77	2.28
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG21	10	2.0	0.77	2.28
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG23	10	2.0	0.77	2.28
(1,232)	1:12:B:ILE:HG22	1:80:B:ILE:HG21	10	2.0	0.77	2.28
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG22	10	2.0	0.77	2.28
(1,232)	1:12:B:ILE:HG22	1:80:B:ILE:HG23	10	2.0	0.77	2.28
(1,232)	1:12:B:ILE:HG23	1:80:B:ILE:HG21	10	2.0	0.77	2.28
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD13	10	1.94	0.31	1.87
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD23	10	1.94	0.31	1.87
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD11	10	1.94	0.31	1.87
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD22	10	1.94	0.31	1.87
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD13	10	1.94	0.31	1.87
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD23	10	1.94	0.31	1.87
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD11	10	1.94	0.31	1.87
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD22	10	1.94	0.31	1.87

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG23	10	1.91	0.37	1.9
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG22	10	1.91	0.37	1.9
(1,1035)	1:63:A:MET:HE1	1:41:A:VAL:HG23	10	1.91	0.37	1.9
(1,1035)	1:63:A:MET:HE2	1:41:A:VAL:HG21	10	1.91	0.37	1.9
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG21	10	1.91	0.37	1.9
(1,1035)	1:63:A:MET:HE1	1:41:A:VAL:HG22	10	1.91	0.37	1.9
(1,1035)	1:63:A:MET:HE1	1:41:A:VAL:HG21	10	1.91	0.37	1.9
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG23	10	1.91	0.37	1.9
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG22	10	1.91	0.37	1.9
(1,1036)	1:63:B:MET:HE1	1:41:B:VAL:HG23	10	1.91	0.37	1.9
(1,1036)	1:63:B:MET:HE2	1:41:B:VAL:HG21	10	1.91	0.37	1.9
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG21	10	1.91	0.37	1.9
(1,1036)	1:63:B:MET:HE1	1:41:B:VAL:HG22	10	1.91	0.37	1.9
(1,1036)	1:63:B:MET:HE1	1:41:B:VAL:HG21	10	1.91	0.37	1.9
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG22	10	1.89	0.39	1.97
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG21	10	1.89	0.39	1.97
(1,1147)	1:32:A:LEU:HG	1:24:A:VAL:HG12	10	1.89	0.39	1.97
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG22	10	1.89	0.38	1.97
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG21	10	1.89	0.38	1.97
(1,1148)	1:32:B:LEU:HG	1:24:B:VAL:HG12	10	1.89	0.38	1.97
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG12	10	1.86	0.21	1.9
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG13	10	1.86	0.21	1.9
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG11	10	1.86	0.21	1.9
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG12	10	1.86	0.21	1.9
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG13	10	1.86	0.21	1.9
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG11	10	1.86	0.21	1.9
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG11	10	1.82	0.33	1.77
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG12	10	1.82	0.33	1.77
(1,513)	1:51:A:LYS:HE3	1:41:A:VAL:HG13	10	1.82	0.33	1.77
(1,513)	1:51:A:LYS:HE3	1:41:A:VAL:HG11	10	1.82	0.33	1.77
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG13	10	1.82	0.33	1.77
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG11	10	1.82	0.32	1.77
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG12	10	1.82	0.32	1.77
(1,514)	1:51:B:LYS:HE3	1:41:B:VAL:HG13	10	1.82	0.32	1.77
(1,514)	1:51:B:LYS:HE3	1:41:B:VAL:HG11	10	1.82	0.32	1.77
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG13	10	1.82	0.32	1.77
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD13	10	1.79	0.53	1.68
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD22	10	1.79	0.53	1.68
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD23	10	1.79	0.53	1.68
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD21	10	1.79	0.53	1.68
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD11	10	1.79	0.53	1.68
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD13	10	1.79	0.53	1.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD22	10	1.79	0.53	1.67
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD23	10	1.79	0.53	1.67
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD21	10	1.79	0.53	1.67
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD11	10	1.79	0.53	1.67
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD12	10	1.75	0.26	1.81
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HG22	10	1.75	0.26	1.81
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD11	10	1.75	0.26	1.81
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD13	10	1.75	0.26	1.81
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HG21	10	1.75	0.26	1.81
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD12	10	1.75	0.26	1.81
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HG22	10	1.75	0.26	1.81
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD11	10	1.75	0.26	1.81
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD13	10	1.75	0.26	1.81
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HG21	10	1.75	0.26	1.81
(1,722)	1:77:B:GLU:HB2	1:74:B:LEU:HD23	10	1.72	0.31	1.67
(1,722)	1:77:B:GLU:HB3	1:66:A:LEU:HD22	10	1.72	0.31	1.67
(1,722)	1:77:B:GLU:HB3	1:66:B:LEU:HD23	10	1.72	0.31	1.67
(1,722)	1:77:B:GLU:HB3	1:66:B:LEU:HD22	10	1.72	0.31	1.67
(1,722)	1:77:B:GLU:HB2	1:66:B:LEU:HD21	10	1.72	0.31	1.67
(1,722)	1:77:B:GLU:HB2	1:74:B:LEU:HD22	10	1.72	0.31	1.67
(1,721)	1:77:A:GLU:HB2	1:74:A:LEU:HD23	10	1.72	0.31	1.67
(1,721)	1:77:A:GLU:HB3	1:66:B:LEU:HD22	10	1.72	0.31	1.67
(1,721)	1:77:A:GLU:HB3	1:66:A:LEU:HD23	10	1.72	0.31	1.67
(1,721)	1:77:A:GLU:HB3	1:66:A:LEU:HD22	10	1.72	0.31	1.67
(1,721)	1:77:A:GLU:HB2	1:66:A:LEU:HD21	10	1.72	0.31	1.67
(1,721)	1:77:A:GLU:HB2	1:74:A:LEU:HD22	10	1.72	0.31	1.67
(1,1208)	1:39:B:GLU:HB3	1:32:B:LEU:HA	10	1.72	0.15	1.69
(1,1208)	1:34:B:GLN:HB2	1:71:B:ASP:HA	10	1.72	0.15	1.69
(1,1207)	1:39:A:GLU:HB3	1:32:A:LEU:HA	10	1.72	0.16	1.68
(1,1207)	1:34:A:GLN:HB2	1:71:A:ASP:HA	10	1.72	0.16	1.68
(1,464)	1:79:B:PHE:HB3	1:81:B:MET:HG2	10	1.67	0.57	1.76
(1,464)	1:11:B:ASN:HB2	1:5:B:MET:HG2	10	1.67	0.57	1.76
(1,464)	1:79:B:PHE:HB2	1:22:B:TYR:HB2	10	1.67	0.57	1.76
(1,464)	1:79:B:PHE:HB3	1:81:B:MET:HG3	10	1.67	0.57	1.76
(1,464)	1:79:B:PHE:HB2	1:67:B:ASP:HB2	10	1.67	0.57	1.76
(1,464)	1:79:B:PHE:HB3	1:67:B:ASP:HB2	10	1.67	0.57	1.76
(1,463)	1:79:A:PHE:HB3	1:81:A:MET:HG2	10	1.67	0.57	1.76
(1,463)	1:11:A:ASN:HB2	1:5:A:MET:HG2	10	1.67	0.57	1.76
(1,463)	1:79:A:PHE:HB2	1:22:A:TYR:HB2	10	1.67	0.57	1.76
(1,463)	1:79:A:PHE:HB3	1:81:A:MET:HG3	10	1.67	0.57	1.76
(1,463)	1:79:A:PHE:HB2	1:67:A:ASP:HB2	10	1.67	0.57	1.76
(1,463)	1:79:A:PHE:HB3	1:67:A:ASP:HB2	10	1.67	0.57	1.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1213)	1:50:A:LYS:HE3	1:49:A:LEU:HB2	10	1.64	0.46	1.76
(1,1213)	1:50:A:LYS:HE2	1:49:A:LEU:HB2	10	1.64	0.46	1.76
(1,1213)	1:49:A:LEU:HB2	1:54:A:LYS:HE3	10	1.64	0.46	1.76
(1,1214)	1:50:B:LYS:HE3	1:49:B:LEU:HB2	10	1.64	0.45	1.75
(1,1214)	1:50:B:LYS:HE2	1:49:B:LEU:HB2	10	1.64	0.45	1.75
(1,1214)	1:49:B:LEU:HB2	1:54:B:LYS:HE3	10	1.64	0.45	1.75
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD23	10	1.59	0.08	1.58
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD22	10	1.59	0.08	1.58
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD21	10	1.59	0.08	1.58
(1,955)	1:21:A:GLN:HB2	1:32:A:LEU:HD22	10	1.59	0.08	1.58
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD23	10	1.59	0.08	1.58
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD22	10	1.59	0.08	1.58
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD21	10	1.59	0.08	1.58
(1,956)	1:21:B:GLN:HB2	1:32:B:LEU:HD22	10	1.59	0.08	1.58
(1,275)	1:19:A:PHE:HB3	1:40:A:LEU:HA	10	1.57	0.17	1.65
(1,275)	1:19:A:PHE:HB2	1:13:A:GLU:HA	10	1.57	0.17	1.65
(1,275)	1:19:A:PHE:HB3	1:13:A:GLU:HA	10	1.57	0.17	1.65
(1,275)	1:19:A:PHE:HB2	1:21:A:GLN:HA	10	1.57	0.17	1.65
(1,276)	1:19:B:PHE:HB3	1:40:B:LEU:HA	10	1.57	0.17	1.65
(1,276)	1:19:B:PHE:HB2	1:13:B:GLU:HA	10	1.57	0.17	1.65
(1,276)	1:19:B:PHE:HB3	1:13:B:GLU:HA	10	1.57	0.17	1.65
(1,276)	1:19:B:PHE:HB2	1:21:B:GLN:HA	10	1.57	0.17	1.65
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD11	10	1.56	0.21	1.62
(1,462)	1:32:B:LEU:HG	1:87:A:THR:HG21	10	1.56	0.21	1.62
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD13	10	1.56	0.21	1.62
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD12	10	1.56	0.21	1.62
(1,462)	1:10:B:ARG:HG2	1:12:B:ILE:HD12	10	1.56	0.21	1.62
(1,462)	1:32:B:LEU:HG	1:87:A:THR:HG22	10	1.56	0.21	1.62
(1,462)	1:32:B:LEU:HG	1:24:B:VAL:HG12	10	1.56	0.21	1.62
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD11	10	1.56	0.21	1.62
(1,461)	1:32:A:LEU:HG	1:87:B:THR:HG21	10	1.56	0.21	1.62
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD13	10	1.56	0.21	1.62
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD12	10	1.56	0.21	1.62
(1,461)	1:10:A:ARG:HG2	1:12:A:ILE:HD12	10	1.56	0.21	1.62
(1,461)	1:32:A:LEU:HG	1:87:B:THR:HG22	10	1.56	0.21	1.62
(1,461)	1:32:A:LEU:HG	1:24:A:VAL:HG12	10	1.56	0.21	1.62
(1,353)	1:58:A:VAL:HG23	1:54:A:LYS:HA	10	1.54	0.26	1.64
(1,353)	1:58:A:VAL:HG22	1:54:A:LYS:HA	10	1.54	0.26	1.64
(1,353)	1:92:A:GLU:HA	1:87:A:THR:HG21	10	1.54	0.26	1.64
(1,353)	1:58:A:VAL:HG21	1:54:A:LYS:HA	10	1.54	0.26	1.64
(1,354)	1:58:B:VAL:HG23	1:54:B:LYS:HA	10	1.54	0.26	1.64
(1,354)	1:58:B:VAL:HG22	1:54:B:LYS:HA	10	1.54	0.26	1.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,354)	1:92:B:GLU:HA	1:87:B:THR:HG21	10	1.54	0.26	1.64
(1,354)	1:58:B:VAL:HG21	1:54:B:LYS:HA	10	1.54	0.26	1.64
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD11	10	1.52	0.21	1.48
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD13	10	1.52	0.21	1.48
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD12	10	1.52	0.21	1.48
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD11	10	1.52	0.21	1.47
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD13	10	1.52	0.21	1.47
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD12	10	1.52	0.21	1.47
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD11	10	1.51	0.22	1.55
(1,105)	1:7:A:GLN:HG3	1:15:B:ILE:HD11	10	1.51	0.22	1.55
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD12	10	1.51	0.22	1.55
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD13	10	1.51	0.22	1.55
(1,105)	1:7:A:GLN:HG3	1:15:B:ILE:HD13	10	1.51	0.22	1.55
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD11	10	1.5	0.23	1.55
(1,106)	1:7:B:GLN:HG3	1:15:A:ILE:HD11	10	1.5	0.23	1.55
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD12	10	1.5	0.23	1.55
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD13	10	1.5	0.23	1.55
(1,106)	1:7:B:GLN:HG3	1:15:A:ILE:HD13	10	1.5	0.23	1.55
(1,835)	1:76:A:PHE:HB2	1:81:B:MET:HB2	10	1.47	0.64	1.38
(1,835)	1:76:A:PHE:HB3	1:29:A:PRO:HB2	10	1.47	0.64	1.38
(1,835)	1:76:A:PHE:HB2	1:81:B:MET:HE3	10	1.47	0.64	1.38
(1,835)	1:76:A:PHE:HB2	1:29:A:PRO:HB2	10	1.47	0.64	1.38
(1,835)	1:76:A:PHE:HB2	1:81:A:MET:HB2	10	1.47	0.64	1.38
(1,521)	1:49:A:LEU:HB3	1:82:A:LEU:HG	10	1.46	0.28	1.42
(1,521)	1:49:A:LEU:HB2	1:86:A:LEU:HG	10	1.46	0.28	1.42
(1,522)	1:49:B:LEU:HB3	1:82:B:LEU:HG	10	1.46	0.28	1.42
(1,522)	1:49:B:LEU:HB2	1:86:B:LEU:HG	10	1.46	0.28	1.42
(1,836)	1:76:B:PHE:HB2	1:81:A:MET:HB2	10	1.46	0.64	1.38
(1,836)	1:76:B:PHE:HB3	1:29:B:PRO:HB2	10	1.46	0.64	1.38
(1,836)	1:76:B:PHE:HB2	1:81:A:MET:HE3	10	1.46	0.64	1.38
(1,836)	1:76:B:PHE:HB2	1:29:B:PRO:HB2	10	1.46	0.64	1.38
(1,836)	1:76:B:PHE:HB2	1:81:B:MET:HB2	10	1.46	0.64	1.38
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	10	1.42	0.23	1.38
(1,4)	1:73:B:GLN:HG2	1:75:B:SER:HB2	10	1.42	0.23	1.38
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	10	1.42	0.23	1.37
(1,3)	1:73:A:GLN:HG2	1:75:A:SER:HB2	10	1.42	0.23	1.37
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD12	10	1.42	0.11	1.4
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD13	10	1.42	0.11	1.4
(1,1387)	1:18:A:THR:H	1:15:A:ILE:HD13	10	1.42	0.11	1.4
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD11	10	1.42	0.11	1.4
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD12	10	1.42	0.11	1.4
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD13	10	1.42	0.11	1.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1388)	1:18:B:THR:H	1:15:B:ILE:HD13	10	1.42	0.11	1.4
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD11	10	1.42	0.11	1.4
(1,225)	1:12:A:ILE:HG22	1:45:B:LEU:HG	10	1.41	0.4	1.56
(1,225)	1:12:A:ILE:HG23	1:45:B:LEU:HG	10	1.41	0.4	1.56
(1,225)	1:12:A:ILE:HG21	1:80:A:ILE:HB	10	1.41	0.4	1.56
(1,225)	1:12:A:ILE:HG21	1:45:B:LEU:HG	10	1.41	0.4	1.56
(1,225)	1:62:A:ILE:HG23	1:32:A:LEU:HB2	10	1.41	0.4	1.56
(1,225)	1:62:A:ILE:HG22	1:32:A:LEU:HB2	10	1.41	0.4	1.56
(1,226)	1:12:B:ILE:HG22	1:45:A:LEU:HG	10	1.41	0.4	1.56
(1,226)	1:12:B:ILE:HG23	1:45:A:LEU:HG	10	1.41	0.4	1.56
(1,226)	1:12:B:ILE:HG21	1:80:B:ILE:HB	10	1.41	0.4	1.56
(1,226)	1:12:B:ILE:HG21	1:45:A:LEU:HG	10	1.41	0.4	1.56
(1,226)	1:62:B:ILE:HG23	1:32:B:LEU:HB2	10	1.41	0.4	1.56
(1,226)	1:62:B:ILE:HG22	1:32:B:LEU:HB2	10	1.41	0.4	1.56
(1,359)	1:46:A:GLN:HB3	1:59:A:ILE:HD13	10	1.38	0.34	1.48
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD13	10	1.38	0.34	1.48
(1,359)	1:77:A:GLU:HB2	1:31:A:THR:HG22	10	1.38	0.34	1.48
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD11	10	1.38	0.34	1.48
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD12	10	1.38	0.34	1.48
(1,359)	1:77:A:GLU:HB2	1:87:B:THR:HG21	10	1.38	0.34	1.48
(1,359)	1:77:A:GLU:HB2	1:31:A:THR:HG23	10	1.38	0.34	1.48
(1,360)	1:46:B:GLN:HB3	1:59:B:ILE:HD13	10	1.38	0.34	1.48
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD13	10	1.38	0.34	1.48
(1,360)	1:77:B:GLU:HB2	1:31:B:THR:HG22	10	1.38	0.34	1.48
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD11	10	1.38	0.34	1.48
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD12	10	1.38	0.34	1.48
(1,360)	1:77:B:GLU:HB2	1:87:A:THR:HG21	10	1.38	0.34	1.48
(1,360)	1:77:B:GLU:HB2	1:31:B:THR:HG23	10	1.38	0.34	1.48
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD13	10	1.36	0.35	1.48
(1,984)	1:48:B:PHE:HB2	1:16:A:ILE:HD12	10	1.36	0.35	1.48
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD11	10	1.36	0.35	1.48
(1,984)	1:48:B:PHE:HB3	1:40:B:LEU:HD11	10	1.36	0.35	1.48
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD12	10	1.36	0.35	1.48
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD13	10	1.35	0.36	1.47
(1,983)	1:48:A:PHE:HB2	1:16:B:ILE:HD12	10	1.35	0.36	1.47
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD11	10	1.35	0.36	1.47
(1,983)	1:48:A:PHE:HB3	1:40:A:LEU:HD11	10	1.35	0.36	1.47
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD12	10	1.35	0.36	1.47
(1,455)	1:7:A:GLN:HB3	1:21:B:GLN:HG2	10	1.34	0.94	1.04
(1,455)	1:7:A:GLN:HB3	1:9:A:GLU:HG3	10	1.34	0.94	1.04
(1,455)	1:7:A:GLN:HB3	1:46:B:GLN:HG2	10	1.34	0.94	1.04
(1,455)	1:7:A:GLN:HB3	1:9:A:GLU:HG2	10	1.34	0.94	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,456)	1:7:B:GLN:HB3	1:21:A:GLN:HG2	10	1.33	0.94	1.04
(1,456)	1:7:B:GLN:HB3	1:9:B:GLU:HG3	10	1.33	0.94	1.04
(1,456)	1:7:B:GLN:HB3	1:46:A:GLN:HG2	10	1.33	0.94	1.04
(1,456)	1:7:B:GLN:HB3	1:9:B:GLU:HG2	10	1.33	0.94	1.04
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG22	10	1.32	0.2	1.34
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG21	10	1.32	0.2	1.34
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG13	10	1.32	0.2	1.34
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG23	10	1.32	0.2	1.34
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG12	10	1.32	0.2	1.34
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG11	10	1.32	0.2	1.34
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG22	10	1.32	0.2	1.34
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG21	10	1.32	0.2	1.34
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG13	10	1.32	0.2	1.34
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG23	10	1.32	0.2	1.34
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG12	10	1.32	0.2	1.34
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG11	10	1.32	0.2	1.34
(1,104)	1:7:B:GLN:HG2	1:15:A:ILE:HG23	10	1.32	0.43	1.42
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD13	10	1.32	0.43	1.42
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD22	10	1.32	0.43	1.42
(1,104)	1:7:B:GLN:HG2	1:15:A:ILE:HG21	10	1.32	0.43	1.42
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD11	10	1.32	0.43	1.42
(1,104)	1:7:B:GLN:HG2	1:15:A:ILE:HG22	10	1.32	0.43	1.42
(1,103)	1:7:A:GLN:HG2	1:15:B:ILE:HG23	10	1.31	0.43	1.42
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD13	10	1.31	0.43	1.42
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD22	10	1.31	0.43	1.42
(1,103)	1:7:A:GLN:HG2	1:15:B:ILE:HG21	10	1.31	0.43	1.42
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD11	10	1.31	0.43	1.42
(1,103)	1:7:A:GLN:HG2	1:15:B:ILE:HG22	10	1.31	0.43	1.42
(1,1216)	1:49:B:LEU:HB2	1:9:A:GLU:HB2	10	1.29	0.21	1.25
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	10	1.29	0.21	1.25
(1,1215)	1:49:A:LEU:HB2	1:9:B:GLU:HB2	10	1.29	0.21	1.25
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	10	1.29	0.21	1.25
(1,561)	1:16:A:ILE:HB	1:93:B:LYS:HB3	10	1.28	0.16	1.27
(1,561)	1:16:A:ILE:HB	1:12:A:ILE:HG12	10	1.28	0.16	1.27
(1,561)	1:16:A:ILE:HB	1:93:B:LYS:HB2	10	1.28	0.16	1.27
(1,288)	1:9:B:GLU:HB3	1:11:B:ASN:HA	10	1.28	0.23	1.3
(1,288)	1:9:B:GLU:HB2	1:11:B:ASN:HA	10	1.28	0.23	1.3
(1,288)	1:64:B:GLU:HB2	1:71:B:ASP:HA	10	1.28	0.23	1.3
(1,287)	1:9:A:GLU:HB3	1:11:A:ASN:HA	10	1.28	0.23	1.3
(1,287)	1:9:A:GLU:HB2	1:11:A:ASN:HA	10	1.28	0.23	1.3
(1,287)	1:64:A:GLU:HB2	1:71:A:ASP:HA	10	1.28	0.23	1.3
(1,562)	1:16:B:ILE:HB	1:93:A:LYS:HB3	10	1.28	0.16	1.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,562)	1:16:B:ILE:HB	1:12:B:ILE:HG12	10	1.28	0.16	1.26
(1,562)	1:16:B:ILE:HB	1:93:A:LYS:HB2	10	1.28	0.16	1.26
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	10	1.27	0.17	1.29
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	10	1.27	0.17	1.3
(1,358)	1:46:B:GLN:HB3	1:39:B:GLU:HA	10	1.27	0.06	1.26
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	10	1.27	0.06	1.26
(1,357)	1:46:A:GLN:HB3	1:39:A:GLU:HA	10	1.27	0.06	1.26
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	10	1.27	0.06	1.26
(1,1545)	1:43:A:LYS:H	1:59:A:ILE:HD11	10	1.27	0.19	1.21
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD13	10	1.27	0.19	1.21
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD12	10	1.27	0.19	1.21
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD11	10	1.27	0.19	1.21
(1,1545)	1:43:A:LYS:H	1:59:A:ILE:HD12	10	1.27	0.19	1.21
(1,1545)	1:43:A:LYS:H	1:59:A:ILE:HD13	10	1.27	0.19	1.21
(1,1546)	1:43:B:LYS:H	1:59:B:ILE:HD11	10	1.26	0.19	1.21
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD13	10	1.26	0.19	1.21
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD12	10	1.26	0.19	1.21
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD11	10	1.26	0.19	1.21
(1,1546)	1:43:B:LYS:H	1:59:B:ILE:HD12	10	1.26	0.19	1.21
(1,1546)	1:43:B:LYS:H	1:59:B:ILE:HD13	10	1.26	0.19	1.21
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	10	1.26	0.25	1.27
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	10	1.26	0.26	1.27
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG22	10	1.24	0.45	1.25
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG21	10	1.24	0.45	1.25
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG23	10	1.24	0.45	1.25
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG22	10	1.24	0.45	1.25
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG21	10	1.24	0.45	1.25
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG23	10	1.24	0.45	1.25
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD11	10	1.23	0.37	1.32
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD12	10	1.23	0.37	1.32
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD13	10	1.23	0.37	1.32
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD11	10	1.23	0.37	1.32
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD12	10	1.23	0.37	1.32
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD13	10	1.23	0.37	1.32
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG2	10	1.21	0.25	1.29
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG3	10	1.21	0.25	1.29
(3,186)	1:19:B:PHE:HB3	1:83:B:MET:HG2	10	1.21	0.25	1.29
(3,186)	1:19:B:PHE:HB3	1:83:B:MET:HG3	10	1.21	0.25	1.29
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG2	10	1.21	0.25	1.29
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG3	10	1.21	0.25	1.29
(3,185)	1:19:A:PHE:HB3	1:83:A:MET:HG2	10	1.21	0.25	1.29
(3,185)	1:19:A:PHE:HB3	1:83:A:MET:HG3	10	1.21	0.25	1.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	10	1.21	0.28	1.16
(1,68)	1:48:B:PHE:HB3	1:13:A:GLU:H	10	1.21	0.28	1.16
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	10	1.2	0.29	1.14
(1,67)	1:48:A:PHE:HB3	1:13:B:GLU:H	10	1.2	0.29	1.14
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD21	10	1.19	0.58	1.52
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD12	10	1.19	0.58	1.52
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD22	10	1.19	0.58	1.52
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD13	10	1.19	0.58	1.52
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD21	10	1.19	0.27	1.17
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD11	10	1.19	0.27	1.17
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD22	10	1.19	0.27	1.17
(1,1301)	1:9:A:GLU:H	1:15:B:ILE:HG23	10	1.19	0.27	1.17
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD13	10	1.19	0.27	1.17
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	10	1.19	0.28	1.16
(1,990)	1:48:B:PHE:HB2	1:12:A:ILE:H	10	1.19	0.28	1.16
(1,990)	1:48:B:PHE:HB3	1:13:A:GLU:H	10	1.19	0.28	1.16
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD21	10	1.19	0.59	1.51
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD12	10	1.19	0.59	1.51
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD22	10	1.19	0.59	1.51
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD13	10	1.19	0.59	1.51
(1,743)	1:87:A:THR:HG21	1:92:A:GLU:HG2	10	1.19	0.14	1.18
(1,743)	1:87:A:THR:HG23	1:92:A:GLU:HG2	10	1.19	0.14	1.18
(1,743)	1:87:A:THR:HG21	1:92:A:GLU:HG3	10	1.19	0.14	1.18
(3,83)	1:87:A:THR:HG21	1:92:A:GLU:HG2	10	1.19	0.14	1.18
(3,83)	1:87:A:THR:HG23	1:92:A:GLU:HG2	10	1.19	0.14	1.18
(3,83)	1:87:A:THR:HG21	1:92:A:GLU:HG3	10	1.19	0.14	1.18
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD21	10	1.19	0.27	1.15
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD11	10	1.19	0.27	1.15
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD22	10	1.19	0.27	1.15
(1,1302)	1:9:B:GLU:H	1:15:A:ILE:HG23	10	1.19	0.27	1.15
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD13	10	1.19	0.27	1.15
(1,744)	1:87:B:THR:HG21	1:92:B:GLU:HG2	10	1.19	0.14	1.18
(1,744)	1:87:B:THR:HG23	1:92:B:GLU:HG2	10	1.19	0.14	1.18
(1,744)	1:87:B:THR:HG21	1:92:B:GLU:HG3	10	1.19	0.14	1.18
(3,84)	1:87:B:THR:HG21	1:92:B:GLU:HG2	10	1.19	0.14	1.18
(3,84)	1:87:B:THR:HG23	1:92:B:GLU:HG2	10	1.19	0.14	1.18
(3,84)	1:87:B:THR:HG21	1:92:B:GLU:HG3	10	1.19	0.14	1.18
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	10	1.19	0.28	1.14
(1,989)	1:48:A:PHE:HB2	1:12:B:ILE:H	10	1.19	0.28	1.14
(1,989)	1:48:A:PHE:HB3	1:13:B:GLU:H	10	1.19	0.28	1.14
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD12	10	1.16	0.16	1.18
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD13	10	1.16	0.16	1.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD11	10	1.16	0.16	1.18
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD12	10	1.16	0.16	1.17
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD13	10	1.16	0.16	1.17
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD11	10	1.16	0.16	1.17
(1,212)	1:12:B:ILE:HG21	1:11:B:ASN:HA	10	1.15	0.02	1.15
(1,212)	1:12:B:ILE:HG22	1:11:B:ASN:HA	10	1.15	0.02	1.15
(1,212)	1:12:B:ILE:HG23	1:11:B:ASN:HA	10	1.15	0.02	1.15
(1,211)	1:12:A:ILE:HG21	1:11:A:ASN:HA	10	1.15	0.02	1.15
(1,211)	1:12:A:ILE:HG22	1:11:A:ASN:HA	10	1.15	0.02	1.15
(1,211)	1:12:A:ILE:HG23	1:11:A:ASN:HA	10	1.15	0.02	1.15
(3,752)	1:59:B:ILE:HG21	1:61:B:HIS:HB3	10	1.14	0.12	1.17
(3,752)	1:59:B:ILE:HG23	1:61:B:HIS:HB3	10	1.14	0.12	1.17
(3,752)	1:59:B:ILE:HG22	1:61:B:HIS:HB2	10	1.14	0.12	1.17
(3,752)	1:59:B:ILE:HG22	1:61:B:HIS:HB3	10	1.14	0.12	1.17
(3,751)	1:59:A:ILE:HG21	1:61:A:HIS:HB3	10	1.14	0.12	1.17
(3,751)	1:59:A:ILE:HG23	1:61:A:HIS:HB3	10	1.14	0.12	1.17
(3,751)	1:59:A:ILE:HG22	1:61:A:HIS:HB2	10	1.14	0.12	1.17
(3,751)	1:59:A:ILE:HG22	1:61:A:HIS:HB3	10	1.14	0.12	1.17
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD23	10	1.13	0.09	1.12
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD22	10	1.13	0.09	1.12
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	10	1.13	0.12	1.18
(3,279)	1:72:A:LYS:HG2	1:73:A:GLN:HB2	10	1.13	0.12	1.18
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD23	10	1.13	0.08	1.12
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD22	10	1.13	0.08	1.12
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	10	1.13	0.12	1.18
(3,280)	1:72:B:LYS:HG2	1:73:B:GLN:HB2	10	1.13	0.12	1.18
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD23	10	1.12	0.09	1.12
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD21	10	1.12	0.09	1.12
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD22	10	1.12	0.09	1.12
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD23	10	1.12	0.09	1.12
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD21	10	1.12	0.09	1.12
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD22	10	1.12	0.09	1.12
(1,229)	1:12:A:ILE:HG23	1:80:A:ILE:HD12	10	1.12	0.21	1.04
(1,229)	1:62:A:ILE:HG22	1:41:A:VAL:HG22	10	1.12	0.21	1.04
(1,229)	1:12:A:ILE:HG21	1:80:A:ILE:HD11	10	1.12	0.21	1.04
(1,229)	1:12:A:ILE:HG21	1:15:A:ILE:HG23	10	1.12	0.21	1.04
(1,229)	1:12:A:ILE:HG22	1:80:A:ILE:HD13	10	1.12	0.21	1.04
(1,229)	1:12:A:ILE:HG21	1:80:A:ILE:HD12	10	1.12	0.21	1.04
(1,229)	1:62:A:ILE:HG23	1:41:A:VAL:HG23	10	1.12	0.21	1.04
(1,229)	1:62:A:ILE:HG21	1:41:A:VAL:HG21	10	1.12	0.21	1.04
(1,229)	1:62:A:ILE:HG21	1:41:A:VAL:HG23	10	1.12	0.21	1.04
(1,230)	1:12:B:ILE:HG23	1:80:B:ILE:HD12	10	1.12	0.21	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,230)	1:62:B:ILE:HG22	1:41:B:VAL:HG22	10	1.12	0.21	1.04
(1,230)	1:12:B:ILE:HG21	1:80:B:ILE:HD11	10	1.12	0.21	1.04
(1,230)	1:12:B:ILE:HG21	1:15:B:ILE:HG23	10	1.12	0.21	1.04
(1,230)	1:12:B:ILE:HG22	1:80:B:ILE:HD13	10	1.12	0.21	1.04
(1,230)	1:12:B:ILE:HG21	1:80:B:ILE:HD12	10	1.12	0.21	1.04
(1,230)	1:62:B:ILE:HG23	1:41:B:VAL:HG23	10	1.12	0.21	1.04
(1,230)	1:62:B:ILE:HG21	1:41:B:VAL:HG21	10	1.12	0.21	1.04
(1,230)	1:62:B:ILE:HG21	1:41:B:VAL:HG23	10	1.12	0.21	1.04
(1,1803)	1:109:A:LEU:H	1:5:B:MET:H	10	1.12	0.56	1.2
(1,1803)	1:109:A:LEU:H	1:113:A:THR:H	10	1.12	0.56	1.2
(1,1803)	1:93:A:LYS:H	1:88:A:TRP:H	10	1.12	0.56	1.2
(1,1803)	1:16:A:ILE:H	1:87:B:THR:H	10	1.12	0.56	1.2
(1,1803)	1:109:A:LEU:H	1:49:A:LEU:H	10	1.12	0.56	1.2
(1,1804)	1:109:B:LEU:H	1:5:A:MET:H	10	1.12	0.55	1.18
(1,1804)	1:109:B:LEU:H	1:113:B:THR:H	10	1.12	0.55	1.18
(1,1804)	1:93:B:LYS:H	1:88:B:TRP:H	10	1.12	0.55	1.18
(1,1804)	1:16:B:ILE:H	1:87:A:THR:H	10	1.12	0.55	1.18
(1,1804)	1:109:B:LEU:H	1:49:B:LEU:H	10	1.12	0.55	1.18
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG3	10	1.1	0.25	1.03
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG2	10	1.1	0.25	1.03
(1,589)	1:85:A:ARG:HG3	1:78:A:GLU:HG2	10	1.1	0.25	1.03
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG3	10	1.1	0.25	1.03
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG2	10	1.1	0.25	1.03
(1,590)	1:85:B:ARG:HG3	1:78:B:GLU:HG2	10	1.1	0.25	1.03
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG22	10	1.1	0.09	1.1
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG23	10	1.1	0.09	1.1
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG21	10	1.1	0.09	1.1
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG22	10	1.1	0.1	1.09
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG23	10	1.1	0.1	1.09
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG21	10	1.1	0.1	1.09
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD21	10	1.09	0.07	1.11
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD23	10	1.09	0.07	1.11
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD22	10	1.09	0.07	1.11
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD21	10	1.09	0.07	1.11
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD23	10	1.09	0.07	1.11
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD22	10	1.09	0.07	1.11
(1,988)	1:48:B:PHE:HB3	1:109:B:LEU:H	10	1.07	0.38	1.24
(1,988)	1:48:B:PHE:HB2	1:109:B:LEU:H	10	1.07	0.38	1.24
(1,988)	1:48:B:PHE:HB2	1:5:A:MET:H	10	1.07	0.38	1.24
(1,987)	1:48:A:PHE:HB3	1:109:A:LEU:H	10	1.07	0.38	1.25
(1,987)	1:48:A:PHE:HB2	1:109:A:LEU:H	10	1.07	0.38	1.25
(1,987)	1:48:A:PHE:HB2	1:5:B:MET:H	10	1.07	0.38	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD13	10	1.05	0.18	1.09
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD12	10	1.05	0.18	1.09
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD23	10	1.05	0.18	1.09
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD21	10	1.05	0.18	1.09
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD22	10	1.05	0.18	1.09
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD11	10	1.05	0.18	1.09
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD13	10	1.05	0.18	1.08
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD12	10	1.05	0.18	1.08
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD23	10	1.05	0.18	1.08
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD21	10	1.05	0.18	1.08
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD22	10	1.05	0.18	1.08
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD11	10	1.05	0.18	1.08
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	10	1.02	0.13	1.06
(1,1137)	1:14:A:THR:HG21	1:12:A:ILE:HA	10	1.02	0.13	1.06
(1,1137)	1:14:A:THR:HG23	1:12:A:ILE:HA	10	1.02	0.13	1.06
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	10	1.02	0.13	1.06
(1,1138)	1:14:B:THR:HG21	1:12:B:ILE:HA	10	1.02	0.13	1.06
(1,1138)	1:14:B:THR:HG23	1:12:B:ILE:HA	10	1.02	0.13	1.06
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD11	10	1.02	0.21	1.0
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD13	10	1.02	0.21	1.0
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD12	10	1.02	0.21	1.0
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD11	10	1.02	0.21	1.0
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD13	10	1.02	0.21	1.0
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD12	10	1.02	0.21	1.0
(1,1224)	1:50:B:LYS:HA	1:45:B:LEU:HA	10	1.01	0.12	0.98
(1,1224)	1:42:B:ARG:HA	1:45:B:LEU:HA	10	1.01	0.12	0.98
(1,1223)	1:50:A:LYS:HA	1:45:A:LEU:HA	10	1.01	0.12	0.98
(1,1223)	1:42:A:ARG:HA	1:45:A:LEU:HA	10	1.01	0.12	0.98
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	10	0.98	0.14	1.0
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	10	0.98	0.14	0.99
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB2	10	0.96	0.15	0.98
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB3	10	0.96	0.15	0.98
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB1	10	0.96	0.15	0.98
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB2	10	0.96	0.15	0.98
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB3	10	0.96	0.15	0.98
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB1	10	0.96	0.15	0.98
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG13	10	0.94	0.16	1.0
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG12	10	0.94	0.16	1.0
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG11	10	0.94	0.16	1.0
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG13	10	0.94	0.16	0.99
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG12	10	0.94	0.16	0.99
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG11	10	0.94	0.16	0.99

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG21	10	0.94	0.07	0.92
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG23	10	0.94	0.07	0.92
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG22	10	0.94	0.07	0.92
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG21	10	0.94	0.07	0.92
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG23	10	0.94	0.07	0.92
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG22	10	0.94	0.07	0.92
(1,393)	1:33:A:ASN:HB2	1:63:A:MET:HG2	10	0.94	0.34	0.86
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG2	10	0.94	0.34	0.86
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG3	10	0.94	0.34	0.86
(1,393)	1:33:A:ASN:HB2	1:63:A:MET:HG3	10	0.94	0.34	0.86
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD23	10	0.94	0.15	0.98
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD22	10	0.94	0.15	0.98
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD21	10	0.94	0.15	0.98
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD23	10	0.93	0.15	0.98
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD22	10	0.93	0.15	0.98
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD21	10	0.93	0.15	0.98
(1,394)	1:33:B:ASN:HB2	1:63:B:MET:HG2	10	0.93	0.34	0.86
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG2	10	0.93	0.34	0.86
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG3	10	0.93	0.34	0.86
(1,394)	1:33:B:ASN:HB2	1:63:B:MET:HG3	10	0.93	0.34	0.86
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	10	0.93	0.04	0.94
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	10	0.93	0.04	0.92
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	10	0.92	0.23	0.96
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	10	0.92	0.23	0.96
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG3	10	0.92	0.48	0.9
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG2	10	0.92	0.48	0.9
(1,356)	1:54:B:LYS:HA	1:50:B:LYS:HD3	10	0.92	0.48	0.9
(1,1509)	1:39:A:GLU:H	1:38:A:LYS:HD3	10	0.92	0.07	0.92
(1,1509)	1:67:A:ASP:H	1:66:A:LEU:HG	10	0.92	0.07	0.92
(1,1509)	1:39:A:GLU:H	1:38:A:LYS:HD2	10	0.92	0.07	0.92
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG3	10	0.92	0.47	0.9
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG2	10	0.92	0.47	0.9
(1,355)	1:54:A:LYS:HA	1:50:A:LYS:HD3	10	0.92	0.47	0.9
(1,69)	1:33:A:ASN:HB2	1:63:A:MET:HG2	10	0.91	0.31	0.86
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG2	10	0.91	0.31	0.86
(1,69)	1:48:A:PHE:HB3	1:53:A:ASN:HB2	10	0.91	0.31	0.86
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG3	10	0.91	0.31	0.86
(1,69)	1:33:A:ASN:HB2	1:63:A:MET:HG3	10	0.91	0.31	0.86
(1,1510)	1:39:B:GLU:H	1:38:B:LYS:HD3	10	0.91	0.07	0.92
(1,1510)	1:67:B:ASP:H	1:66:B:LEU:HG	10	0.91	0.07	0.92
(1,1510)	1:39:B:GLU:H	1:38:B:LYS:HD2	10	0.91	0.07	0.92
(1,70)	1:33:B:ASN:HB2	1:63:B:MET:HG2	10	0.91	0.3	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG2	10	0.91	0.3	0.86
(1,70)	1:48:B:PHE:HB3	1:53:B:ASN:HB2	10	0.91	0.3	0.86
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG3	10	0.91	0.3	0.86
(1,70)	1:33:B:ASN:HB2	1:63:B:MET:HG3	10	0.91	0.3	0.86
(1,911)	1:66:A:LEU:HD12	1:64:A:GLU:HA	10	0.89	0.37	0.92
(1,911)	1:66:A:LEU:HD22	1:64:A:GLU:HA	10	0.89	0.37	0.92
(1,911)	1:66:A:LEU:HD13	1:64:A:GLU:HA	10	0.89	0.37	0.92
(1,911)	1:66:A:LEU:HD11	1:64:A:GLU:HA	10	0.89	0.37	0.92
(1,912)	1:66:B:LEU:HD12	1:64:B:GLU:HA	10	0.89	0.37	0.92
(1,912)	1:66:B:LEU:HD22	1:64:B:GLU:HA	10	0.89	0.37	0.92
(1,912)	1:66:B:LEU:HD13	1:64:B:GLU:HA	10	0.89	0.37	0.92
(1,912)	1:66:B:LEU:HD11	1:64:B:GLU:HA	10	0.89	0.37	0.92
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD23	10	0.87	0.09	0.85
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD22	10	0.87	0.09	0.85
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD21	10	0.87	0.09	0.85
(1,616)	1:42:B:ARG:HA	1:45:B:LEU:HD11	10	0.87	0.09	0.85
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD23	10	0.87	0.09	0.85
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD22	10	0.87	0.09	0.85
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD21	10	0.87	0.09	0.85
(1,615)	1:42:A:ARG:HA	1:45:A:LEU:HD11	10	0.87	0.09	0.85
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	10	0.87	0.1	0.82
(1,566)	1:42:B:ARG:HA	1:49:B:LEU:H	10	0.87	0.1	0.82
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	10	0.87	0.1	0.82
(1,565)	1:42:A:ARG:HA	1:49:A:LEU:H	10	0.87	0.1	0.82
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB3	10	0.86	0.38	0.76
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB2	10	0.86	0.38	0.76
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB3	10	0.86	0.39	0.76
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB2	10	0.86	0.39	0.76
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD12	10	0.86	0.09	0.89
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD23	10	0.86	0.09	0.89
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD13	10	0.86	0.09	0.89
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD11	10	0.86	0.09	0.89
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD22	10	0.86	0.09	0.89
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD21	10	0.86	0.09	0.89
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD12	10	0.86	0.09	0.9
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD23	10	0.86	0.09	0.9
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD13	10	0.86	0.09	0.9
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD11	10	0.86	0.09	0.9
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD22	10	0.86	0.09	0.9
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD21	10	0.86	0.09	0.9
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	10	0.83	0.23	0.79
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	10	0.83	0.24	0.79

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,600)	1:18:B:THR:HG22	1:11:A:ASN:HB2	10	0.81	0.24	0.77
(1,600)	1:18:B:THR:HG23	1:43:B:LYS:HE3	10	0.81	0.24	0.77
(1,600)	1:18:B:THR:HG21	1:11:A:ASN:HB2	10	0.81	0.24	0.77
(1,600)	1:18:B:THR:HG21	1:43:B:LYS:HE2	10	0.81	0.24	0.77
(1,600)	1:18:B:THR:HG23	1:11:A:ASN:HB3	10	0.81	0.24	0.77
(1,600)	1:18:B:THR:HG21	1:11:A:ASN:HB3	10	0.81	0.24	0.77
(1,600)	1:18:B:THR:HG21	1:43:B:LYS:HE3	10	0.81	0.24	0.77
(1,599)	1:18:A:THR:HG22	1:11:B:ASN:HB2	10	0.81	0.24	0.76
(1,599)	1:18:A:THR:HG23	1:43:A:LYS:HE3	10	0.81	0.24	0.76
(1,599)	1:18:A:THR:HG21	1:11:B:ASN:HB2	10	0.81	0.24	0.76
(1,599)	1:18:A:THR:HG21	1:43:A:LYS:HE2	10	0.81	0.24	0.76
(1,599)	1:18:A:THR:HG23	1:11:B:ASN:HB3	10	0.81	0.24	0.76
(1,599)	1:18:A:THR:HG21	1:11:B:ASN:HB3	10	0.81	0.24	0.76
(1,599)	1:18:A:THR:HG21	1:43:A:LYS:HE3	10	0.81	0.24	0.76
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD21	10	0.79	0.27	0.67
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD22	10	0.79	0.27	0.67
(1,1297)	1:8:A:LEU:H	1:15:B:ILE:HG23	10	0.79	0.27	0.67
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD23	10	0.79	0.27	0.67
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	10	0.79	0.34	0.73
(1,82)	1:46:B:GLN:HG2	1:8:A:LEU:H	10	0.79	0.34	0.73
(1,130)	1:16:B:ILE:HD11	1:17:B:ASN:HA	10	0.79	0.08	0.8
(1,130)	1:16:B:ILE:HD12	1:17:B:ASN:HA	10	0.79	0.08	0.8
(1,130)	1:16:B:ILE:HD13	1:17:B:ASN:HA	10	0.79	0.08	0.8
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD21	10	0.78	0.27	0.66
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD22	10	0.78	0.27	0.66
(1,1298)	1:8:B:LEU:H	1:15:A:ILE:HG23	10	0.78	0.27	0.66
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD23	10	0.78	0.27	0.66
(1,129)	1:16:A:ILE:HD11	1:17:A:ASN:HA	10	0.78	0.08	0.8
(1,129)	1:16:A:ILE:HD12	1:17:A:ASN:HA	10	0.78	0.08	0.8
(1,129)	1:16:A:ILE:HD13	1:17:A:ASN:HA	10	0.78	0.08	0.8
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	10	0.78	0.34	0.7
(1,81)	1:46:A:GLN:HG2	1:8:B:LEU:H	10	0.78	0.34	0.7
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	10	0.75	0.11	0.74
(1,1590)	1:10:B:ARG:H	1:12:B:ILE:HA	10	0.75	0.11	0.74
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	10	0.75	0.11	0.74
(1,1589)	1:10:A:ARG:H	1:12:A:ILE:HA	10	0.75	0.11	0.74
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	10	0.74	0.23	0.76
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG3	10	0.74	0.23	0.76
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	10	0.74	0.23	0.74
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG3	10	0.74	0.23	0.74
(3,90)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	10	0.74	0.2	0.72
(3,90)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	10	0.74	0.2	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,90)	1:7:B:GLN:HG2	1:44:A:ASP:HB2	10	0.74	0.2	0.72
(3,89)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	10	0.74	0.19	0.73
(3,89)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	10	0.74	0.19	0.73
(3,89)	1:7:A:GLN:HG2	1:44:B:ASP:HB2	10	0.74	0.19	0.73
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD21	10	0.7	0.15	0.63
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD22	10	0.7	0.15	0.63
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD23	10	0.7	0.15	0.63
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE1	10	0.7	0.16	0.67
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE2	10	0.7	0.16	0.67
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE3	10	0.7	0.16	0.67
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE1	10	0.7	0.16	0.68
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE2	10	0.7	0.16	0.68
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE3	10	0.7	0.16	0.68
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD21	10	0.7	0.14	0.62
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD22	10	0.7	0.14	0.62
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD23	10	0.7	0.14	0.62
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	10	0.68	0.13	0.64
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	10	0.68	0.13	0.65
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG3	10	0.67	0.22	0.62
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG2	10	0.67	0.22	0.62
(1,811)	1:21:A:GLN:HG3	1:39:A:GLU:HG2	10	0.67	0.22	0.62
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG3	10	0.67	0.22	0.62
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG2	10	0.67	0.22	0.62
(1,812)	1:21:B:GLN:HG3	1:39:B:GLU:HG2	10	0.67	0.22	0.62
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG23	10	0.67	0.02	0.68
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG22	10	0.67	0.02	0.68
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG21	10	0.67	0.02	0.68
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	10	0.67	0.03	0.66
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	10	0.67	0.02	0.66
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG23	10	0.67	0.02	0.67
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG22	10	0.67	0.02	0.67
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG21	10	0.67	0.02	0.67
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG21	10	0.66	0.01	0.66
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG22	10	0.66	0.01	0.66
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG23	10	0.66	0.01	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG21	10	0.66	0.01	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG22	10	0.66	0.01	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG23	10	0.66	0.01	0.66
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB2	10	0.66	0.19	0.74
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB3	10	0.66	0.19	0.74
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB2	10	0.66	0.19	0.74
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB3	10	0.66	0.19	0.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB2	10	0.66	0.19	0.74
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB3	10	0.66	0.19	0.74
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB2	10	0.66	0.19	0.74
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB3	10	0.66	0.19	0.74
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD13	10	0.65	0.35	0.55
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD23	10	0.65	0.35	0.55
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD11	10	0.65	0.35	0.55
(1,1581)	1:50:A:LYS:H	1:45:A:LEU:HD22	10	0.65	0.35	0.55
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD21	10	0.65	0.35	0.55
(1,1581)	1:50:A:LYS:H	1:45:A:LEU:HD23	10	0.65	0.35	0.55
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD13	10	0.65	0.34	0.56
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD23	10	0.65	0.34	0.56
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD11	10	0.65	0.34	0.56
(1,1582)	1:50:B:LYS:H	1:45:B:LEU:HD22	10	0.65	0.34	0.56
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD21	10	0.65	0.34	0.56
(1,1582)	1:50:B:LYS:H	1:45:B:LEU:HD23	10	0.65	0.34	0.56
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD22	10	0.65	0.26	0.66
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD13	10	0.65	0.26	0.66
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD23	10	0.65	0.26	0.66
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD22	10	0.65	0.26	0.66
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD13	10	0.65	0.26	0.66
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD23	10	0.65	0.26	0.66
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	10	0.65	0.1	0.66
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	10	0.65	0.11	0.66
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG23	10	0.64	0.02	0.64
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG22	10	0.64	0.02	0.64
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG21	10	0.64	0.02	0.64
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG23	10	0.64	0.02	0.65
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG22	10	0.64	0.02	0.65
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG21	10	0.64	0.02	0.65
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	10	0.64	0.08	0.66
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	10	0.64	0.08	0.64
(3,667)	1:63:A:MET:HE3	1:32:A:LEU:HB2	10	0.64	0.23	0.52
(3,667)	1:63:A:MET:HE1	1:32:A:LEU:HB2	10	0.64	0.23	0.52
(3,667)	1:63:A:MET:HE2	1:32:A:LEU:HB2	10	0.64	0.23	0.52
(3,667)	1:63:A:MET:HE1	1:32:A:LEU:HB3	10	0.64	0.23	0.52
(3,668)	1:63:B:MET:HE3	1:32:B:LEU:HB2	10	0.64	0.23	0.52
(3,668)	1:63:B:MET:HE1	1:32:B:LEU:HB2	10	0.64	0.23	0.52
(3,668)	1:63:B:MET:HE2	1:32:B:LEU:HB2	10	0.64	0.23	0.52
(3,668)	1:63:B:MET:HE1	1:32:B:LEU:HB3	10	0.64	0.23	0.52
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG22	10	0.64	0.07	0.68
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG21	10	0.64	0.07	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1693)	1:62:A:ILE:H	1:58:A:VAL:HG13	10	0.64	0.07	0.68
(1,1693)	1:62:A:ILE:H	1:58:A:VAL:HG11	10	0.64	0.07	0.68
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG23	10	0.64	0.07	0.68
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG22	10	0.64	0.07	0.68
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG21	10	0.64	0.07	0.68
(1,1694)	1:62:B:ILE:H	1:58:B:VAL:HG13	10	0.64	0.07	0.68
(1,1694)	1:62:B:ILE:H	1:58:B:VAL:HG11	10	0.64	0.07	0.68
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG23	10	0.64	0.07	0.68
(1,974)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	10	0.64	0.28	0.6
(1,974)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	10	0.64	0.28	0.6
(1,974)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	10	0.64	0.28	0.6
(1,974)	1:7:B:GLN:HG2	1:44:A:ASP:HB2	10	0.64	0.28	0.6
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD13	10	0.64	0.19	0.72
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD11	10	0.64	0.19	0.72
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD12	10	0.64	0.19	0.72
(1,1709)	1:79:A:PHE:H	1:66:A:LEU:HD22	10	0.64	0.19	0.72
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD22	10	0.64	0.19	0.72
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD13	10	0.64	0.19	0.72
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD11	10	0.64	0.19	0.72
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD12	10	0.64	0.19	0.72
(1,1710)	1:79:B:PHE:H	1:66:B:LEU:HD22	10	0.64	0.19	0.72
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD22	10	0.64	0.19	0.72
(1,973)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	10	0.63	0.28	0.6
(1,973)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	10	0.63	0.28	0.6
(1,973)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	10	0.63	0.28	0.6
(1,973)	1:7:A:GLN:HG2	1:44:B:ASP:HB2	10	0.63	0.28	0.6
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG2	10	0.63	0.15	0.65
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG3	10	0.63	0.15	0.65
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG2	10	0.63	0.15	0.66
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG3	10	0.63	0.15	0.66
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG2	10	0.63	0.15	0.65
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG3	10	0.63	0.15	0.65
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG2	10	0.63	0.15	0.66
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG3	10	0.63	0.15	0.66
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	10	0.63	0.28	0.58
(1,948)	1:86:B:LEU:HA	1:83:B:MET:HB3	10	0.63	0.28	0.58
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	10	0.63	0.28	0.58
(1,947)	1:86:A:LEU:HA	1:83:A:MET:HB3	10	0.63	0.28	0.58
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	10	0.62	0.24	0.65
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG3	10	0.62	0.24	0.65
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HB3	10	0.62	0.24	0.65
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG13	10	0.62	0.05	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG11	10	0.62	0.05	0.64
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG12	10	0.62	0.05	0.64
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG13	10	0.62	0.05	0.63
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG11	10	0.62	0.05	0.63
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG12	10	0.62	0.05	0.63
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	10	0.6	0.18	0.57
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	10	0.6	0.18	0.57
(1,336)	1:41:B:VAL:HG11	1:48:B:PHE:H	10	0.6	0.24	0.59
(1,336)	1:41:B:VAL:HG12	1:48:B:PHE:H	10	0.6	0.24	0.59
(1,336)	1:41:B:VAL:HG13	1:48:B:PHE:H	10	0.6	0.24	0.59
(1,335)	1:41:A:VAL:HG11	1:48:A:PHE:H	10	0.59	0.24	0.6
(1,335)	1:41:A:VAL:HG12	1:48:A:PHE:H	10	0.59	0.24	0.6
(1,335)	1:41:A:VAL:HG13	1:48:A:PHE:H	10	0.59	0.24	0.6
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	10	0.58	0.08	0.6
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	10	0.58	0.08	0.6
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	10	0.58	0.08	0.6
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	10	0.58	0.08	0.6
(1,372)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	10	0.58	0.26	0.55
(1,372)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	10	0.58	0.26	0.55
(1,372)	1:7:B:GLN:HG2	1:17:A:ASN:HB3	10	0.58	0.26	0.55
(1,372)	1:7:B:GLN:HG2	1:17:A:ASN:HB2	10	0.58	0.26	0.55
(1,372)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	10	0.58	0.26	0.55
(1,371)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	10	0.58	0.26	0.55
(1,371)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	10	0.58	0.26	0.55
(1,371)	1:7:A:GLN:HG2	1:17:B:ASN:HB3	10	0.58	0.26	0.55
(1,371)	1:7:A:GLN:HG2	1:17:B:ASN:HB2	10	0.58	0.26	0.55
(1,371)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	10	0.58	0.26	0.55
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	10	0.57	0.14	0.56
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	10	0.57	0.14	0.56
(1,679)	1:37:A:PHE:HB2	1:62:A:ILE:HG23	10	0.56	0.16	0.49
(1,679)	1:37:A:PHE:HB3	1:62:A:ILE:HG21	10	0.56	0.16	0.49
(1,679)	1:37:A:PHE:HB2	1:62:A:ILE:HG21	10	0.56	0.16	0.49
(1,679)	1:37:A:PHE:HB3	1:62:A:ILE:HG23	10	0.56	0.16	0.49
(1,679)	1:37:A:PHE:HB2	1:62:A:ILE:HG22	10	0.56	0.16	0.49
(1,680)	1:37:B:PHE:HB2	1:62:B:ILE:HG23	10	0.56	0.16	0.48
(1,680)	1:37:B:PHE:HB3	1:62:B:ILE:HG21	10	0.56	0.16	0.48
(1,680)	1:37:B:PHE:HB2	1:62:B:ILE:HG21	10	0.56	0.16	0.48
(1,680)	1:37:B:PHE:HB3	1:62:B:ILE:HG23	10	0.56	0.16	0.48
(1,680)	1:37:B:PHE:HB2	1:62:B:ILE:HG22	10	0.56	0.16	0.48
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	10	0.56	0.25	0.52
(1,439)	1:10:A:ARG:HG2	1:11:A:ASN:HB2	10	0.56	0.25	0.52
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB3	10	0.56	0.25	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	10	0.56	0.25	0.52
(1,440)	1:10:B:ARG:HG2	1:11:B:ASN:HB2	10	0.56	0.25	0.52
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB3	10	0.56	0.25	0.52
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG21	10	0.55	0.13	0.52
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG23	10	0.55	0.13	0.52
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG22	10	0.55	0.13	0.52
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG21	10	0.55	0.13	0.52
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG23	10	0.55	0.13	0.52
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG22	10	0.55	0.13	0.52
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	10	0.53	0.13	0.5
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	10	0.53	0.13	0.5
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD23	10	0.53	0.18	0.45
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD21	10	0.53	0.18	0.45
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD22	10	0.53	0.18	0.45
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD23	10	0.53	0.18	0.46
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD21	10	0.53	0.18	0.46
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD22	10	0.53	0.18	0.46
(1,214)	1:62:B:ILE:HG23	1:63:B:MET:HA	10	0.52	0.11	0.55
(1,214)	1:62:B:ILE:HG21	1:63:B:MET:HA	10	0.52	0.11	0.55
(1,214)	1:62:B:ILE:HG22	1:63:B:MET:HA	10	0.52	0.11	0.55
(1,328)	1:66:B:LEU:HD23	1:67:B:ASP:HA	10	0.52	0.16	0.57
(1,328)	1:66:B:LEU:HD22	1:67:B:ASP:HA	10	0.52	0.16	0.57
(1,328)	1:66:B:LEU:HD21	1:67:B:ASP:HA	10	0.52	0.16	0.57
(1,328)	1:66:B:LEU:HD13	1:67:B:ASP:HA	10	0.52	0.16	0.57
(3,584)	1:66:B:LEU:HD23	1:67:B:ASP:HA	10	0.52	0.16	0.57
(3,584)	1:66:B:LEU:HD22	1:67:B:ASP:HA	10	0.52	0.16	0.57
(3,584)	1:66:B:LEU:HD21	1:67:B:ASP:HA	10	0.52	0.16	0.57
(3,584)	1:66:B:LEU:HD13	1:67:B:ASP:HA	10	0.52	0.16	0.57
(1,213)	1:62:A:ILE:HG23	1:63:A:MET:HA	10	0.52	0.11	0.55
(1,213)	1:62:A:ILE:HG21	1:63:A:MET:HA	10	0.52	0.11	0.55
(1,213)	1:62:A:ILE:HG22	1:63:A:MET:HA	10	0.52	0.11	0.55
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	10	0.52	0.09	0.55
(1,1082)	1:37:B:PHE:HA	1:35:B:GLY:HA2	10	0.52	0.09	0.55
(1,1082)	1:79:B:PHE:HA	1:83:B:MET:HA	10	0.52	0.09	0.55
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	10	0.52	0.09	0.55
(1,1081)	1:37:A:PHE:HA	1:35:A:GLY:HA2	10	0.52	0.09	0.55
(1,1081)	1:79:A:PHE:HA	1:83:A:MET:HA	10	0.52	0.09	0.55
(1,327)	1:66:A:LEU:HD23	1:67:A:ASP:HA	10	0.52	0.16	0.57
(1,327)	1:66:A:LEU:HD22	1:67:A:ASP:HA	10	0.52	0.16	0.57
(1,327)	1:66:A:LEU:HD21	1:67:A:ASP:HA	10	0.52	0.16	0.57
(1,327)	1:66:A:LEU:HD13	1:67:A:ASP:HA	10	0.52	0.16	0.57
(3,583)	1:66:A:LEU:HD23	1:67:A:ASP:HA	10	0.52	0.16	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,583)	1:66:A:LEU:HD22	1:67:A:ASP:HA	10	0.52	0.16	0.57
(3,583)	1:66:A:LEU:HD21	1:67:A:ASP:HA	10	0.52	0.16	0.57
(3,583)	1:66:A:LEU:HD13	1:67:A:ASP:HA	10	0.52	0.16	0.57
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	10	0.51	0.05	0.53
(3,745)	1:24:A:VAL:HG13	1:25:A:LYS:HG3	10	0.51	0.11	0.53
(3,745)	1:24:A:VAL:HG11	1:25:A:LYS:HG3	10	0.51	0.11	0.53
(3,745)	1:24:A:VAL:HG12	1:25:A:LYS:HG3	10	0.51	0.11	0.53
(3,746)	1:24:B:VAL:HG13	1:25:B:LYS:HG3	10	0.51	0.11	0.53
(3,746)	1:24:B:VAL:HG11	1:25:B:LYS:HG3	10	0.51	0.11	0.53
(3,746)	1:24:B:VAL:HG12	1:25:B:LYS:HG3	10	0.51	0.11	0.53
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	10	0.51	0.06	0.52
(1,646)	1:86:B:LEU:HA	1:49:B:LEU:HA	10	0.51	0.19	0.54
(1,646)	1:53:B:ASN:HA	1:49:B:LEU:HA	10	0.51	0.19	0.54
(1,645)	1:86:A:LEU:HA	1:49:A:LEU:HA	10	0.5	0.19	0.53
(1,645)	1:53:A:ASN:HA	1:49:A:LEU:HA	10	0.5	0.19	0.53
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB3	10	0.49	0.16	0.47
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	10	0.49	0.16	0.47
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	10	0.48	0.27	0.46
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	10	0.48	0.27	0.46
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB3	10	0.48	0.15	0.46
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	10	0.48	0.15	0.46
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	10	0.47	0.08	0.47
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	10	0.47	0.08	0.48
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD13	10	0.45	0.13	0.41
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD11	10	0.45	0.13	0.41
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD12	10	0.45	0.13	0.41
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD13	10	0.45	0.13	0.41
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD11	10	0.45	0.13	0.41
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD12	10	0.45	0.13	0.41
(3,92)	1:7:B:GLN:HG2	1:6:B:SER:HB3	10	0.45	0.21	0.55
(3,92)	1:7:B:GLN:HG3	1:6:B:SER:HB3	10	0.45	0.21	0.55
(3,91)	1:7:A:GLN:HG2	1:6:A:SER:HB3	10	0.45	0.21	0.54
(3,91)	1:7:A:GLN:HG3	1:6:A:SER:HB3	10	0.45	0.21	0.54
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	10	0.45	0.1	0.45
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	10	0.45	0.1	0.45
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	10	0.45	0.1	0.45
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	10	0.45	0.1	0.45
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE3	10	0.44	0.24	0.36
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE1	10	0.44	0.24	0.36
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE2	10	0.44	0.24	0.36
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	10	0.44	0.04	0.45
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG2	10	0.44	0.04	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	10	0.44	0.04	0.44
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG2	10	0.44	0.04	0.44
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE3	10	0.44	0.24	0.36
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE1	10	0.44	0.24	0.36
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE2	10	0.44	0.24	0.36
(1,247)	1:63:A:MET:HB2	1:61:A:HIS:HB3	10	0.44	0.12	0.47
(1,247)	1:63:A:MET:HB3	1:61:A:HIS:HB3	10	0.44	0.12	0.47
(1,247)	1:63:A:MET:HB2	1:61:A:HIS:HB2	10	0.44	0.12	0.47
(1,248)	1:63:B:MET:HB2	1:61:B:HIS:HB3	10	0.44	0.12	0.46
(1,248)	1:63:B:MET:HB3	1:61:B:HIS:HB3	10	0.44	0.12	0.46
(1,248)	1:63:B:MET:HB2	1:61:B:HIS:HB2	10	0.44	0.12	0.46
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	10	0.44	0.09	0.43
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG3	10	0.44	0.09	0.43
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	10	0.43	0.09	0.42
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG3	10	0.43	0.09	0.42
(3,251)	1:33:A:ASN:HB2	1:72:A:LYS:HA	10	0.42	0.12	0.38
(3,251)	1:33:A:ASN:HB3	1:72:A:LYS:HA	10	0.42	0.12	0.38
(3,252)	1:33:B:ASN:HB2	1:72:B:LYS:HA	10	0.42	0.12	0.38
(3,252)	1:33:B:ASN:HB3	1:72:B:LYS:HA	10	0.42	0.12	0.38
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	10	0.41	0.29	0.3
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	10	0.41	0.29	0.3
(3,42)	1:58:B:VAL:HG21	1:57:B:LYS:HB2	10	0.4	0.09	0.38
(3,42)	1:58:B:VAL:HG13	1:57:B:LYS:HB2	10	0.4	0.09	0.38
(3,42)	1:58:B:VAL:HG23	1:57:B:LYS:HB2	10	0.4	0.09	0.38
(3,42)	1:58:B:VAL:HG22	1:57:B:LYS:HB2	10	0.4	0.09	0.38
(3,41)	1:58:A:VAL:HG21	1:57:A:LYS:HB2	10	0.4	0.09	0.38
(3,41)	1:58:A:VAL:HG13	1:57:A:LYS:HB2	10	0.4	0.09	0.38
(3,41)	1:58:A:VAL:HG23	1:57:A:LYS:HB2	10	0.4	0.09	0.38
(3,41)	1:58:A:VAL:HG22	1:57:A:LYS:HB2	10	0.4	0.09	0.38
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD12	10	0.39	0.05	0.42
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD13	10	0.39	0.05	0.42
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD11	10	0.39	0.05	0.42
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD12	10	0.39	0.05	0.42
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD13	10	0.39	0.05	0.42
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD11	10	0.39	0.05	0.42
(1,185)	1:60:A:GLU:HG2	1:61:A:HIS:HA	10	0.39	0.1	0.42
(1,185)	1:60:A:GLU:HG3	1:61:A:HIS:HA	10	0.39	0.1	0.42
(1,186)	1:60:B:GLU:HG2	1:61:B:HIS:HA	10	0.38	0.1	0.42
(1,186)	1:60:B:GLU:HG3	1:61:B:HIS:HA	10	0.38	0.1	0.42
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD22	10	0.35	0.13	0.35
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD21	10	0.35	0.13	0.35
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD23	10	0.35	0.13	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD22	10	0.35	0.13	0.35
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD21	10	0.35	0.13	0.35
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD23	10	0.35	0.13	0.35
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD12	10	0.35	0.09	0.36
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD13	10	0.35	0.09	0.36
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD11	10	0.35	0.09	0.36
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD12	10	0.34	0.09	0.36
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD13	10	0.34	0.09	0.36
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD11	10	0.34	0.09	0.36
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG11	10	0.34	0.13	0.39
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG12	10	0.34	0.13	0.39
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG13	10	0.34	0.13	0.39
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG11	10	0.34	0.13	0.4
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG12	10	0.34	0.13	0.4
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG13	10	0.34	0.13	0.4
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	10	0.3	0.05	0.3
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	10	0.3	0.05	0.29
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	10	0.3	0.15	0.26
(3,629)	1:48:A:PHE:HB3	1:45:A:LEU:HA	10	0.3	0.15	0.26
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	10	0.29	0.14	0.26
(3,630)	1:48:B:PHE:HB3	1:45:B:LEU:HA	10	0.29	0.14	0.26
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	10	0.29	0.04	0.29
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB3	10	0.29	0.04	0.29
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	10	0.29	0.04	0.29
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB3	10	0.29	0.04	0.29
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	10	0.28	0.02	0.28
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	10	0.28	0.02	0.28
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG13	10	0.27	0.02	0.27
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG11	10	0.27	0.02	0.27
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG12	10	0.27	0.02	0.27
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG13	10	0.27	0.02	0.26
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG11	10	0.27	0.02	0.26
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG12	10	0.27	0.02	0.26
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	10	0.23	0.02	0.24
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	10	0.23	0.02	0.24
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	10	0.21	0.05	0.2
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	10	0.21	0.05	0.2
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	10	0.21	0.05	0.18
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	10	0.21	0.05	0.18
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	10	0.21	0.05	0.22
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	10	0.2	0.05	0.21
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB3	10	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB1	10	0.16	0.03	0.15
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB2	10	0.16	0.03	0.15
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	10	0.16	0.03	0.17
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB3	10	0.16	0.04	0.15
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB1	10	0.16	0.04	0.15
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB2	10	0.16	0.04	0.15
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	10	0.16	0.03	0.16
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	10	0.14	0.03	0.14
(1,1077)	1:31:A:THR:HG22	1:25:A:LYS:HG3	9	2.45	0.82	2.7
(1,1077)	1:31:A:THR:HG22	1:68:A:THR:HG22	9	2.45	0.82	2.7
(1,1077)	1:31:A:THR:HG23	1:25:A:LYS:HG3	9	2.45	0.82	2.7
(1,1077)	1:31:A:THR:HG21	1:68:A:THR:HG23	9	2.45	0.82	2.7
(1,1077)	1:31:A:THR:HG23	1:66:A:LEU:HB3	9	2.45	0.82	2.7
(1,1077)	1:31:A:THR:HG21	1:25:A:LYS:HG3	9	2.45	0.82	2.7
(1,1078)	1:31:B:THR:HG22	1:25:B:LYS:HG3	9	2.45	0.82	2.7
(1,1078)	1:31:B:THR:HG22	1:68:B:THR:HG22	9	2.45	0.82	2.7
(1,1078)	1:31:B:THR:HG23	1:25:B:LYS:HG3	9	2.45	0.82	2.7
(1,1078)	1:31:B:THR:HG21	1:68:B:THR:HG23	9	2.45	0.82	2.7
(1,1078)	1:31:B:THR:HG23	1:66:B:LEU:HB3	9	2.45	0.82	2.7
(1,1078)	1:31:B:THR:HG21	1:25:B:LYS:HG3	9	2.45	0.82	2.7
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	9	2.07	1.34	2.65
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	9	2.07	1.34	2.66
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG3	9	1.38	0.32	1.5
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG2	9	1.38	0.32	1.5
(1,442)	1:10:B:ARG:HG2	1:4:B:LYS:HG3	9	1.38	0.32	1.5
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG3	9	1.38	0.32	1.5
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG2	9	1.38	0.32	1.5
(1,441)	1:10:A:ARG:HG2	1:4:A:LYS:HG3	9	1.38	0.32	1.5
(1,872)	1:34:B:GLN:HB2	1:64:B:GLU:HG3	9	1.38	0.45	1.4
(1,872)	1:34:B:GLN:HB2	1:71:B:ASP:HB3	9	1.38	0.45	1.4
(1,871)	1:34:A:GLN:HB2	1:64:A:GLU:HG3	9	1.37	0.45	1.39
(1,871)	1:34:A:GLN:HB2	1:71:A:ASP:HB3	9	1.37	0.45	1.39
(1,754)	1:111:B:GLU:HG2	1:4:A:LYS:HE3	9	1.37	0.68	1.19
(1,754)	1:92:B:GLU:HG2	1:30:A:ASP:HB2	9	1.37	0.68	1.19
(1,754)	1:111:B:GLU:HG3	1:4:A:LYS:HE3	9	1.37	0.68	1.19
(1,754)	1:111:B:GLU:HG3	1:51:B:LYS:HE2	9	1.37	0.68	1.19
(1,754)	1:111:B:GLU:HG3	1:4:A:LYS:HE2	9	1.37	0.68	1.19
(1,754)	1:92:B:GLU:HG3	1:51:B:LYS:HE3	9	1.37	0.68	1.19
(1,753)	1:111:A:GLU:HG2	1:4:B:LYS:HE3	9	1.36	0.68	1.2
(1,753)	1:92:A:GLU:HG2	1:30:B:ASP:HB2	9	1.36	0.68	1.2
(1,753)	1:111:A:GLU:HG3	1:4:B:LYS:HE3	9	1.36	0.68	1.2
(1,753)	1:111:A:GLU:HG3	1:51:A:LYS:HE2	9	1.36	0.68	1.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,753)	1:111:A:GLU:HG3	1:4:B:LYS:HE2	9	1.36	0.68	1.2
(1,753)	1:92:A:GLU:HG3	1:51:A:LYS:HE3	9	1.36	0.68	1.2
(1,138)	1:16:B:ILE:HD12	1:93:A:LYS:HE3	9	1.35	1.04	1.05
(1,138)	1:16:B:ILE:HD12	1:11:B:ASN:HB2	9	1.35	1.04	1.05
(1,138)	1:16:B:ILE:HD13	1:11:B:ASN:HB2	9	1.35	1.04	1.05
(1,138)	1:16:B:ILE:HD13	1:93:A:LYS:HE2	9	1.35	1.04	1.05
(1,138)	1:80:B:ILE:HD11	1:85:A:ARG:HD2	9	1.35	1.04	1.05
(1,138)	1:16:B:ILE:HD11	1:11:B:ASN:HB3	9	1.35	1.04	1.05
(1,138)	1:16:B:ILE:HD13	1:11:B:ASN:HB3	9	1.35	1.04	1.05
(1,137)	1:16:A:ILE:HD12	1:93:B:LYS:HE3	9	1.35	1.04	1.05
(1,137)	1:16:A:ILE:HD12	1:11:A:ASN:HB2	9	1.35	1.04	1.05
(1,137)	1:16:A:ILE:HD13	1:11:A:ASN:HB2	9	1.35	1.04	1.05
(1,137)	1:16:A:ILE:HD13	1:93:B:LYS:HE2	9	1.35	1.04	1.05
(1,137)	1:80:A:ILE:HD11	1:85:B:ARG:HD2	9	1.35	1.04	1.05
(1,137)	1:16:A:ILE:HD11	1:11:A:ASN:HB3	9	1.35	1.04	1.05
(1,137)	1:16:A:ILE:HD13	1:11:A:ASN:HB3	9	1.35	1.04	1.05
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG11	9	1.27	0.48	1.33
(1,511)	1:51:A:LYS:HE2	1:58:A:VAL:HG22	9	1.27	0.48	1.33
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG12	9	1.27	0.48	1.33
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG13	9	1.27	0.48	1.33
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG11	9	1.27	0.48	1.33
(1,512)	1:51:B:LYS:HE2	1:58:B:VAL:HG22	9	1.27	0.48	1.33
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG12	9	1.27	0.48	1.33
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG13	9	1.27	0.48	1.33
(1,1820)	1:21:B:GLN:H	1:40:B:LEU:HG	9	1.25	0.22	1.27
(1,1820)	1:94:B:MET:H	1:89:B:ALA:HB2	9	1.25	0.22	1.27
(1,1820)	1:94:B:MET:H	1:89:B:ALA:HB3	9	1.25	0.22	1.27
(1,1819)	1:21:A:GLN:H	1:40:A:LEU:HG	9	1.25	0.22	1.27
(1,1819)	1:94:A:MET:H	1:89:A:ALA:HB2	9	1.25	0.22	1.27
(1,1819)	1:94:A:MET:H	1:89:A:ALA:HB3	9	1.25	0.22	1.27
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG23	9	1.11	0.36	1.31
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG21	9	1.11	0.36	1.31
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG22	9	1.11	0.36	1.31
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG23	9	1.1	0.36	1.31
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG21	9	1.1	0.36	1.31
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG22	9	1.1	0.36	1.31
(1,24)	1:65:B:ASP:HA	1:72:B:LYS:HA	9	1.06	0.63	0.81
(1,24)	1:96:B:GLU:HA	1:107:B:PRO:HD2	9	1.06	0.63	0.81
(1,24)	1:96:B:GLU:HA	1:107:B:PRO:HD3	9	1.06	0.63	0.81
(1,24)	1:93:B:LYS:HA	1:107:B:PRO:HD3	9	1.06	0.63	0.81
(1,24)	1:93:B:LYS:HA	1:107:B:PRO:HD2	9	1.06	0.63	0.81
(1,23)	1:65:A:ASP:HA	1:72:A:LYS:HA	9	1.06	0.63	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,23)	1:96:A:GLU:HA	1:107:A:PRO:HD2	9	1.06	0.63	0.82
(1,23)	1:96:A:GLU:HA	1:107:A:PRO:HD3	9	1.06	0.63	0.82
(1,23)	1:93:A:LYS:HA	1:107:A:PRO:HD3	9	1.06	0.63	0.82
(1,23)	1:93:A:LYS:HA	1:107:A:PRO:HD2	9	1.06	0.63	0.82
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	9	1.02	0.28	1.04
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	9	1.02	0.28	1.04
(1,1218)	1:87:B:THR:HG22	1:83:B:MET:HB3	9	1.0	0.25	1.04
(1,1218)	1:87:B:THR:HG22	1:15:A:ILE:HB	9	1.0	0.25	1.04
(1,1218)	1:87:B:THR:HG21	1:83:B:MET:HB3	9	1.0	0.25	1.04
(1,1218)	1:87:B:THR:HG23	1:15:A:ILE:HB	9	1.0	0.25	1.04
(1,1217)	1:87:A:THR:HG22	1:83:A:MET:HB3	9	0.99	0.25	1.04
(1,1217)	1:87:A:THR:HG22	1:15:B:ILE:HB	9	0.99	0.25	1.04
(1,1217)	1:87:A:THR:HG21	1:83:A:MET:HB3	9	0.99	0.25	1.04
(1,1217)	1:87:A:THR:HG23	1:15:B:ILE:HB	9	0.99	0.25	1.04
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG13	9	0.97	0.25	1.04
(1,1707)	1:79:A:PHE:H	1:87:B:THR:HG21	9	0.97	0.25	1.04
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG12	9	0.97	0.25	1.04
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG13	9	0.97	0.25	1.04
(1,1708)	1:79:B:PHE:H	1:87:A:THR:HG21	9	0.97	0.25	1.04
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG12	9	0.97	0.25	1.04
(1,1781)	1:89:A:ALA:H	1:85:A:ARG:HG2	9	0.91	0.23	0.86
(1,1781)	1:89:A:ALA:H	1:93:A:LYS:HB2	9	0.91	0.23	0.86
(1,1781)	1:89:A:ALA:H	1:16:B:ILE:HG12	9	0.91	0.23	0.86
(1,1782)	1:89:B:ALA:H	1:85:B:ARG:HG2	9	0.91	0.23	0.86
(1,1782)	1:89:B:ALA:H	1:93:B:LYS:HB2	9	0.91	0.23	0.86
(1,1782)	1:89:B:ALA:H	1:16:A:ILE:HG12	9	0.91	0.23	0.86
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	9	0.87	0.13	0.87
(1,477)	1:63:A:MET:HB2	1:37:A:PHE:HB3	9	0.87	0.13	0.87
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	9	0.87	0.13	0.87
(1,478)	1:63:B:MET:HB2	1:37:B:PHE:HB3	9	0.87	0.13	0.87
(1,994)	1:109:B:LEU:HD11	1:47:B:ASN:HB2	9	0.86	0.39	0.93
(1,994)	1:8:B:LEU:HD21	1:22:A:TYR:HB2	9	0.86	0.39	0.93
(1,994)	1:109:B:LEU:HD21	1:47:B:ASN:HB2	9	0.86	0.39	0.93
(1,994)	1:109:B:LEU:HD21	1:47:B:ASN:HB3	9	0.86	0.39	0.93
(1,994)	1:109:B:LEU:HD13	1:47:B:ASN:HB3	9	0.86	0.39	0.93
(1,994)	1:109:B:LEU:HD22	1:47:B:ASN:HB3	9	0.86	0.39	0.93
(1,994)	1:8:B:LEU:HD22	1:22:A:TYR:HB2	9	0.86	0.39	0.93
(1,994)	1:109:B:LEU:HD22	1:47:B:ASN:HB2	9	0.86	0.39	0.93
(1,993)	1:109:A:LEU:HD11	1:47:A:ASN:HB2	9	0.86	0.4	0.92
(1,993)	1:8:A:LEU:HD21	1:22:B:TYR:HB2	9	0.86	0.4	0.92
(1,993)	1:109:A:LEU:HD21	1:47:A:ASN:HB2	9	0.86	0.4	0.92
(1,993)	1:109:A:LEU:HD21	1:47:A:ASN:HB3	9	0.86	0.4	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,993)	1:109:A:LEU:HD13	1:47:A:ASN:HB3	9	0.86	0.4	0.92
(1,993)	1:109:A:LEU:HD22	1:47:A:ASN:HB3	9	0.86	0.4	0.92
(1,993)	1:8:A:LEU:HD22	1:22:B:TYR:HB2	9	0.86	0.4	0.92
(1,993)	1:109:A:LEU:HD22	1:47:A:ASN:HB2	9	0.86	0.4	0.92
(1,1826)	1:21:B:GLN:H	1:17:B:ASN:HB3	9	0.82	0.17	0.86
(1,1826)	1:16:B:ILE:H	1:17:B:ASN:HB2	9	0.82	0.17	0.86
(1,1826)	1:94:B:MET:H	1:93:B:LYS:HE3	9	0.82	0.17	0.86
(1,1826)	1:94:B:MET:H	1:93:B:LYS:HE2	9	0.82	0.17	0.86
(1,1826)	1:94:B:MET:H	1:95:B:HIS:HB3	9	0.82	0.17	0.86
(1,1825)	1:21:A:GLN:H	1:17:A:ASN:HB3	9	0.82	0.17	0.86
(1,1825)	1:16:A:ILE:H	1:17:A:ASN:HB2	9	0.82	0.17	0.86
(1,1825)	1:94:A:MET:H	1:93:A:LYS:HE3	9	0.82	0.17	0.86
(1,1825)	1:94:A:MET:H	1:93:A:LYS:HE2	9	0.82	0.17	0.86
(1,1825)	1:94:A:MET:H	1:95:A:HIS:HB3	9	0.82	0.17	0.86
(1,458)	1:111:B:GLU:HA	1:50:B:LYS:HB3	9	0.82	0.4	0.7
(1,458)	1:111:B:GLU:HA	1:10:A:ARG:HG2	9	0.82	0.4	0.7
(1,458)	1:111:B:GLU:HA	1:50:B:LYS:HB2	9	0.82	0.4	0.7
(1,796)	1:111:B:GLU:HA	1:50:B:LYS:HB3	9	0.82	0.4	0.7
(1,796)	1:111:B:GLU:HA	1:10:A:ARG:HG2	9	0.82	0.4	0.7
(1,796)	1:111:B:GLU:HA	1:50:B:LYS:HB2	9	0.82	0.4	0.7
(1,457)	1:111:A:GLU:HA	1:50:A:LYS:HB3	9	0.82	0.4	0.69
(1,457)	1:111:A:GLU:HA	1:10:B:ARG:HG2	9	0.82	0.4	0.69
(1,457)	1:111:A:GLU:HA	1:50:A:LYS:HB2	9	0.82	0.4	0.69
(1,795)	1:111:A:GLU:HA	1:50:A:LYS:HB3	9	0.82	0.4	0.69
(1,795)	1:111:A:GLU:HA	1:10:B:ARG:HG2	9	0.82	0.4	0.69
(1,795)	1:111:A:GLU:HA	1:50:A:LYS:HB2	9	0.82	0.4	0.69
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD23	9	0.81	0.28	0.88
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD12	9	0.81	0.28	0.88
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD13	9	0.81	0.28	0.88
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD21	9	0.81	0.28	0.88
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD11	9	0.81	0.28	0.88
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD22	9	0.81	0.28	0.88
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD23	9	0.81	0.28	0.88
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD12	9	0.81	0.28	0.88
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD13	9	0.81	0.28	0.88
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD21	9	0.81	0.28	0.88
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD11	9	0.81	0.28	0.88
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD22	9	0.81	0.28	0.88
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD22	9	0.8	0.23	0.9
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD21	9	0.8	0.23	0.9
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD23	9	0.8	0.23	0.9
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD12	9	0.8	0.23	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD22	9	0.8	0.23	0.9
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD21	9	0.8	0.23	0.9
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD23	9	0.8	0.23	0.9
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD12	9	0.8	0.23	0.9
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD21	9	0.71	0.19	0.77
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD11	9	0.71	0.19	0.77
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD12	9	0.71	0.19	0.77
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD22	9	0.71	0.19	0.77
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD13	9	0.71	0.19	0.77
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD21	9	0.71	0.2	0.78
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD11	9	0.71	0.2	0.78
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD12	9	0.71	0.2	0.78
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD22	9	0.71	0.2	0.78
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD13	9	0.71	0.2	0.78
(3,220)	1:66:B:LEU:HD23	1:74:B:LEU:HA	9	0.71	0.4	0.73
(3,220)	1:66:B:LEU:HD11	1:74:B:LEU:HA	9	0.71	0.4	0.73
(3,220)	1:66:B:LEU:HD12	1:74:B:LEU:HA	9	0.71	0.4	0.73
(3,220)	1:66:B:LEU:HD13	1:74:B:LEU:HA	9	0.71	0.4	0.73
(3,220)	1:66:B:LEU:HD21	1:74:B:LEU:HA	9	0.71	0.4	0.73
(3,220)	1:66:B:LEU:HD22	1:74:B:LEU:HA	9	0.71	0.4	0.73
(3,219)	1:66:A:LEU:HD23	1:74:A:LEU:HA	9	0.71	0.4	0.72
(3,219)	1:66:A:LEU:HD11	1:74:A:LEU:HA	9	0.71	0.4	0.72
(3,219)	1:66:A:LEU:HD12	1:74:A:LEU:HA	9	0.71	0.4	0.72
(3,219)	1:66:A:LEU:HD13	1:74:A:LEU:HA	9	0.71	0.4	0.72
(3,219)	1:66:A:LEU:HD21	1:74:A:LEU:HA	9	0.71	0.4	0.72
(3,219)	1:66:A:LEU:HD22	1:74:A:LEU:HA	9	0.71	0.4	0.72
(1,37)	1:58:A:VAL:HG23	1:53:A:ASN:HA	9	0.69	0.25	0.72
(1,37)	1:58:A:VAL:HG12	1:61:A:HIS:HA	9	0.69	0.25	0.72
(1,37)	1:58:A:VAL:HG13	1:61:A:HIS:HA	9	0.69	0.25	0.72
(1,37)	1:58:A:VAL:HG13	1:53:A:ASN:HA	9	0.69	0.25	0.72
(1,37)	1:58:A:VAL:HG22	1:53:A:ASN:HA	9	0.69	0.25	0.72
(1,38)	1:58:B:VAL:HG23	1:53:B:ASN:HA	9	0.69	0.25	0.72
(1,38)	1:58:B:VAL:HG12	1:61:B:HIS:HA	9	0.69	0.25	0.72
(1,38)	1:58:B:VAL:HG13	1:61:B:HIS:HA	9	0.69	0.25	0.72
(1,38)	1:58:B:VAL:HG13	1:53:B:ASN:HA	9	0.69	0.25	0.72
(1,38)	1:58:B:VAL:HG22	1:53:B:ASN:HA	9	0.69	0.25	0.72
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	9	0.68	0.17	0.72
(1,556)	1:47:B:ASN:HA	1:53:B:ASN:H	9	0.68	0.17	0.72
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG2	9	0.68	0.18	0.69
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG3	9	0.68	0.18	0.69
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HB3	9	0.68	0.18	0.69
(1,555)	1:47:A:ASN:HA	1:5:B:MET:H	9	0.67	0.17	0.73

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,555)	1:47:A:ASN:HA	1:53:A:ASN:H	9	0.67	0.17	0.73
(1,348)	1:5:B:MET:HG3	1:4:B:LYS:HE3	9	0.67	0.36	0.67
(1,348)	1:5:B:MET:HG2	1:4:B:LYS:HE3	9	0.67	0.36	0.67
(1,348)	1:5:B:MET:HG3	1:4:B:LYS:HE2	9	0.67	0.36	0.67
(1,347)	1:5:A:MET:HG3	1:4:A:LYS:HE3	9	0.67	0.35	0.68
(1,347)	1:5:A:MET:HG2	1:4:A:LYS:HE3	9	0.67	0.35	0.68
(1,347)	1:5:A:MET:HG3	1:4:A:LYS:HE2	9	0.67	0.35	0.68
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD21	9	0.65	0.17	0.62
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD23	9	0.65	0.17	0.62
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD22	9	0.65	0.17	0.62
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD12	9	0.65	0.17	0.62
(1,598)	1:85:B:ARG:HG3	1:66:B:LEU:HD23	9	0.65	0.17	0.62
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD21	9	0.65	0.17	0.61
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD23	9	0.65	0.17	0.61
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD22	9	0.65	0.17	0.61
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD12	9	0.65	0.17	0.61
(1,597)	1:85:A:ARG:HG3	1:66:A:LEU:HD23	9	0.65	0.17	0.61
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	9	0.64	0.16	0.7
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG12	9	0.64	0.16	0.7
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	9	0.64	0.16	0.7
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG12	9	0.64	0.16	0.7
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	9	0.63	0.27	0.65
(1,1389)	1:5:A:MET:H	1:110:B:GLY:H	9	0.63	0.27	0.65
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	9	0.63	0.16	0.62
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	9	0.63	0.26	0.64
(1,1390)	1:5:B:MET:H	1:110:A:GLY:H	9	0.63	0.26	0.64
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	9	0.63	0.16	0.62
(1,613)	1:36:A:GLU:HA	1:25:A:LYS:HD3	9	0.62	0.2	0.74
(1,613)	1:51:A:LYS:HA	1:51:A:LYS:HD3	9	0.62	0.2	0.74
(1,613)	1:36:A:GLU:HA	1:25:A:LYS:HD2	9	0.62	0.2	0.74
(1,613)	1:50:A:LYS:HD2	1:50:A:LYS:HA	9	0.62	0.2	0.74
(1,613)	1:50:A:LYS:HD3	1:50:A:LYS:HA	9	0.62	0.2	0.74
(1,614)	1:36:B:GLU:HA	1:25:B:LYS:HD3	9	0.62	0.2	0.74
(1,614)	1:51:B:LYS:HA	1:51:B:LYS:HD3	9	0.62	0.2	0.74
(1,614)	1:36:B:GLU:HA	1:25:B:LYS:HD2	9	0.62	0.2	0.74
(1,614)	1:50:B:LYS:HD2	1:50:B:LYS:HA	9	0.62	0.2	0.74
(1,614)	1:50:B:LYS:HD3	1:50:B:LYS:HA	9	0.62	0.2	0.74
(1,809)	1:68:A:THR:H	1:74:A:LEU:HG	9	0.62	0.24	0.65
(1,809)	1:74:A:LEU:HG	1:38:A:LYS:H	9	0.62	0.24	0.65
(1,810)	1:68:B:THR:H	1:74:B:LEU:HG	9	0.62	0.24	0.65
(1,810)	1:74:B:LEU:HG	1:38:B:LYS:H	9	0.62	0.24	0.65
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	9	0.59	0.28	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,714)	1:21:B:GLN:HG2	1:40:B:LEU:HB2	9	0.59	0.28	0.57
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	9	0.59	0.28	0.57
(3,780)	1:21:B:GLN:HG2	1:40:B:LEU:HB2	9	0.59	0.28	0.57
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	9	0.59	0.28	0.57
(1,713)	1:21:A:GLN:HG2	1:40:A:LEU:HB2	9	0.59	0.28	0.57
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	9	0.59	0.28	0.57
(3,779)	1:21:A:GLN:HG2	1:40:A:LEU:HB2	9	0.59	0.28	0.57
(3,641)	1:8:A:LEU:HD21	1:15:B:ILE:HD12	9	0.57	0.22	0.64
(3,641)	1:8:A:LEU:HD13	1:15:B:ILE:HD12	9	0.57	0.22	0.64
(3,641)	1:8:A:LEU:HD11	1:15:B:ILE:HD11	9	0.57	0.22	0.64
(3,641)	1:8:A:LEU:HD23	1:15:B:ILE:HD12	9	0.57	0.22	0.64
(3,641)	1:8:A:LEU:HD23	1:15:B:ILE:HD11	9	0.57	0.22	0.64
(3,641)	1:8:A:LEU:HD12	1:15:B:ILE:HD11	9	0.57	0.22	0.64
(3,641)	1:8:A:LEU:HD13	1:15:B:ILE:HD11	9	0.57	0.22	0.64
(3,641)	1:8:A:LEU:HD22	1:15:B:ILE:HD12	9	0.57	0.22	0.64
(3,960)	1:75:B:SER:H	1:63:B:MET:HE2	9	0.57	0.21	0.54
(3,960)	1:75:B:SER:H	1:63:B:MET:HE1	9	0.57	0.21	0.54
(3,960)	1:75:B:SER:H	1:63:B:MET:HE3	9	0.57	0.21	0.54
(3,642)	1:8:B:LEU:HD21	1:15:A:ILE:HD12	9	0.57	0.22	0.64
(3,642)	1:8:B:LEU:HD13	1:15:A:ILE:HD12	9	0.57	0.22	0.64
(3,642)	1:8:B:LEU:HD11	1:15:A:ILE:HD11	9	0.57	0.22	0.64
(3,642)	1:8:B:LEU:HD23	1:15:A:ILE:HD12	9	0.57	0.22	0.64
(3,642)	1:8:B:LEU:HD23	1:15:A:ILE:HD11	9	0.57	0.22	0.64
(3,642)	1:8:B:LEU:HD12	1:15:A:ILE:HD11	9	0.57	0.22	0.64
(3,642)	1:8:B:LEU:HD13	1:15:A:ILE:HD11	9	0.57	0.22	0.64
(3,642)	1:8:B:LEU:HD22	1:15:A:ILE:HD12	9	0.57	0.22	0.64
(3,959)	1:75:A:SER:H	1:63:A:MET:HE2	9	0.57	0.21	0.54
(3,959)	1:75:A:SER:H	1:63:A:MET:HE1	9	0.57	0.21	0.54
(3,959)	1:75:A:SER:H	1:63:A:MET:HE3	9	0.57	0.21	0.54
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE3	9	0.56	0.17	0.59
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE2	9	0.56	0.17	0.59
(1,568)	1:42:B:ARG:HA	1:50:B:LYS:HE3	9	0.56	0.17	0.59
(1,568)	1:42:B:ARG:HA	1:54:B:LYS:HE3	9	0.56	0.17	0.59
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE3	9	0.56	0.17	0.59
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE2	9	0.56	0.17	0.59
(1,567)	1:42:A:ARG:HA	1:50:A:LYS:HE3	9	0.56	0.17	0.59
(1,567)	1:42:A:ARG:HA	1:54:A:LYS:HE3	9	0.56	0.17	0.59
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	9	0.53	0.15	0.54
(3,116)	1:75:B:SER:HB2	1:67:B:ASP:HA	9	0.53	0.15	0.54
(1,603)	1:18:A:THR:HG22	1:21:A:GLN:HG2	9	0.52	0.13	0.56
(1,603)	1:18:A:THR:HG23	1:21:A:GLN:HG2	9	0.52	0.13	0.56
(1,603)	1:18:A:THR:HG21	1:21:A:GLN:HG2	9	0.52	0.13	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	9	0.52	0.14	0.53
(3,115)	1:75:A:SER:HB2	1:67:A:ASP:HA	9	0.52	0.14	0.53
(1,604)	1:18:B:THR:HG22	1:21:B:GLN:HG2	9	0.52	0.13	0.56
(1,604)	1:18:B:THR:HG23	1:21:B:GLN:HG2	9	0.52	0.13	0.56
(1,604)	1:18:B:THR:HG21	1:21:B:GLN:HG2	9	0.52	0.13	0.56
(1,756)	1:111:B:GLU:HG2	1:108:B:GLY:HA3	9	0.49	0.34	0.41
(1,756)	1:111:B:GLU:HG3	1:108:B:GLY:HA2	9	0.49	0.34	0.41
(1,756)	1:111:B:GLU:HG2	1:108:B:GLY:HA2	9	0.49	0.34	0.41
(1,756)	1:96:B:GLU:HG3	1:97:B:GLY:HA3	9	0.49	0.34	0.41
(1,756)	1:111:B:GLU:HG3	1:108:B:GLY:HA3	9	0.49	0.34	0.41
(1,756)	1:96:B:GLU:HG2	1:97:B:GLY:HA3	9	0.49	0.34	0.41
(1,755)	1:111:A:GLU:HG2	1:108:A:GLY:HA3	9	0.49	0.34	0.41
(1,755)	1:111:A:GLU:HG3	1:108:A:GLY:HA2	9	0.49	0.34	0.41
(1,755)	1:111:A:GLU:HG2	1:108:A:GLY:HA2	9	0.49	0.34	0.41
(1,755)	1:96:A:GLU:HG3	1:97:A:GLY:HA3	9	0.49	0.34	0.41
(1,755)	1:111:A:GLU:HG3	1:108:A:GLY:HA3	9	0.49	0.34	0.41
(1,755)	1:96:A:GLU:HG2	1:97:A:GLY:HA3	9	0.49	0.34	0.41
(1,1227)	1:76:A:PHE:H	1:80:A:ILE:HB	9	0.47	0.12	0.47
(1,1227)	1:76:A:PHE:H	1:32:A:LEU:HB2	9	0.47	0.12	0.47
(1,27)	1:87:A:THR:HG21	1:85:A:ARG:HA	9	0.47	0.21	0.46
(1,27)	1:58:A:VAL:HG13	1:53:A:ASN:HA	9	0.47	0.21	0.46
(1,27)	1:87:A:THR:HG23	1:85:A:ARG:HA	9	0.47	0.21	0.46
(1,1228)	1:76:B:PHE:H	1:80:B:ILE:HB	9	0.47	0.12	0.47
(1,1228)	1:76:B:PHE:H	1:32:B:LEU:HB2	9	0.47	0.12	0.47
(1,28)	1:87:B:THR:HG21	1:85:B:ARG:HA	9	0.47	0.21	0.46
(1,28)	1:58:B:VAL:HG13	1:53:B:ASN:HA	9	0.47	0.21	0.46
(1,28)	1:87:B:THR:HG23	1:85:B:ARG:HA	9	0.47	0.21	0.46
(1,1308)	1:10:B:ARG:H	1:11:B:ASN:HB2	9	0.45	0.27	0.33
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD2	9	0.45	0.27	0.33
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD3	9	0.45	0.27	0.33
(1,1045)	1:85:A:ARG:HA	1:77:B:GLU:HA	9	0.45	0.14	0.45
(1,1045)	1:53:A:ASN:HA	1:38:A:LYS:HA	9	0.45	0.14	0.45
(1,1046)	1:85:B:ARG:HA	1:77:A:GLU:HA	9	0.45	0.13	0.45
(1,1046)	1:53:B:ASN:HA	1:38:B:LYS:HA	9	0.45	0.13	0.45
(1,1307)	1:10:A:ARG:H	1:11:A:ASN:HB2	9	0.45	0.28	0.32
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD2	9	0.45	0.28	0.32
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD3	9	0.45	0.28	0.32
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG2	9	0.44	0.06	0.43
(1,1122)	1:84:B:ALA:HA	1:81:B:MET:HG2	9	0.44	0.06	0.43
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG3	9	0.44	0.06	0.43
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG2	9	0.44	0.06	0.43
(1,1121)	1:84:A:ALA:HA	1:81:A:MET:HG2	9	0.44	0.06	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG3	9	0.44	0.06	0.43
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD21	9	0.42	0.15	0.39
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD23	9	0.42	0.15	0.39
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD22	9	0.42	0.15	0.39
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD21	9	0.42	0.15	0.39
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD23	9	0.42	0.15	0.39
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD22	9	0.42	0.15	0.39
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD11	9	0.42	0.15	0.41
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD12	9	0.42	0.15	0.41
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD13	9	0.42	0.15	0.41
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD11	9	0.41	0.14	0.41
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD12	9	0.41	0.14	0.41
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD13	9	0.41	0.14	0.41
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	9	0.4	0.25	0.27
(3,366)	1:85:B:ARG:HG2	1:77:A:GLU:HA	9	0.4	0.25	0.27
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	9	0.4	0.25	0.25
(3,365)	1:85:A:ARG:HG2	1:77:B:GLU:HA	9	0.4	0.25	0.25
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE3	9	0.39	0.14	0.38
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE2	9	0.39	0.14	0.38
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE3	9	0.39	0.14	0.38
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE2	9	0.39	0.14	0.38
(1,1317)	1:13:A:GLU:H	1:12:A:ILE:HG13	9	0.37	0.08	0.38
(1,1317)	1:11:A:ASN:H	1:12:A:ILE:HG13	9	0.37	0.08	0.38
(1,1318)	1:13:B:GLU:H	1:12:B:ILE:HG13	9	0.37	0.08	0.38
(1,1318)	1:11:B:ASN:H	1:12:B:ILE:HG13	9	0.37	0.08	0.38
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	9	0.37	0.2	0.31
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	9	0.36	0.14	0.41
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	9	0.36	0.14	0.41
(1,367)	1:34:A:GLN:HG2	1:38:A:LYS:HA	9	0.34	0.11	0.35
(1,367)	1:34:A:GLN:HG3	1:38:A:LYS:HA	9	0.34	0.11	0.35
(1,368)	1:34:B:GLN:HG2	1:38:B:LYS:HA	9	0.34	0.11	0.35
(1,368)	1:34:B:GLN:HG3	1:38:B:LYS:HA	9	0.34	0.11	0.35
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	9	0.33	0.12	0.34
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG13	9	0.33	0.12	0.34
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	9	0.33	0.12	0.33
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG13	9	0.33	0.12	0.33
(1,1327)	1:12:A:ILE:H	1:45:B:LEU:HD23	9	0.33	0.14	0.3
(1,1327)	1:12:A:ILE:H	1:45:B:LEU:HD22	9	0.33	0.14	0.3
(1,1327)	1:12:A:ILE:H	1:86:B:LEU:HD12	9	0.33	0.14	0.3
(1,1327)	1:12:A:ILE:H	1:86:B:LEU:HD22	9	0.33	0.14	0.3
(1,1327)	1:12:A:ILE:H	1:86:B:LEU:HD21	9	0.33	0.14	0.3
(1,1328)	1:12:B:ILE:H	1:45:A:LEU:HD23	9	0.33	0.14	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1328)	1:12:B:ILE:H	1:45:A:LEU:HD22	9	0.33	0.14	0.3
(1,1328)	1:12:B:ILE:H	1:86:A:LEU:HD12	9	0.33	0.14	0.3
(1,1328)	1:12:B:ILE:H	1:45:A:LEU:HD21	9	0.33	0.14	0.3
(1,1328)	1:12:B:ILE:H	1:86:A:LEU:HD22	9	0.33	0.14	0.3
(1,1328)	1:12:B:ILE:H	1:86:A:LEU:HD21	9	0.33	0.14	0.3
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD21	9	0.32	0.09	0.31
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD23	9	0.32	0.09	0.31
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD22	9	0.32	0.09	0.31
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD21	9	0.32	0.1	0.31
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD23	9	0.32	0.1	0.31
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD22	9	0.32	0.1	0.31
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD11	9	0.32	0.09	0.31
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD13	9	0.32	0.09	0.31
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD12	9	0.32	0.09	0.31
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD11	9	0.32	0.09	0.31
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD13	9	0.32	0.09	0.31
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD12	9	0.32	0.09	0.31
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG21	9	0.32	0.1	0.29
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG22	9	0.32	0.1	0.29
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG23	9	0.32	0.1	0.29
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG21	9	0.31	0.1	0.29
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG22	9	0.31	0.1	0.29
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG23	9	0.31	0.1	0.29
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	9	0.31	0.08	0.3
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	9	0.31	0.08	0.3
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB1	9	0.29	0.2	0.23
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB2	9	0.29	0.2	0.23
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB3	9	0.29	0.2	0.23
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB1	9	0.29	0.2	0.23
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB2	9	0.29	0.2	0.23
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB3	9	0.29	0.2	0.23
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	9	0.28	0.07	0.29
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	9	0.28	0.07	0.28
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE1	9	0.28	0.05	0.3
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE3	9	0.28	0.05	0.3
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE2	9	0.28	0.05	0.3
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE1	9	0.27	0.05	0.3
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE3	9	0.27	0.05	0.3
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE2	9	0.27	0.05	0.3
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE3	9	0.27	0.08	0.3
(1,1838)	1:103:B:HIS:H	1:104:B:HIS:HB2	9	0.27	0.08	0.3
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE2	9	0.27	0.08	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG13	9	0.27	0.04	0.28
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG12	9	0.27	0.04	0.28
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG13	9	0.27	0.04	0.28
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG12	9	0.27	0.04	0.28
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE3	9	0.27	0.08	0.3
(1,1837)	1:103:A:HIS:H	1:104:A:HIS:HB2	9	0.27	0.08	0.3
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE2	9	0.27	0.08	0.3
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD11	9	0.27	0.12	0.2
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD12	9	0.27	0.12	0.2
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD13	9	0.27	0.12	0.2
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD22	9	0.27	0.12	0.2
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD23	9	0.27	0.12	0.2
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD11	9	0.27	0.12	0.2
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD12	9	0.27	0.12	0.2
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD13	9	0.27	0.12	0.2
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD22	9	0.27	0.12	0.2
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD23	9	0.27	0.12	0.2
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	9	0.27	0.09	0.26
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	9	0.27	0.09	0.27
(3,33)	1:87:A:THR:HG21	1:88:A:TRP:HA	9	0.23	0.07	0.21
(3,33)	1:87:A:THR:HG23	1:88:A:TRP:HA	9	0.23	0.07	0.21
(3,34)	1:87:B:THR:HG21	1:88:B:TRP:HA	9	0.23	0.07	0.21
(3,34)	1:87:B:THR:HG23	1:88:B:TRP:HA	9	0.23	0.07	0.21
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	9	0.22	0.08	0.23
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	9	0.22	0.08	0.23
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB2	9	0.21	0.06	0.21
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB3	9	0.21	0.06	0.21
(3,339)	1:57:A:LYS:HG2	1:56:A:GLU:HB3	9	0.21	0.06	0.21
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB2	9	0.21	0.06	0.21
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB3	9	0.21	0.06	0.21
(3,340)	1:57:B:LYS:HG2	1:56:B:GLU:HB3	9	0.21	0.06	0.21
(1,338)	1:41:B:VAL:HG12	1:42:B:ARG:HA	9	0.2	0.02	0.2
(1,338)	1:41:B:VAL:HG13	1:42:B:ARG:HA	9	0.2	0.02	0.2
(1,338)	1:41:B:VAL:HG11	1:42:B:ARG:HA	9	0.2	0.02	0.2
(1,337)	1:41:A:VAL:HG12	1:42:A:ARG:HA	9	0.2	0.02	0.2
(1,337)	1:41:A:VAL:HG13	1:42:A:ARG:HA	9	0.2	0.02	0.2
(1,337)	1:41:A:VAL:HG11	1:42:A:ARG:HA	9	0.2	0.02	0.2
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	9	0.18	0.07	0.2
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG2	9	0.18	0.02	0.18
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG3	9	0.18	0.02	0.18
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG2	9	0.18	0.02	0.18
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG3	9	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	8	1.95	0.13	1.94
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD12	8	1.95	0.13	1.94
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD11	8	1.95	0.13	1.94
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	8	1.95	0.13	1.94
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD12	8	1.95	0.13	1.94
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD11	8	1.95	0.13	1.94
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	8	1.95	0.13	1.94
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD12	8	1.95	0.13	1.94
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD11	8	1.95	0.13	1.94
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	8	1.95	0.13	1.94
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD12	8	1.95	0.13	1.94
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD11	8	1.95	0.13	1.94
(1,1006)	1:109:B:LEU:HD12	1:86:B:LEU:H	8	1.34	0.42	1.34
(1,1006)	1:8:B:LEU:HD21	1:22:A:TYR:H	8	1.34	0.42	1.34
(1,1006)	1:109:B:LEU:HD22	1:86:B:LEU:H	8	1.34	0.42	1.34
(1,1006)	1:8:B:LEU:HD13	1:22:A:TYR:H	8	1.34	0.42	1.34
(1,1006)	1:109:B:LEU:HD13	1:86:B:LEU:H	8	1.34	0.42	1.34
(1,1006)	1:8:B:LEU:HD12	1:22:A:TYR:H	8	1.34	0.42	1.34
(1,1005)	1:109:A:LEU:HD12	1:86:A:LEU:H	8	1.34	0.42	1.34
(1,1005)	1:8:A:LEU:HD21	1:22:B:TYR:H	8	1.34	0.42	1.34
(1,1005)	1:109:A:LEU:HD22	1:86:A:LEU:H	8	1.34	0.42	1.34
(1,1005)	1:8:A:LEU:HD13	1:22:B:TYR:H	8	1.34	0.42	1.34
(1,1005)	1:109:A:LEU:HD13	1:86:A:LEU:H	8	1.34	0.42	1.34
(1,1005)	1:8:A:LEU:HD12	1:22:B:TYR:H	8	1.34	0.42	1.34
(1,769)	1:59:A:ILE:HD11	1:42:A:ARG:HD2	8	1.09	0.37	1.12
(1,769)	1:59:A:ILE:HD12	1:42:A:ARG:HD2	8	1.09	0.37	1.12
(1,769)	1:37:A:PHE:HB3	1:59:A:ILE:HD11	8	1.09	0.37	1.12
(1,769)	1:37:A:PHE:HB3	1:59:A:ILE:HD13	8	1.09	0.37	1.12
(1,769)	1:37:A:PHE:HB3	1:59:A:ILE:HD12	8	1.09	0.37	1.12
(1,770)	1:59:B:ILE:HD11	1:42:B:ARG:HD2	8	1.09	0.38	1.12
(1,770)	1:59:B:ILE:HD12	1:42:B:ARG:HD2	8	1.09	0.38	1.12
(1,770)	1:37:B:PHE:HB3	1:59:B:ILE:HD11	8	1.09	0.38	1.12
(1,770)	1:37:B:PHE:HB3	1:59:B:ILE:HD13	8	1.09	0.38	1.12
(1,770)	1:37:B:PHE:HB3	1:59:B:ILE:HD12	8	1.09	0.38	1.12
(1,991)	1:8:A:LEU:HD22	1:20:B:HIS:HB2	8	0.92	0.54	1.0
(1,991)	1:8:A:LEU:HD11	1:20:B:HIS:HB3	8	0.92	0.54	1.0
(1,991)	1:8:A:LEU:HD23	1:48:B:PHE:HB2	8	0.92	0.54	1.0
(1,991)	1:8:A:LEU:HD23	1:48:B:PHE:HB3	8	0.92	0.54	1.0
(1,991)	1:8:A:LEU:HD21	1:48:B:PHE:HB2	8	0.92	0.54	1.0
(1,991)	1:8:A:LEU:HD23	1:80:B:ILE:HA	8	0.92	0.54	1.0
(1,992)	1:8:B:LEU:HD22	1:20:A:HIS:HB2	8	0.92	0.54	1.0
(1,992)	1:8:B:LEU:HD11	1:20:A:HIS:HB3	8	0.92	0.54	1.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,992)	1:8:B:LEU:HD23	1:48:A:PHE:HB2	8	0.92	0.54	1.0
(1,992)	1:8:B:LEU:HD23	1:48:A:PHE:HB3	8	0.92	0.54	1.0
(1,992)	1:8:B:LEU:HD21	1:48:A:PHE:HB2	8	0.92	0.54	1.0
(1,992)	1:8:B:LEU:HD23	1:80:A:ILE:HA	8	0.92	0.54	1.0
(1,1098)	1:59:B:ILE:HG22	1:42:B:ARG:HD2	8	0.91	0.55	1.08
(1,1098)	1:59:B:ILE:HG23	1:42:B:ARG:HD2	8	0.91	0.55	1.08
(1,1098)	1:59:B:ILE:HG22	1:42:B:ARG:HD3	8	0.91	0.55	1.08
(1,1097)	1:59:A:ILE:HG22	1:42:A:ARG:HD2	8	0.91	0.56	1.08
(1,1097)	1:59:A:ILE:HG23	1:42:A:ARG:HD2	8	0.91	0.56	1.08
(1,1097)	1:59:A:ILE:HG22	1:42:A:ARG:HD3	8	0.91	0.56	1.08
(1,1573)	1:48:A:PHE:H	1:41:A:VAL:HA	8	0.9	0.24	0.96
(1,1573)	1:75:A:SER:H	1:68:A:THR:HA	8	0.9	0.24	0.96
(1,1574)	1:48:B:PHE:H	1:41:B:VAL:HA	8	0.89	0.24	0.95
(1,1574)	1:75:B:SER:H	1:68:B:THR:HA	8	0.89	0.24	0.95
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD13	8	0.89	0.5	0.85
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD12	8	0.89	0.5	0.85
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD21	8	0.89	0.5	0.85
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD13	8	0.88	0.5	0.84
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD12	8	0.88	0.5	0.84
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD21	8	0.88	0.5	0.84
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	8	0.86	0.23	0.78
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	8	0.86	0.23	0.78
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	8	0.86	0.23	0.78
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	8	0.86	0.23	0.78
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	8	0.85	0.15	0.89
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	8	0.85	0.15	0.88
(1,862)	1:25:B:LYS:HD3	1:33:B:ASN:HB3	8	0.82	0.44	0.84
(1,862)	1:25:B:LYS:HD2	1:33:B:ASN:HB3	8	0.82	0.44	0.84
(1,862)	1:25:B:LYS:HD2	1:33:B:ASN:HB2	8	0.82	0.44	0.84
(1,862)	1:25:B:LYS:HD3	1:33:B:ASN:HB2	8	0.82	0.44	0.84
(1,862)	1:25:B:LYS:HD2	1:43:B:LYS:HE3	8	0.82	0.44	0.84
(1,861)	1:25:A:LYS:HD3	1:33:A:ASN:HB3	8	0.81	0.44	0.84
(1,861)	1:25:A:LYS:HD2	1:33:A:ASN:HB3	8	0.81	0.44	0.84
(1,861)	1:25:A:LYS:HD2	1:33:A:ASN:HB2	8	0.81	0.44	0.84
(1,861)	1:25:A:LYS:HD3	1:33:A:ASN:HB2	8	0.81	0.44	0.84
(1,861)	1:25:A:LYS:HD2	1:43:A:LYS:HE3	8	0.81	0.44	0.84
(1,1797)	1:5:A:MET:H	1:4:A:LYS:HE3	8	0.74	0.16	0.81
(1,1797)	1:16:A:ILE:H	1:17:A:ASN:HB2	8	0.74	0.16	0.81
(1,1797)	1:109:A:LEU:H	1:93:A:LYS:HE2	8	0.74	0.16	0.81
(1,1797)	1:94:A:MET:H	1:93:A:LYS:HE2	8	0.74	0.16	0.81
(1,1798)	1:5:B:MET:H	1:4:B:LYS:HE3	8	0.74	0.16	0.81
(1,1798)	1:16:B:ILE:H	1:17:B:ASN:HB2	8	0.74	0.16	0.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1798)	1:109:B:LEU:H	1:93:B:LYS:HE2	8	0.74	0.16	0.81
(1,1798)	1:94:B:MET:H	1:93:B:LYS:HE2	8	0.74	0.16	0.81
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD22	8	0.72	0.48	0.58
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD23	8	0.72	0.48	0.58
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD13	8	0.72	0.48	0.58
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD12	8	0.72	0.48	0.58
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD11	8	0.72	0.48	0.58
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD21	8	0.72	0.48	0.58
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD22	8	0.72	0.48	0.58
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD23	8	0.72	0.48	0.58
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD13	8	0.72	0.48	0.58
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD12	8	0.72	0.48	0.58
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD11	8	0.72	0.48	0.58
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD21	8	0.72	0.48	0.58
(1,390)	1:16:B:ILE:HD12	1:10:B:ARG:HA	8	0.7	0.45	0.58
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD23	8	0.7	0.45	0.58
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD13	8	0.7	0.45	0.58
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD12	8	0.7	0.45	0.58
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD11	8	0.7	0.45	0.58
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD22	8	0.7	0.45	0.58
(1,390)	1:16:B:ILE:HD13	1:10:B:ARG:HA	8	0.7	0.45	0.58
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD21	8	0.7	0.45	0.58
(1,389)	1:16:A:ILE:HD12	1:10:A:ARG:HA	8	0.7	0.46	0.58
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD23	8	0.7	0.46	0.58
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD13	8	0.7	0.46	0.58
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD12	8	0.7	0.46	0.58
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD11	8	0.7	0.46	0.58
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD22	8	0.7	0.46	0.58
(1,389)	1:16:A:ILE:HD13	1:10:A:ARG:HA	8	0.7	0.46	0.58
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD21	8	0.7	0.46	0.58
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	8	0.67	0.04	0.67
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	8	0.67	0.04	0.67
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD13	8	0.63	0.13	0.64
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD12	8	0.63	0.13	0.64
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD11	8	0.63	0.13	0.64
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD13	8	0.62	0.13	0.64
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD12	8	0.62	0.13	0.64
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD11	8	0.62	0.13	0.64
(1,1543)	1:43:A:LYS:H	1:42:A:ARG:HG2	8	0.61	0.23	0.55
(1,1543)	1:43:A:LYS:H	1:42:A:ARG:HG3	8	0.61	0.23	0.55
(1,1543)	1:43:A:LYS:H	1:43:A:LYS:HD2	8	0.61	0.23	0.55
(1,1544)	1:43:B:LYS:H	1:42:B:ARG:HG2	8	0.61	0.24	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1544)	1:43:B:LYS:H	1:42:B:ARG:HG3	8	0.61	0.24	0.55
(1,1544)	1:43:B:LYS:H	1:43:B:LYS:HD2	8	0.61	0.24	0.55
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD13	8	0.6	0.07	0.6
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD12	8	0.6	0.07	0.6
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG2	8	0.59	0.12	0.62
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG3	8	0.59	0.12	0.62
(1,1183)	1:96:A:GLU:HB2	1:93:A:LYS:HD2	8	0.59	0.27	0.46
(1,1183)	1:56:A:GLU:HB2	1:57:A:LYS:HD3	8	0.59	0.27	0.46
(1,1183)	1:96:A:GLU:HB2	1:93:A:LYS:HD3	8	0.59	0.27	0.46
(1,1183)	1:56:A:GLU:HB3	1:57:A:LYS:HD3	8	0.59	0.27	0.46
(1,1183)	1:81:A:MET:HB3	1:85:A:ARG:HG3	8	0.59	0.27	0.46
(1,1183)	1:56:A:GLU:HB3	1:57:A:LYS:HD2	8	0.59	0.27	0.46
(1,1184)	1:96:B:GLU:HB2	1:93:B:LYS:HD2	8	0.59	0.28	0.46
(1,1184)	1:56:B:GLU:HB2	1:57:B:LYS:HD3	8	0.59	0.28	0.46
(1,1184)	1:96:B:GLU:HB2	1:93:B:LYS:HD3	8	0.59	0.28	0.46
(1,1184)	1:56:B:GLU:HB3	1:57:B:LYS:HD3	8	0.59	0.28	0.46
(1,1184)	1:81:B:MET:HB3	1:85:B:ARG:HG3	8	0.59	0.28	0.46
(1,1184)	1:56:B:GLU:HB3	1:57:B:LYS:HD2	8	0.59	0.28	0.46
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD13	8	0.59	0.07	0.59
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD12	8	0.59	0.07	0.59
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG2	8	0.59	0.12	0.62
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG3	8	0.59	0.12	0.62
(1,479)	1:63:A:MET:HB2	1:59:A:ILE:HD12	8	0.55	0.37	0.4
(1,479)	1:63:A:MET:HB2	1:62:A:ILE:HD12	8	0.55	0.37	0.4
(1,479)	1:36:A:GLU:HB2	1:31:A:THR:HG23	8	0.55	0.37	0.4
(1,479)	1:36:A:GLU:HB2	1:31:A:THR:HG22	8	0.55	0.37	0.4
(1,479)	1:63:A:MET:HB2	1:62:A:ILE:HD13	8	0.55	0.37	0.4
(1,479)	1:63:A:MET:HB2	1:82:A:LEU:HD23	8	0.55	0.37	0.4
(1,480)	1:63:B:MET:HB2	1:59:B:ILE:HD12	8	0.55	0.36	0.4
(1,480)	1:63:B:MET:HB2	1:62:B:ILE:HD12	8	0.55	0.36	0.4
(1,480)	1:36:B:GLU:HB2	1:31:B:THR:HG23	8	0.55	0.36	0.4
(1,480)	1:36:B:GLU:HB2	1:31:B:THR:HG22	8	0.55	0.36	0.4
(1,480)	1:63:B:MET:HB2	1:62:B:ILE:HD13	8	0.55	0.36	0.4
(1,480)	1:63:B:MET:HB2	1:82:B:LEU:HD23	8	0.55	0.36	0.4
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD22	8	0.55	0.24	0.55
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD23	8	0.55	0.24	0.55
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD21	8	0.55	0.24	0.55
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD22	8	0.55	0.24	0.54
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD23	8	0.55	0.24	0.54
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD21	8	0.55	0.24	0.54
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE3	8	0.49	0.21	0.45
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE2	8	0.49	0.21	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,234)	1:46:B:GLN:HA	1:44:B:ASP:HB2	8	0.49	0.21	0.45
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE3	8	0.49	0.21	0.44
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE2	8	0.49	0.21	0.44
(1,233)	1:46:A:GLN:HA	1:44:A:ASP:HB2	8	0.49	0.21	0.44
(3,491)	1:59:A:ILE:HD13	1:52:A:GLU:HG2	8	0.48	0.2	0.5
(3,491)	1:59:A:ILE:HD12	1:52:A:GLU:HG3	8	0.48	0.2	0.5
(3,491)	1:59:A:ILE:HD11	1:52:A:GLU:HG2	8	0.48	0.2	0.5
(3,491)	1:59:A:ILE:HD12	1:52:A:GLU:HG2	8	0.48	0.2	0.5
(3,492)	1:59:B:ILE:HD13	1:52:B:GLU:HG2	8	0.48	0.2	0.5
(3,492)	1:59:B:ILE:HD12	1:52:B:GLU:HG3	8	0.48	0.2	0.5
(3,492)	1:59:B:ILE:HD11	1:52:B:GLU:HG2	8	0.48	0.2	0.5
(3,492)	1:59:B:ILE:HD12	1:52:B:GLU:HG2	8	0.48	0.2	0.5
(3,600)	1:53:B:ASN:HB3	1:46:B:GLN:HG3	8	0.45	0.26	0.43
(3,600)	1:53:B:ASN:HB2	1:46:B:GLN:HG3	8	0.45	0.26	0.43
(3,599)	1:53:A:ASN:HB3	1:46:A:GLN:HG3	8	0.45	0.26	0.43
(3,599)	1:53:A:ASN:HB2	1:46:A:GLN:HG3	8	0.45	0.26	0.43
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG21	8	0.45	0.09	0.46
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG23	8	0.45	0.09	0.46
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG22	8	0.45	0.09	0.46
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG21	8	0.45	0.09	0.46
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG23	8	0.45	0.09	0.46
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG22	8	0.45	0.09	0.46
(1,671)	1:49:A:LEU:HG	1:53:A:ASN:H	8	0.44	0.08	0.46
(1,671)	1:8:A:LEU:HG	1:15:B:ILE:H	8	0.44	0.08	0.46
(1,672)	1:49:B:LEU:HG	1:53:B:ASN:H	8	0.44	0.08	0.46
(1,672)	1:8:B:LEU:HG	1:15:A:ILE:H	8	0.44	0.08	0.46
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG22	8	0.43	0.13	0.46
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG21	8	0.43	0.13	0.46
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG23	8	0.43	0.13	0.46
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG22	8	0.43	0.13	0.46
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG21	8	0.43	0.13	0.46
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG23	8	0.43	0.13	0.46
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG21	8	0.4	0.07	0.4
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG22	8	0.4	0.07	0.4
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG23	8	0.4	0.07	0.4
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG21	8	0.4	0.07	0.4
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG22	8	0.4	0.07	0.4
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG23	8	0.4	0.07	0.4
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	8	0.39	0.2	0.36
(1,395)	1:33:A:ASN:HB2	1:34:A:GLN:HG2	8	0.38	0.23	0.32
(1,395)	1:33:A:ASN:HB3	1:34:A:GLN:HG2	8	0.38	0.23	0.32
(1,395)	1:33:A:ASN:HB2	1:71:A:ASP:HB3	8	0.38	0.23	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,396)	1:33:B:ASN:HB2	1:34:B:GLN:HG2	8	0.38	0.22	0.32
(1,396)	1:33:B:ASN:HB3	1:34:B:GLN:HG2	8	0.38	0.22	0.32
(1,396)	1:33:B:ASN:HB2	1:71:B:ASP:HB3	8	0.38	0.22	0.32
(1,549)	1:32:A:LEU:HA	1:32:A:LEU:HG	8	0.36	0.1	0.4
(1,549)	1:32:A:LEU:HA	1:36:A:GLU:HB2	8	0.36	0.1	0.4
(1,550)	1:32:B:LEU:HA	1:32:B:LEU:HG	8	0.36	0.1	0.4
(1,550)	1:32:B:LEU:HA	1:36:B:GLU:HB2	8	0.36	0.1	0.4
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG22	8	0.33	0.09	0.36
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG23	8	0.33	0.09	0.36
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG22	8	0.33	0.09	0.36
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG23	8	0.33	0.09	0.36
(3,131)	1:78:A:GLU:HB2	1:31:A:THR:HA	8	0.31	0.1	0.31
(3,131)	1:78:A:GLU:HB3	1:31:A:THR:HA	8	0.31	0.1	0.31
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	8	0.31	0.09	0.32
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	8	0.31	0.09	0.33
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	8	0.31	0.09	0.32
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	8	0.31	0.09	0.33
(3,132)	1:78:B:GLU:HB2	1:31:B:THR:HA	8	0.3	0.1	0.3
(3,132)	1:78:B:GLU:HB3	1:31:B:THR:HA	8	0.3	0.1	0.3
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	8	0.3	0.17	0.24
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG21	8	0.3	0.13	0.29
(1,1368)	1:93:B:LYS:H	1:109:B:LEU:HD22	8	0.3	0.13	0.29
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG22	8	0.3	0.13	0.29
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG23	8	0.3	0.13	0.29
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG21	8	0.3	0.12	0.29
(1,1367)	1:93:A:LYS:H	1:109:A:LEU:HD22	8	0.3	0.12	0.29
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG22	8	0.3	0.12	0.29
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG23	8	0.3	0.12	0.29
(3,378)	1:25:B:LYS:HD3	1:32:B:LEU:HA	8	0.24	0.06	0.26
(3,378)	1:25:B:LYS:HD2	1:32:B:LEU:HA	8	0.24	0.06	0.26
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD3	8	0.23	0.05	0.22
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD2	8	0.23	0.05	0.22
(3,377)	1:25:A:LYS:HD3	1:32:A:LEU:HA	8	0.23	0.07	0.25
(3,377)	1:25:A:LYS:HD2	1:32:A:LEU:HA	8	0.23	0.07	0.25
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD3	8	0.23	0.05	0.22
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD2	8	0.23	0.05	0.22
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	8	0.22	0.07	0.2
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	8	0.22	0.07	0.2
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG3	8	0.21	0.05	0.2
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG2	8	0.21	0.05	0.2
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG3	8	0.21	0.06	0.2
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG2	8	0.21	0.06	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	8	0.19	0.06	0.2
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	8	0.19	0.06	0.18
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	8	0.19	0.06	0.2
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	8	0.19	0.06	0.2
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	8	0.19	0.06	0.18
(1,806)	1:74:B:LEU:HG	1:73:B:GLN:HG2	8	0.19	0.04	0.18
(1,806)	1:74:B:LEU:HG	1:34:B:GLN:HB2	8	0.19	0.04	0.18
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG3	8	0.19	0.03	0.19
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG2	8	0.19	0.03	0.19
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG3	8	0.18	0.03	0.2
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG2	8	0.18	0.03	0.2
(1,805)	1:74:A:LEU:HG	1:73:A:GLN:HG2	8	0.18	0.04	0.18
(1,805)	1:74:A:LEU:HG	1:34:A:GLN:HB2	8	0.18	0.04	0.18
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG23	8	0.15	0.03	0.15
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG21	8	0.15	0.03	0.15
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG22	8	0.15	0.03	0.15
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG23	8	0.15	0.03	0.15
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG21	8	0.15	0.03	0.15
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG22	8	0.15	0.03	0.15
(1,623)	1:42:A:ARG:HA	1:44:A:ASP:HB2	7	1.14	0.33	1.14
(1,623)	1:21:A:GLN:HA	1:25:A:LYS:HE3	7	1.14	0.33	1.14
(1,623)	1:19:A:PHE:HB2	1:21:A:GLN:HA	7	1.14	0.33	1.14
(1,624)	1:42:B:ARG:HA	1:44:B:ASP:HB2	7	1.14	0.33	1.14
(1,624)	1:21:B:GLN:HA	1:25:B:LYS:HE3	7	1.14	0.33	1.14
(1,624)	1:19:B:PHE:HB2	1:21:B:GLN:HA	7	1.14	0.33	1.14
(1,758)	1:111:B:GLU:HG2	1:107:B:PRO:HD2	7	0.94	0.31	0.79
(1,758)	1:96:B:GLU:HG2	1:107:B:PRO:HD2	7	0.94	0.31	0.79
(1,758)	1:111:B:GLU:HG2	1:107:B:PRO:HD3	7	0.94	0.31	0.79
(1,757)	1:111:A:GLU:HG2	1:107:A:PRO:HD2	7	0.94	0.31	0.79
(1,757)	1:96:A:GLU:HG2	1:107:A:PRO:HD2	7	0.94	0.31	0.79
(1,757)	1:111:A:GLU:HG2	1:107:A:PRO:HD3	7	0.94	0.31	0.79
(1,690)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	7	0.75	0.35	0.68
(1,690)	1:107:B:PRO:HG3	1:112:B:GLY:HA3	7	0.75	0.35	0.68
(1,689)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	7	0.75	0.35	0.68
(1,689)	1:107:A:PRO:HG3	1:112:A:GLY:HA3	7	0.75	0.35	0.68
(1,534)	1:86:B:LEU:HD22	1:89:B:ALA:HA	7	0.74	0.11	0.71
(1,534)	1:86:B:LEU:HD12	1:89:B:ALA:HA	7	0.74	0.11	0.71
(1,534)	1:86:B:LEU:HD23	1:89:B:ALA:HA	7	0.74	0.11	0.71
(1,534)	1:86:B:LEU:HD21	1:89:B:ALA:HA	7	0.74	0.11	0.71
(1,533)	1:86:A:LEU:HD22	1:89:A:ALA:HA	7	0.74	0.11	0.7
(1,533)	1:86:A:LEU:HD22	1:13:B:GLU:HA	7	0.74	0.11	0.7
(1,533)	1:86:A:LEU:HD23	1:89:A:ALA:HA	7	0.74	0.11	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,533)	1:86:A:LEU:HD21	1:89:A:ALA:HA	7	0.74	0.11	0.7
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB3	7	0.67	0.28	0.53
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB2	7	0.67	0.28	0.53
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB3	7	0.67	0.29	0.51
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB2	7	0.67	0.29	0.51
(1,261)	1:49:A:LEU:HG	1:89:A:ALA:HB3	7	0.65	0.27	0.53
(1,261)	1:8:A:LEU:HG	1:40:B:LEU:HG	7	0.65	0.27	0.53
(1,261)	1:49:A:LEU:HG	1:89:A:ALA:HB1	7	0.65	0.27	0.53
(1,262)	1:49:B:LEU:HG	1:89:B:ALA:HB3	7	0.64	0.28	0.52
(1,262)	1:8:B:LEU:HG	1:40:A:LEU:HG	7	0.64	0.28	0.52
(1,262)	1:49:B:LEU:HG	1:89:B:ALA:HB1	7	0.64	0.28	0.52
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD21	7	0.64	0.06	0.67
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD22	7	0.64	0.06	0.67
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD23	7	0.64	0.06	0.67
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD21	7	0.64	0.07	0.68
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD22	7	0.64	0.07	0.68
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD23	7	0.64	0.07	0.68
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD21	7	0.63	0.06	0.66
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD22	7	0.63	0.06	0.66
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD23	7	0.63	0.06	0.66
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD21	7	0.63	0.07	0.67
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD22	7	0.63	0.07	0.67
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD23	7	0.63	0.07	0.67
(3,15)	1:101:A:PRO:HG2	1:102:A:GLY:HA2	7	0.62	0.22	0.64
(3,15)	1:101:A:PRO:HG3	1:102:A:GLY:HA2	7	0.62	0.22	0.64
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG21	7	0.61	0.13	0.66
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG23	7	0.61	0.13	0.66
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG22	7	0.61	0.13	0.66
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG21	7	0.61	0.12	0.66
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG23	7	0.61	0.12	0.66
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG22	7	0.61	0.12	0.66
(3,16)	1:101:B:PRO:HG2	1:102:B:GLY:HA2	7	0.61	0.22	0.64
(3,16)	1:101:B:PRO:HG3	1:102:B:GLY:HA2	7	0.61	0.22	0.64
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG2	7	0.59	0.08	0.64
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG3	7	0.59	0.08	0.64
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG2	7	0.59	0.08	0.64
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG3	7	0.59	0.08	0.64
(1,267)	1:66:A:LEU:HG	1:85:A:ARG:HB2	7	0.57	0.19	0.57
(1,267)	1:8:A:LEU:HG	1:15:B:ILE:HB	7	0.57	0.19	0.57
(1,268)	1:66:B:LEU:HG	1:85:B:ARG:HB2	7	0.56	0.19	0.56
(1,268)	1:8:B:LEU:HG	1:15:A:ILE:HB	7	0.56	0.19	0.56
(1,49)	1:64:A:GLU:HG3	1:71:A:ASP:HA	7	0.52	0.22	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,49)	1:13:A:GLU:HG2	1:17:A:ASN:HA	7	0.52	0.22	0.47
(1,49)	1:64:A:GLU:HG2	1:71:A:ASP:HA	7	0.52	0.22	0.47
(1,50)	1:64:B:GLU:HG3	1:71:B:ASP:HA	7	0.52	0.23	0.46
(1,50)	1:13:B:GLU:HG2	1:17:B:ASN:HA	7	0.52	0.23	0.46
(1,50)	1:64:B:GLU:HG2	1:71:B:ASP:HA	7	0.52	0.23	0.46
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD11	7	0.46	0.19	0.45
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD12	7	0.46	0.19	0.45
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD13	7	0.46	0.19	0.45
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD11	7	0.45	0.19	0.45
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD12	7	0.45	0.19	0.45
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD13	7	0.45	0.19	0.45
(1,1858)	1:110:B:GLY:H	1:111:B:GLU:HA	7	0.45	0.17	0.52
(1,1858)	1:108:B:GLY:H	1:111:B:GLU:HA	7	0.45	0.17	0.52
(1,1857)	1:110:A:GLY:H	1:111:A:GLU:HA	7	0.45	0.16	0.52
(1,1857)	1:108:A:GLY:H	1:111:A:GLU:HA	7	0.45	0.16	0.52
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB2	7	0.43	0.14	0.39
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB3	7	0.43	0.14	0.39
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB2	7	0.43	0.14	0.39
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB3	7	0.43	0.14	0.39
(1,139)	1:16:A:ILE:HD12	1:13:A:GLU:HG2	7	0.39	0.21	0.36
(1,139)	1:16:A:ILE:HD13	1:13:A:GLU:HG2	7	0.39	0.21	0.36
(1,139)	1:16:A:ILE:HD13	1:13:A:GLU:HB3	7	0.39	0.21	0.36
(1,139)	1:16:A:ILE:HD11	1:13:A:GLU:HG2	7	0.39	0.21	0.36
(1,140)	1:16:B:ILE:HD12	1:13:B:GLU:HG2	7	0.39	0.22	0.37
(1,140)	1:16:B:ILE:HD13	1:13:B:GLU:HG2	7	0.39	0.22	0.37
(1,140)	1:16:B:ILE:HD13	1:13:B:GLU:HB3	7	0.39	0.22	0.37
(1,140)	1:16:B:ILE:HD11	1:13:B:GLU:HG2	7	0.39	0.22	0.37
(3,485)	1:96:A:GLU:HG3	1:97:A:GLY:H	7	0.36	0.08	0.37
(3,485)	1:96:A:GLU:HG2	1:97:A:GLY:H	7	0.36	0.08	0.37
(3,486)	1:96:B:GLU:HG3	1:97:B:GLY:H	7	0.35	0.07	0.36
(3,486)	1:96:B:GLU:HG2	1:97:B:GLY:H	7	0.35	0.07	0.36
(1,1401)	1:20:A:HIS:H	1:87:B:THR:HG22	7	0.35	0.17	0.32
(1,1401)	1:20:A:HIS:H	1:87:B:THR:HG23	7	0.35	0.17	0.32
(1,1401)	1:20:A:HIS:H	1:24:A:VAL:HG12	7	0.35	0.17	0.32
(1,1401)	1:20:A:HIS:H	1:8:B:LEU:HD21	7	0.35	0.17	0.32
(1,1401)	1:20:A:HIS:H	1:24:A:VAL:HG11	7	0.35	0.17	0.32
(3,659)	1:72:A:LYS:HB3	1:64:A:GLU:HA	7	0.35	0.17	0.47
(1,1402)	1:20:B:HIS:H	1:87:A:THR:HG22	7	0.34	0.17	0.31
(1,1402)	1:20:B:HIS:H	1:87:A:THR:HG23	7	0.34	0.17	0.31
(1,1402)	1:20:B:HIS:H	1:24:B:VAL:HG12	7	0.34	0.17	0.31
(1,1402)	1:20:B:HIS:H	1:8:A:LEU:HD21	7	0.34	0.17	0.31
(1,1402)	1:20:B:HIS:H	1:24:B:VAL:HG11	7	0.34	0.17	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,11)	1:98:A:ASP:HA	1:96:A:GLU:HA	7	0.33	0.17	0.24
(1,1760)	1:24:B:VAL:H	1:25:B:LYS:HG3	7	0.31	0.1	0.33
(1,1759)	1:24:A:VAL:H	1:25:A:LYS:HG3	7	0.31	0.1	0.33
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD11	7	0.28	0.14	0.2
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD13	7	0.28	0.14	0.2
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD12	7	0.28	0.14	0.2
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD11	7	0.28	0.14	0.2
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD13	7	0.28	0.14	0.2
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD12	7	0.28	0.14	0.2
(1,1048)	1:53:B:ASN:HA	1:59:B:ILE:HA	7	0.27	0.1	0.23
(1,1047)	1:53:A:ASN:HA	1:59:A:ILE:HA	7	0.27	0.1	0.23
(1,1369)	1:17:A:ASN:H	1:15:A:ILE:HG13	7	0.27	0.14	0.22
(1,1370)	1:17:B:ASN:H	1:15:B:ILE:HG13	7	0.27	0.14	0.21
(3,691)	1:32:A:LEU:HA	1:36:A:GLU:HB2	7	0.24	0.1	0.24
(3,692)	1:32:B:LEU:HA	1:36:B:GLU:HB2	7	0.24	0.1	0.24
(1,896)	1:81:B:MET:HB2	1:80:A:ILE:HG12	7	0.22	0.05	0.21
(1,896)	1:81:B:MET:HB2	1:80:B:ILE:HG13	7	0.22	0.05	0.21
(1,896)	1:81:B:MET:HB3	1:80:A:ILE:HG12	7	0.22	0.05	0.21
(1,1178)	1:81:B:MET:HB2	1:80:A:ILE:HG12	7	0.22	0.05	0.21
(1,1178)	1:81:B:MET:HB2	1:80:B:ILE:HG13	7	0.22	0.05	0.21
(1,1178)	1:81:B:MET:HB3	1:80:A:ILE:HG12	7	0.22	0.05	0.21
(1,1180)	1:81:B:MET:HB2	1:80:A:ILE:HG12	7	0.22	0.05	0.21
(1,1180)	1:81:B:MET:HB2	1:80:B:ILE:HG13	7	0.22	0.05	0.21
(1,1180)	1:81:B:MET:HB3	1:80:A:ILE:HG12	7	0.22	0.05	0.21
(1,895)	1:81:A:MET:HB2	1:80:B:ILE:HG12	7	0.22	0.05	0.19
(1,895)	1:81:A:MET:HB2	1:80:A:ILE:HG13	7	0.22	0.05	0.19
(1,895)	1:81:A:MET:HB3	1:80:B:ILE:HG12	7	0.22	0.05	0.19
(1,1177)	1:81:A:MET:HB2	1:80:B:ILE:HG12	7	0.22	0.05	0.19
(1,1177)	1:81:A:MET:HB2	1:80:A:ILE:HG13	7	0.22	0.05	0.19
(1,1177)	1:81:A:MET:HB3	1:80:B:ILE:HG12	7	0.22	0.05	0.19
(1,1179)	1:81:A:MET:HB2	1:80:B:ILE:HG12	7	0.22	0.05	0.19
(1,1179)	1:81:A:MET:HB2	1:80:A:ILE:HG13	7	0.22	0.05	0.19
(1,1179)	1:81:A:MET:HB3	1:80:B:ILE:HG12	7	0.22	0.05	0.19
(2,64)	1:82:A:LEU:H	1:78:A:GLU:O	7	0.2	0.03	0.2
(3,320)	1:51:B:LYS:HE2	1:51:B:LYS:H	7	0.2	0.04	0.18
(3,320)	1:51:B:LYS:HE3	1:51:B:LYS:H	7	0.2	0.04	0.18
(3,319)	1:51:A:LYS:HE2	1:51:A:LYS:H	7	0.2	0.05	0.17
(3,319)	1:51:A:LYS:HE3	1:51:A:LYS:H	7	0.2	0.05	0.17
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG23	7	0.19	0.06	0.18
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG22	7	0.19	0.06	0.18
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG21	7	0.19	0.06	0.18
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG23	7	0.19	0.06	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG22	7	0.19	0.06	0.18
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG21	7	0.19	0.06	0.18
(4,61)	1:25:A:LYS:HA	1:21:A:GLN:HA	7	0.17	0.04	0.19
(4,62)	1:25:B:LYS:HA	1:21:B:GLN:HA	7	0.17	0.03	0.18
(1,961)	1:21:A:GLN:HB3	1:22:A:TYR:HB2	7	0.17	0.07	0.15
(1,961)	1:21:A:GLN:HB2	1:22:A:TYR:HB2	7	0.17	0.07	0.15
(2,42)	1:53:A:ASN:H	1:50:A:LYS:O	7	0.14	0.03	0.13
(3,793)	1:107:A:PRO:HG3	1:93:A:LYS:HG2	6	1.99	2.79	0.88
(3,793)	1:107:A:PRO:HG2	1:93:A:LYS:HG3	6	1.99	2.79	0.88
(3,793)	1:107:A:PRO:HG2	1:93:A:LYS:HG2	6	1.99	2.79	0.88
(3,794)	1:107:B:PRO:HG3	1:93:B:LYS:HG2	6	1.99	2.79	0.88
(3,794)	1:107:B:PRO:HG2	1:93:B:LYS:HG3	6	1.99	2.79	0.88
(3,794)	1:107:B:PRO:HG2	1:93:B:LYS:HG2	6	1.99	2.79	0.88
(1,42)	1:78:B:GLU:HG3	1:76:B:PHE:HA	6	1.19	0.47	1.36
(1,42)	1:78:B:GLU:HG2	1:76:B:PHE:HA	6	1.19	0.47	1.36
(1,41)	1:78:A:GLU:HG3	1:76:A:PHE:HA	6	1.19	0.48	1.36
(1,41)	1:78:A:GLU:HG2	1:76:A:PHE:HA	6	1.19	0.48	1.36
(1,1497)	1:38:A:LYS:H	1:59:A:ILE:HD12	6	0.85	0.1	0.86
(1,1497)	1:38:A:LYS:H	1:59:A:ILE:HD11	6	0.85	0.1	0.86
(1,1497)	1:38:A:LYS:H	1:59:A:ILE:HD13	6	0.85	0.1	0.86
(1,1497)	1:44:A:ASP:H	1:49:A:LEU:HD11	6	0.85	0.1	0.86
(1,1497)	1:44:A:ASP:H	1:49:A:LEU:HD12	6	0.85	0.1	0.86
(1,1498)	1:38:B:LYS:H	1:59:B:ILE:HD12	6	0.85	0.1	0.86
(1,1498)	1:38:B:LYS:H	1:59:B:ILE:HD11	6	0.85	0.1	0.86
(1,1498)	1:38:B:LYS:H	1:59:B:ILE:HD13	6	0.85	0.1	0.86
(1,1498)	1:44:B:ASP:H	1:49:B:LEU:HD11	6	0.85	0.1	0.86
(1,1498)	1:44:B:ASP:H	1:49:B:LEU:HD12	6	0.85	0.1	0.86
(1,697)	1:107:A:PRO:HG3	1:93:A:LYS:HG2	6	0.8	0.29	0.88
(1,697)	1:74:A:LEU:HG	1:40:A:LEU:HB3	6	0.8	0.29	0.88
(1,697)	1:107:A:PRO:HG2	1:93:A:LYS:HG3	6	0.8	0.29	0.88
(1,697)	1:107:A:PRO:HG2	1:93:A:LYS:HG2	6	0.8	0.29	0.88
(1,698)	1:107:B:PRO:HG3	1:93:B:LYS:HG2	6	0.8	0.29	0.88
(1,698)	1:74:B:LEU:HG	1:40:B:LEU:HB3	6	0.8	0.29	0.88
(1,698)	1:107:B:PRO:HG2	1:93:B:LYS:HG3	6	0.8	0.29	0.88
(1,698)	1:107:B:PRO:HG2	1:93:B:LYS:HG2	6	0.8	0.29	0.88
(1,693)	1:74:A:LEU:HG	1:78:A:GLU:HG3	6	0.75	0.42	0.9
(1,693)	1:74:A:LEU:HG	1:78:A:GLU:HG2	6	0.75	0.42	0.9
(1,693)	1:74:A:LEU:HG	1:64:A:GLU:HG3	6	0.75	0.42	0.9
(1,694)	1:74:B:LEU:HG	1:78:B:GLU:HG3	6	0.75	0.42	0.9
(1,694)	1:74:B:LEU:HG	1:78:B:GLU:HG2	6	0.75	0.42	0.9
(1,694)	1:74:B:LEU:HG	1:64:B:GLU:HG3	6	0.75	0.42	0.9
(1,1196)	1:98:B:ASP:HA	1:104:B:HIS:HB3	6	0.73	0.35	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1196)	1:98:B:ASP:HA	1:104:B:HIS:HB2	6	0.73	0.35	0.67
(1,1196)	1:98:B:ASP:HA	1:95:B:HIS:HB3	6	0.73	0.35	0.67
(1,1195)	1:98:A:ASP:HA	1:104:A:HIS:HB3	6	0.73	0.35	0.67
(1,1195)	1:98:A:ASP:HA	1:104:A:HIS:HB2	6	0.73	0.35	0.67
(1,1195)	1:98:A:ASP:HA	1:95:A:HIS:HB3	6	0.73	0.35	0.67
(1,280)	1:19:B:PHE:HB3	1:32:B:LEU:HB2	6	0.73	0.24	0.78
(1,280)	1:19:B:PHE:HB2	1:32:B:LEU:HB2	6	0.73	0.24	0.78
(1,279)	1:19:A:PHE:HB3	1:32:A:LEU:HB2	6	0.73	0.24	0.78
(1,279)	1:19:A:PHE:HB2	1:32:A:LEU:HB2	6	0.73	0.24	0.78
(1,19)	1:93:A:LYS:HA	1:109:A:LEU:HG	6	0.66	0.21	0.65
(1,20)	1:93:B:LYS:HA	1:109:B:LEU:HG	6	0.66	0.22	0.65
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD23	6	0.63	0.26	0.6
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD12	6	0.63	0.26	0.6
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD13	6	0.63	0.26	0.6
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD11	6	0.63	0.26	0.6
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD23	6	0.63	0.26	0.6
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD12	6	0.63	0.26	0.6
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD13	6	0.63	0.26	0.6
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD11	6	0.63	0.26	0.6
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD21	6	0.6	0.21	0.67
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD13	6	0.6	0.21	0.67
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD12	6	0.6	0.21	0.67
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD21	6	0.59	0.21	0.67
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD13	6	0.59	0.21	0.67
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD12	6	0.59	0.21	0.67
(1,1135)	1:57:A:LYS:HE3	1:60:A:GLU:HG3	6	0.58	0.36	0.55
(1,1135)	1:5:A:MET:HG2	1:4:A:LYS:HE3	6	0.58	0.36	0.55
(1,1135)	1:5:A:MET:HG3	1:4:A:LYS:HE3	6	0.58	0.36	0.55
(1,1135)	1:5:A:MET:HG3	1:4:A:LYS:HE2	6	0.58	0.36	0.55
(1,1136)	1:57:B:LYS:HE3	1:60:B:GLU:HG3	6	0.58	0.36	0.54
(1,1136)	1:5:B:MET:HG2	1:4:B:LYS:HE3	6	0.58	0.36	0.54
(1,1136)	1:5:B:MET:HG3	1:4:B:LYS:HE3	6	0.58	0.36	0.54
(1,1136)	1:5:B:MET:HG3	1:4:B:LYS:HE2	6	0.58	0.36	0.54
(1,1270)	1:48:B:PHE:H	1:4:A:LYS:HE3	6	0.56	0.35	0.55
(1,1270)	1:48:B:PHE:H	1:51:B:LYS:HE2	6	0.56	0.35	0.55
(1,1421)	1:22:A:TYR:H	1:36:A:GLU:HG2	6	0.56	0.29	0.52
(1,1421)	1:22:A:TYR:H	1:36:A:GLU:HG3	6	0.56	0.29	0.52
(1,1269)	1:48:A:PHE:H	1:4:B:LYS:HE3	6	0.55	0.35	0.55
(1,1269)	1:48:A:PHE:H	1:51:A:LYS:HE2	6	0.55	0.35	0.55
(1,1422)	1:22:B:TYR:H	1:36:B:GLU:HG2	6	0.55	0.29	0.52
(1,1422)	1:22:B:TYR:H	1:36:B:GLU:HG3	6	0.55	0.29	0.52
(3,1466)	1:110:B:GLY:H	1:108:B:GLY:HA3	6	0.55	0.3	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1466)	1:110:B:GLY:H	1:108:B:GLY:HA2	6	0.55	0.3	0.57
(3,1465)	1:110:A:GLY:H	1:108:A:GLY:HA3	6	0.54	0.29	0.56
(3,1465)	1:110:A:GLY:H	1:108:A:GLY:HA2	6	0.54	0.29	0.56
(1,189)	1:77:A:GLU:HA	1:87:B:THR:HG22	6	0.51	0.26	0.42
(1,189)	1:77:A:GLU:HA	1:87:B:THR:HG21	6	0.51	0.26	0.42
(1,190)	1:77:B:GLU:HA	1:87:A:THR:HG22	6	0.51	0.26	0.43
(1,190)	1:77:B:GLU:HA	1:87:A:THR:HG21	6	0.51	0.26	0.43
(1,1153)	1:32:A:LEU:HG	1:36:A:GLU:HG2	6	0.5	0.16	0.52
(1,1153)	1:32:A:LEU:HG	1:36:A:GLU:HG3	6	0.5	0.16	0.52
(1,1154)	1:32:B:LEU:HG	1:36:B:GLU:HG2	6	0.49	0.16	0.51
(1,1154)	1:32:B:LEU:HG	1:36:B:GLU:HG3	6	0.49	0.16	0.51
(1,96)	1:7:B:GLN:HG3	1:18:A:THR:HB	6	0.47	0.21	0.57
(1,96)	1:7:B:GLN:HG2	1:18:A:THR:HB	6	0.47	0.21	0.57
(3,246)	1:7:B:GLN:HG3	1:18:A:THR:HB	6	0.47	0.21	0.57
(3,246)	1:7:B:GLN:HG2	1:18:A:THR:HB	6	0.47	0.21	0.57
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG22	6	0.46	0.32	0.38
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG23	6	0.46	0.32	0.38
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG21	6	0.46	0.32	0.38
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG22	6	0.46	0.32	0.38
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG23	6	0.46	0.32	0.38
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG21	6	0.46	0.32	0.38
(3,525)	1:76:A:PHE:HB3	1:16:A:ILE:HA	6	0.46	0.24	0.37
(3,525)	1:76:A:PHE:HB2	1:16:A:ILE:HA	6	0.46	0.24	0.37
(3,526)	1:76:B:PHE:HB3	1:16:B:ILE:HA	6	0.46	0.24	0.38
(3,526)	1:76:B:PHE:HB2	1:16:B:ILE:HA	6	0.46	0.24	0.38
(1,660)	1:8:B:LEU:HG	1:83:A:MET:HG3	6	0.43	0.16	0.49
(1,660)	1:7:B:GLN:HG2	1:8:B:LEU:HG	6	0.43	0.16	0.49
(1,660)	1:7:B:GLN:HG3	1:8:B:LEU:HG	6	0.43	0.16	0.49
(1,659)	1:8:A:LEU:HG	1:83:B:MET:HG3	6	0.43	0.16	0.49
(1,659)	1:7:A:GLN:HG2	1:8:A:LEU:HG	6	0.43	0.16	0.49
(1,659)	1:7:A:GLN:HG3	1:8:A:LEU:HG	6	0.43	0.16	0.49
(3,163)	1:13:A:GLU:HB3	1:14:A:THR:HG21	6	0.43	0.32	0.32
(3,163)	1:13:A:GLU:HB2	1:14:A:THR:HG21	6	0.43	0.32	0.32
(3,163)	1:13:A:GLU:HB3	1:14:A:THR:HG22	6	0.43	0.32	0.32
(3,164)	1:13:B:GLU:HB3	1:14:B:THR:HG21	6	0.43	0.32	0.32
(3,164)	1:13:B:GLU:HB2	1:14:B:THR:HG21	6	0.43	0.32	0.32
(3,164)	1:13:B:GLU:HB3	1:14:B:THR:HG22	6	0.43	0.32	0.32
(1,923)	1:87:A:THR:HA	1:86:A:LEU:HG	6	0.42	0.05	0.42
(1,924)	1:87:B:THR:HA	1:86:B:LEU:HG	6	0.42	0.05	0.42
(1,72)	1:48:B:PHE:HB2	1:9:A:GLU:HB3	6	0.41	0.07	0.39
(1,72)	1:33:B:ASN:HB3	1:73:B:GLN:HG2	6	0.41	0.07	0.39
(1,71)	1:48:A:PHE:HB2	1:9:B:GLU:HB3	6	0.41	0.07	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,71)	1:33:A:ASN:HB3	1:73:A:GLN:HG2	6	0.41	0.07	0.38
(1,1149)	1:32:A:LEU:HG	1:40:A:LEU:HB2	6	0.4	0.13	0.44
(1,1150)	1:32:B:LEU:HG	1:40:B:LEU:HB2	6	0.4	0.13	0.44
(3,660)	1:72:B:LYS:HB3	1:64:B:GLU:HA	6	0.39	0.15	0.48
(1,94)	1:34:B:GLN:HG3	1:63:B:MET:H	6	0.38	0.21	0.38
(1,378)	1:34:B:GLN:HG3	1:63:B:MET:H	6	0.38	0.21	0.38
(1,93)	1:34:A:GLN:HG3	1:63:A:MET:H	6	0.37	0.22	0.38
(1,377)	1:34:A:GLN:HG3	1:63:A:MET:H	6	0.37	0.22	0.38
(3,437)	1:37:A:PHE:HB2	1:63:A:MET:HE3	6	0.33	0.05	0.34
(3,437)	1:37:A:PHE:HB3	1:63:A:MET:HE3	6	0.33	0.05	0.34
(3,437)	1:37:A:PHE:HB2	1:63:A:MET:HE2	6	0.33	0.05	0.34
(3,437)	1:37:A:PHE:HB2	1:63:A:MET:HE1	6	0.33	0.05	0.34
(3,438)	1:37:B:PHE:HB2	1:63:B:MET:HE3	6	0.33	0.05	0.33
(3,438)	1:37:B:PHE:HB3	1:63:B:MET:HE3	6	0.33	0.05	0.33
(3,438)	1:37:B:PHE:HB2	1:63:B:MET:HE2	6	0.33	0.05	0.33
(3,438)	1:37:B:PHE:HB2	1:63:B:MET:HE1	6	0.33	0.05	0.33
(1,1791)	1:16:A:ILE:H	1:12:A:ILE:HG21	6	0.3	0.14	0.29
(1,1791)	1:93:A:LYS:H	1:109:A:LEU:HD22	6	0.3	0.14	0.29
(1,1791)	1:16:A:ILE:H	1:12:A:ILE:HG22	6	0.3	0.14	0.29
(1,1791)	1:16:A:ILE:H	1:12:A:ILE:HG23	6	0.3	0.14	0.29
(1,1792)	1:16:B:ILE:H	1:12:B:ILE:HG21	6	0.3	0.14	0.29
(1,1792)	1:93:B:LYS:H	1:109:B:LEU:HD22	6	0.3	0.14	0.29
(1,1792)	1:16:B:ILE:H	1:12:B:ILE:HG22	6	0.3	0.14	0.29
(1,1792)	1:16:B:ILE:H	1:12:B:ILE:HG23	6	0.3	0.14	0.29
(3,602)	1:46:B:GLN:HG3	1:4:A:LYS:HE3	6	0.27	0.12	0.22
(3,602)	1:46:B:GLN:HG3	1:4:A:LYS:HE2	6	0.27	0.12	0.22
(1,1199)	1:60:A:GLU:HB2	1:59:A:ILE:HG21	6	0.26	0.06	0.29
(1,1199)	1:60:A:GLU:HB2	1:59:A:ILE:HG22	6	0.26	0.06	0.29
(1,1200)	1:60:B:GLU:HB2	1:59:B:ILE:HG21	6	0.26	0.06	0.29
(1,1200)	1:60:B:GLU:HB2	1:59:B:ILE:HG22	6	0.26	0.06	0.29
(3,601)	1:46:A:GLN:HG3	1:4:B:LYS:HE3	6	0.26	0.11	0.22
(3,601)	1:46:A:GLN:HG3	1:4:B:LYS:HE2	6	0.26	0.11	0.22
(3,6)	1:73:B:GLN:HG3	1:72:B:LYS:HG2	6	0.24	0.11	0.2
(3,6)	1:73:B:GLN:HG3	1:72:B:LYS:HG3	6	0.24	0.11	0.2
(3,5)	1:73:A:GLN:HG3	1:72:A:LYS:HG2	6	0.24	0.11	0.2
(3,5)	1:73:A:GLN:HG3	1:72:A:LYS:HG3	6	0.24	0.11	0.2
(3,1381)	1:71:A:ASP:H	1:72:A:LYS:HE3	6	0.24	0.11	0.22
(3,1381)	1:71:A:ASP:H	1:72:A:LYS:HE2	6	0.24	0.11	0.22
(3,1382)	1:71:B:ASP:H	1:72:B:LYS:HE3	6	0.24	0.11	0.22
(3,1382)	1:71:B:ASP:H	1:72:B:LYS:HE2	6	0.24	0.11	0.22
(3,13)	1:111:A:GLU:HA	1:111:A:GLU:HG3	6	0.24	0.07	0.24
(3,13)	1:111:A:GLU:HA	1:111:A:GLU:HG2	6	0.24	0.07	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,14)	1:111:B:GLU:HA	1:111:B:GLU:HG3	6	0.24	0.07	0.24
(3,14)	1:111:B:GLU:HA	1:111:B:GLU:HG2	6	0.24	0.07	0.24
(3,872)	1:6:B:SER:H	1:5:B:MET:HG2	6	0.23	0.05	0.24
(3,872)	1:6:B:SER:H	1:5:B:MET:HG3	6	0.23	0.05	0.24
(3,871)	1:6:A:SER:H	1:5:A:MET:HG2	6	0.23	0.05	0.24
(3,871)	1:6:A:SER:H	1:5:A:MET:HG3	6	0.23	0.05	0.24
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG22	6	0.22	0.1	0.16
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG23	6	0.22	0.1	0.16
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG21	6	0.22	0.1	0.16
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG22	6	0.22	0.11	0.16
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG23	6	0.22	0.11	0.16
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG21	6	0.22	0.11	0.16
(1,165)	1:41:A:VAL:HB	1:37:A:PHE:HB3	6	0.2	0.05	0.18
(1,166)	1:41:B:VAL:HB	1:37:B:PHE:HB3	6	0.2	0.05	0.18
(1,1431)	1:23:A:SER:H	1:21:A:GLN:H	6	0.19	0.04	0.18
(1,1432)	1:23:B:SER:H	1:21:B:GLN:H	6	0.19	0.04	0.18
(1,962)	1:21:B:GLN:HB3	1:22:B:TYR:HB2	6	0.18	0.07	0.16
(1,962)	1:21:B:GLN:HB2	1:22:B:TYR:HB2	6	0.18	0.07	0.16
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD22	6	0.16	0.05	0.14
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD23	6	0.16	0.05	0.14
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD21	6	0.16	0.05	0.14
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD22	6	0.16	0.05	0.15
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD23	6	0.16	0.05	0.15
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD21	6	0.16	0.05	0.15
(2,26)	1:22:A:TYR:H	1:18:A:THR:O	6	0.14	0.02	0.14
(1,55)	1:13:A:GLU:HG2	1:109:B:LEU:HD11	5	1.26	0.91	1.25
(1,55)	1:13:A:GLU:HG2	1:86:B:LEU:HD13	5	1.26	0.91	1.25
(1,55)	1:13:A:GLU:HG3	1:109:B:LEU:HD21	5	1.26	0.91	1.25
(1,56)	1:13:B:GLU:HG2	1:109:A:LEU:HD11	5	1.26	0.92	1.24
(1,56)	1:13:B:GLU:HG2	1:86:A:LEU:HD13	5	1.26	0.92	1.24
(1,56)	1:13:B:GLU:HG3	1:109:A:LEU:HD21	5	1.26	0.92	1.24
(1,907)	1:86:A:LEU:HB2	1:9:B:GLU:HG2	5	1.25	0.77	1.31
(1,907)	1:86:A:LEU:HB3	1:13:B:GLU:HG2	5	1.25	0.77	1.31
(1,907)	1:86:A:LEU:HB3	1:9:B:GLU:HG3	5	1.25	0.77	1.31
(1,907)	1:86:A:LEU:HB2	1:9:B:GLU:HG3	5	1.25	0.77	1.31
(1,908)	1:86:B:LEU:HB2	1:9:A:GLU:HG2	5	1.25	0.77	1.3
(1,908)	1:86:B:LEU:HB3	1:13:A:GLU:HG2	5	1.25	0.77	1.3
(1,908)	1:86:B:LEU:HB3	1:9:A:GLU:HG3	5	1.25	0.77	1.3
(1,908)	1:86:B:LEU:HB2	1:9:A:GLU:HG3	5	1.25	0.77	1.3
(3,494)	1:59:B:ILE:HD12	1:38:B:LYS:HE2	5	1.07	0.46	1.13
(3,494)	1:59:B:ILE:HD11	1:38:B:LYS:HE2	5	1.07	0.46	1.13
(3,494)	1:59:B:ILE:HD13	1:38:B:LYS:HE2	5	1.07	0.46	1.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,494)	1:59:B:ILE:HD13	1:38:B:LYS:HE3	5	1.07	0.46	1.13
(3,493)	1:59:A:ILE:HD12	1:38:A:LYS:HE2	5	1.07	0.47	1.13
(3,493)	1:59:A:ILE:HD11	1:38:A:LYS:HE2	5	1.07	0.47	1.13
(3,493)	1:59:A:ILE:HD13	1:38:A:LYS:HE2	5	1.07	0.47	1.13
(3,493)	1:59:A:ILE:HD13	1:38:A:LYS:HE3	5	1.07	0.47	1.13
(1,400)	1:63:B:MET:HB3	1:72:B:LYS:HE2	5	0.96	0.7	0.79
(1,399)	1:63:A:MET:HB3	1:72:A:LYS:HE2	5	0.96	0.71	0.79
(1,1547)	1:43:A:LYS:H	1:8:B:LEU:HD13	5	0.88	0.16	0.95
(1,1547)	1:43:A:LYS:H	1:40:A:LEU:HG	5	0.88	0.16	0.95
(1,1548)	1:43:B:LYS:H	1:8:A:LEU:HD13	5	0.87	0.17	0.95
(1,1548)	1:43:B:LYS:H	1:40:B:LEU:HG	5	0.87	0.17	0.95
(1,1521)	1:41:A:VAL:H	1:42:A:ARG:HG3	5	0.82	0.11	0.8
(1,1521)	1:41:A:VAL:H	1:49:A:LEU:HB2	5	0.82	0.11	0.8
(1,1521)	1:41:A:VAL:H	1:43:A:LYS:HD2	5	0.82	0.11	0.8
(1,1522)	1:41:B:VAL:H	1:42:B:ARG:HG3	5	0.82	0.11	0.8
(1,1522)	1:41:B:VAL:H	1:49:B:LEU:HB2	5	0.82	0.11	0.8
(1,1522)	1:41:B:VAL:H	1:43:B:LYS:HD2	5	0.82	0.11	0.8
(3,515)	1:21:A:GLN:HG3	1:25:A:LYS:HE3	5	0.81	0.12	0.74
(3,515)	1:21:A:GLN:HG3	1:25:A:LYS:HE2	5	0.81	0.12	0.74
(3,516)	1:21:B:GLN:HG3	1:25:B:LYS:HE3	5	0.81	0.12	0.74
(3,516)	1:21:B:GLN:HG3	1:25:B:LYS:HE2	5	0.81	0.12	0.74
(3,719)	1:31:A:THR:HG22	1:74:A:LEU:HB2	5	0.79	0.11	0.76
(3,719)	1:31:A:THR:HG23	1:74:A:LEU:HB2	5	0.79	0.11	0.76
(3,719)	1:31:A:THR:HG21	1:74:A:LEU:HB2	5	0.79	0.11	0.76
(3,720)	1:31:B:THR:HG22	1:74:B:LEU:HB2	5	0.79	0.11	0.76
(3,720)	1:31:B:THR:HG23	1:74:B:LEU:HB2	5	0.79	0.11	0.76
(3,720)	1:31:B:THR:HG21	1:74:B:LEU:HB2	5	0.79	0.11	0.76
(3,1507)	1:113:A:THR:H	1:107:A:PRO:HD2	5	0.73	0.21	0.71
(3,1507)	1:113:A:THR:H	1:107:A:PRO:HD3	5	0.73	0.21	0.71
(3,1508)	1:113:B:THR:H	1:107:B:PRO:HD2	5	0.73	0.21	0.7
(3,1508)	1:113:B:THR:H	1:107:B:PRO:HD3	5	0.73	0.21	0.7
(1,117)	1:66:A:LEU:HG	1:62:A:ILE:HD11	5	0.67	0.46	0.48
(1,117)	1:66:A:LEU:HG	1:62:A:ILE:HD12	5	0.67	0.46	0.48
(1,118)	1:66:B:LEU:HG	1:62:B:ILE:HD11	5	0.67	0.46	0.48
(1,118)	1:66:B:LEU:HG	1:62:B:ILE:HD12	5	0.67	0.46	0.48
(1,223)	1:62:A:ILE:HG22	1:66:A:LEU:HG	5	0.65	0.34	0.7
(1,223)	1:62:A:ILE:HG23	1:66:A:LEU:HG	5	0.65	0.34	0.7
(1,223)	1:62:A:ILE:HG21	1:66:A:LEU:HG	5	0.65	0.34	0.7
(1,223)	1:12:A:ILE:HG21	1:83:B:MET:HE1	5	0.65	0.34	0.7
(1,224)	1:62:B:ILE:HG22	1:66:B:LEU:HG	5	0.65	0.35	0.69
(1,224)	1:62:B:ILE:HG23	1:66:B:LEU:HG	5	0.65	0.35	0.69
(1,224)	1:62:B:ILE:HG21	1:66:B:LEU:HG	5	0.65	0.35	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,224)	1:12:B:ILE:HG21	1:83:A:MET:HE1	5	0.65	0.35	0.69
(1,1527)	1:42:A:ARG:H	1:42:A:ARG:HG3	5	0.62	0.03	0.63
(1,1527)	1:42:A:ARG:H	1:42:A:ARG:HG2	5	0.62	0.03	0.63
(1,1528)	1:42:B:ARG:H	1:42:B:ARG:HG3	5	0.62	0.02	0.63
(1,1528)	1:42:B:ARG:H	1:42:B:ARG:HG2	5	0.62	0.02	0.63
(3,802)	1:29:B:PRO:HD2	1:30:B:ASP:HB2	5	0.61	0.5	0.27
(3,802)	1:29:B:PRO:HD3	1:30:B:ASP:HB2	5	0.61	0.5	0.27
(3,801)	1:29:A:PRO:HD2	1:30:A:ASP:HB2	5	0.59	0.47	0.27
(3,801)	1:29:A:PRO:HD3	1:30:A:ASP:HB2	5	0.59	0.47	0.27
(1,687)	1:107:A:PRO:HG2	1:109:A:LEU:H	5	0.59	0.22	0.62
(1,688)	1:107:B:PRO:HG2	1:109:B:LEU:H	5	0.59	0.21	0.62
(3,245)	1:7:A:GLN:HG3	1:18:B:THR:HB	5	0.56	0.16	0.58
(3,245)	1:7:A:GLN:HG2	1:18:B:THR:HB	5	0.56	0.16	0.58
(1,95)	1:7:A:GLN:HG3	1:6:A:SER:HA	5	0.55	0.15	0.58
(1,95)	1:7:A:GLN:HG3	1:18:B:THR:HB	5	0.55	0.15	0.58
(1,95)	1:7:A:GLN:HG2	1:18:B:THR:HB	5	0.55	0.15	0.58
(1,1674)	1:66:B:LEU:H	1:63:B:MET:HE1	5	0.53	0.17	0.53
(1,1674)	1:66:B:LEU:H	1:62:B:ILE:HG12	5	0.53	0.17	0.53
(1,1673)	1:66:A:LEU:H	1:63:A:MET:HE1	5	0.52	0.18	0.52
(1,1673)	1:66:A:LEU:H	1:62:A:ILE:HG12	5	0.52	0.18	0.52
(1,65)	1:74:A:LEU:HG	1:62:A:ILE:HG21	5	0.49	0.19	0.4
(1,65)	1:74:A:LEU:HG	1:62:A:ILE:HG22	5	0.49	0.19	0.4
(1,65)	1:74:A:LEU:HG	1:62:A:ILE:HG23	5	0.49	0.19	0.4
(1,66)	1:74:B:LEU:HG	1:62:B:ILE:HG21	5	0.48	0.2	0.39
(1,66)	1:74:B:LEU:HG	1:62:B:ILE:HG22	5	0.48	0.2	0.39
(1,66)	1:74:B:LEU:HG	1:62:B:ILE:HG23	5	0.48	0.2	0.39
(1,317)	1:82:A:LEU:HB3	1:80:A:ILE:HD13	5	0.43	0.16	0.37
(1,317)	1:82:A:LEU:HB3	1:80:A:ILE:HD11	5	0.43	0.16	0.37
(1,317)	1:82:A:LEU:HB3	1:80:A:ILE:HD12	5	0.43	0.16	0.37
(1,317)	1:82:A:LEU:HB3	1:80:B:ILE:HD11	5	0.43	0.16	0.37
(1,318)	1:82:B:LEU:HB3	1:80:B:ILE:HD13	5	0.43	0.16	0.37
(1,318)	1:82:B:LEU:HB3	1:80:B:ILE:HD11	5	0.43	0.16	0.37
(1,318)	1:82:B:LEU:HB3	1:80:B:ILE:HD12	5	0.43	0.16	0.37
(1,318)	1:82:B:LEU:HB3	1:80:A:ILE:HD11	5	0.43	0.16	0.37
(3,739)	1:59:A:ILE:HG23	1:58:A:VAL:HG13	5	0.37	0.06	0.33
(3,739)	1:59:A:ILE:HG23	1:58:A:VAL:HG12	5	0.37	0.06	0.33
(3,739)	1:59:A:ILE:HG21	1:58:A:VAL:HG13	5	0.37	0.06	0.33
(3,740)	1:59:B:ILE:HG23	1:58:B:VAL:HG13	5	0.37	0.06	0.33
(3,740)	1:59:B:ILE:HG23	1:58:B:VAL:HG12	5	0.37	0.06	0.33
(3,740)	1:59:B:ILE:HG21	1:58:B:VAL:HG13	5	0.37	0.06	0.33
(3,725)	1:38:A:LYS:HA	1:42:A:ARG:HD2	5	0.36	0.07	0.36
(3,1468)	1:110:B:GLY:H	1:48:B:PHE:HB3	5	0.36	0.13	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1468)	1:110:B:GLY:H	1:48:B:PHE:HB2	5	0.36	0.13	0.41
(3,726)	1:38:B:LYS:HA	1:42:B:ARG:HD2	5	0.36	0.07	0.35
(3,1467)	1:110:A:GLY:H	1:48:A:PHE:HB3	5	0.36	0.13	0.41
(3,1467)	1:110:A:GLY:H	1:48:A:PHE:HB2	5	0.36	0.13	0.41
(3,628)	1:48:B:PHE:HB2	1:9:A:GLU:HG3	5	0.33	0.15	0.34
(3,628)	1:48:B:PHE:HB2	1:9:A:GLU:HG2	5	0.33	0.15	0.34
(3,627)	1:48:A:PHE:HB2	1:9:B:GLU:HG3	5	0.33	0.15	0.33
(3,627)	1:48:A:PHE:HB2	1:9:B:GLU:HG2	5	0.33	0.15	0.33
(3,530)	1:67:B:ASP:HB3	1:64:B:GLU:HG3	5	0.33	0.16	0.33
(3,530)	1:67:B:ASP:HB2	1:64:B:GLU:HG2	5	0.33	0.16	0.33
(3,529)	1:67:A:ASP:HB3	1:64:A:GLU:HG3	5	0.32	0.16	0.31
(3,529)	1:67:A:ASP:HB2	1:64:A:GLU:HG2	5	0.32	0.16	0.31
(3,565)	1:111:A:GLU:HB2	1:108:A:GLY:HA3	5	0.3	0.1	0.3
(3,565)	1:111:A:GLU:HB2	1:108:A:GLY:HA2	5	0.3	0.1	0.3
(3,566)	1:111:B:GLU:HB2	1:108:B:GLY:HA3	5	0.3	0.1	0.3
(3,566)	1:111:B:GLU:HB2	1:108:B:GLY:HA2	5	0.3	0.1	0.3
(3,1442)	1:87:B:THR:H	1:16:A:ILE:HD13	5	0.3	0.05	0.31
(3,1442)	1:87:B:THR:H	1:16:A:ILE:HD11	5	0.3	0.05	0.31
(3,1442)	1:87:B:THR:H	1:16:A:ILE:HD12	5	0.3	0.05	0.31
(3,1441)	1:87:A:THR:H	1:16:B:ILE:HD13	5	0.29	0.06	0.3
(3,1441)	1:87:A:THR:H	1:16:B:ILE:HD11	5	0.29	0.06	0.3
(3,1441)	1:87:A:THR:H	1:16:B:ILE:HD12	5	0.29	0.06	0.3
(1,741)	1:81:A:MET:HA	1:84:A:ALA:HB3	5	0.26	0.12	0.29
(1,741)	1:81:A:MET:HA	1:84:A:ALA:HB1	5	0.26	0.12	0.29
(1,741)	1:4:A:LYS:HA	1:4:A:LYS:HG2	5	0.26	0.12	0.29
(1,741)	1:81:A:MET:HA	1:84:A:ALA:HB2	5	0.26	0.12	0.29
(1,742)	1:81:B:MET:HA	1:84:B:ALA:HB3	5	0.26	0.12	0.29
(1,742)	1:81:B:MET:HA	1:84:B:ALA:HB1	5	0.26	0.12	0.29
(1,742)	1:4:B:LYS:HA	1:4:B:LYS:HG2	5	0.26	0.12	0.29
(1,742)	1:81:B:MET:HA	1:84:B:ALA:HB2	5	0.26	0.12	0.29
(3,673)	1:73:A:GLN:H	1:63:A:MET:HE3	5	0.26	0.05	0.29
(3,673)	1:73:A:GLN:H	1:63:A:MET:HE1	5	0.26	0.05	0.29
(3,673)	1:73:A:GLN:H	1:63:A:MET:HE2	5	0.26	0.05	0.29
(3,674)	1:73:B:GLN:H	1:63:B:MET:HE3	5	0.26	0.05	0.28
(3,674)	1:73:B:GLN:H	1:63:B:MET:HE1	5	0.26	0.05	0.28
(3,674)	1:73:B:GLN:H	1:63:B:MET:HE2	5	0.26	0.05	0.28
(1,1591)	1:10:A:ARG:H	1:14:A:THR:H	5	0.22	0.05	0.19
(1,1592)	1:10:B:ARG:H	1:14:B:THR:H	5	0.22	0.05	0.19
(3,1448)	1:88:B:TRP:H	1:77:A:GLU:HG3	5	0.2	0.09	0.14
(3,1448)	1:88:B:TRP:H	1:77:A:GLU:HG2	5	0.2	0.09	0.14
(1,123)	1:45:A:LEU:HG	1:9:B:GLU:HA	5	0.19	0.04	0.17
(1,124)	1:45:B:LEU:HG	1:9:A:GLU:HA	5	0.19	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1735)	1:82:A:LEU:H	1:86:A:LEU:H	5	0.19	0.05	0.18
(1,1436)	1:23:B:SER:H	1:19:B:PHE:H	5	0.18	0.04	0.2
(1,1769)	1:87:A:THR:H	1:82:A:LEU:HD13	5	0.18	0.11	0.13
(1,1769)	1:87:A:THR:H	1:82:A:LEU:HD12	5	0.18	0.11	0.13
(1,1769)	1:87:A:THR:H	1:82:A:LEU:HD11	5	0.18	0.11	0.13
(1,1435)	1:23:A:SER:H	1:19:A:PHE:H	5	0.18	0.04	0.21
(1,1736)	1:82:B:LEU:H	1:86:B:LEU:H	5	0.18	0.04	0.17
(3,265)	1:42:A:ARG:HB2	1:43:A:LYS:H	5	0.14	0.02	0.16
(3,265)	1:42:A:ARG:HB3	1:43:A:LYS:H	5	0.14	0.02	0.16
(1,1540)	1:42:B:ARG:H	1:40:B:LEU:H	5	0.14	0.02	0.14
(2,2)	1:32:A:LEU:N	1:74:A:LEU:O	5	0.12	0.02	0.11
(1,1056)	1:33:B:ASN:HB3	1:31:B:THR:HG22	4	1.29	0.44	1.36
(1,1056)	1:33:B:ASN:HB2	1:31:B:THR:HG21	4	1.29	0.44	1.36
(1,1056)	1:33:B:ASN:HB2	1:31:B:THR:HG23	4	1.29	0.44	1.36
(1,1056)	1:33:B:ASN:HB3	1:31:B:THR:HG21	4	1.29	0.44	1.36
(3,256)	1:33:B:ASN:HB3	1:31:B:THR:HG22	4	1.29	0.44	1.36
(3,256)	1:33:B:ASN:HB2	1:31:B:THR:HG21	4	1.29	0.44	1.36
(3,256)	1:33:B:ASN:HB2	1:31:B:THR:HG23	4	1.29	0.44	1.36
(3,256)	1:33:B:ASN:HB3	1:31:B:THR:HG21	4	1.29	0.44	1.36
(1,771)	1:58:A:VAL:HA	1:59:A:ILE:HD13	4	1.29	0.04	1.28
(1,771)	1:58:A:VAL:HA	1:59:A:ILE:HD12	4	1.29	0.04	1.28
(1,771)	1:58:A:VAL:HA	1:59:A:ILE:HD11	4	1.29	0.04	1.28
(1,772)	1:58:B:VAL:HA	1:59:B:ILE:HD13	4	1.28	0.04	1.28
(1,772)	1:58:B:VAL:HA	1:59:B:ILE:HD12	4	1.28	0.04	1.28
(1,772)	1:58:B:VAL:HA	1:59:B:ILE:HD11	4	1.28	0.04	1.28
(1,1055)	1:33:A:ASN:HB3	1:31:A:THR:HG22	4	1.28	0.44	1.35
(1,1055)	1:33:A:ASN:HB2	1:31:A:THR:HG21	4	1.28	0.44	1.35
(1,1055)	1:33:A:ASN:HB2	1:31:A:THR:HG23	4	1.28	0.44	1.35
(1,1055)	1:33:A:ASN:HB3	1:31:A:THR:HG21	4	1.28	0.44	1.35
(3,255)	1:33:A:ASN:HB3	1:31:A:THR:HG22	4	1.28	0.44	1.35
(3,255)	1:33:A:ASN:HB2	1:31:A:THR:HG21	4	1.28	0.44	1.35
(3,255)	1:33:A:ASN:HB2	1:31:A:THR:HG23	4	1.28	0.44	1.35
(3,255)	1:33:A:ASN:HB3	1:31:A:THR:HG21	4	1.28	0.44	1.35
(1,719)	1:77:A:GLU:HB3	1:68:A:THR:HG23	4	0.77	0.49	0.6
(1,719)	1:77:A:GLU:HB2	1:68:A:THR:HG23	4	0.77	0.49	0.6
(1,719)	1:77:A:GLU:HB3	1:68:A:THR:HG22	4	0.77	0.49	0.6
(1,719)	1:77:A:GLU:HB2	1:68:A:THR:HG22	4	0.77	0.49	0.6
(1,720)	1:77:B:GLU:HB3	1:68:B:THR:HG23	4	0.77	0.49	0.6
(1,720)	1:77:B:GLU:HB2	1:68:B:THR:HG23	4	0.77	0.49	0.6
(1,720)	1:77:B:GLU:HB3	1:68:B:THR:HG22	4	0.77	0.49	0.6
(1,720)	1:77:B:GLU:HB2	1:68:B:THR:HG22	4	0.77	0.49	0.6
(3,275)	1:53:A:ASN:HB2	1:52:A:GLU:HG2	4	0.75	0.13	0.77

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,275)	1:53:A:ASN:HB3	1:52:A:GLU:HG2	4	0.75	0.13	0.77
(3,275)	1:53:A:ASN:HB2	1:52:A:GLU:HG3	4	0.75	0.13	0.77
(3,276)	1:53:B:ASN:HB2	1:52:B:GLU:HG2	4	0.75	0.13	0.77
(3,276)	1:53:B:ASN:HB3	1:52:B:GLU:HG2	4	0.75	0.13	0.77
(3,276)	1:53:B:ASN:HB2	1:52:B:GLU:HG3	4	0.75	0.13	0.77
(1,995)	1:109:A:LEU:HD12	1:93:A:LYS:HD3	4	0.75	0.1	0.76
(1,995)	1:109:A:LEU:HD22	1:93:A:LYS:HB2	4	0.75	0.1	0.76
(1,995)	1:109:A:LEU:HD12	1:93:A:LYS:HB3	4	0.75	0.1	0.76
(1,995)	1:109:A:LEU:HD11	1:93:A:LYS:HB2	4	0.75	0.1	0.76
(1,996)	1:109:B:LEU:HD12	1:93:B:LYS:HD3	4	0.75	0.09	0.76
(1,996)	1:109:B:LEU:HD22	1:93:B:LYS:HB2	4	0.75	0.09	0.76
(1,996)	1:109:B:LEU:HD12	1:93:B:LYS:HB3	4	0.75	0.09	0.76
(1,996)	1:109:B:LEU:HD11	1:93:B:LYS:HB2	4	0.75	0.09	0.76
(1,471)	1:79:A:PHE:HB3	1:81:A:MET:HG2	4	0.74	0.31	0.76
(1,471)	1:79:A:PHE:HB3	1:76:A:PHE:HB3	4	0.74	0.31	0.76
(1,472)	1:79:B:PHE:HB3	1:81:B:MET:HG2	4	0.74	0.31	0.76
(1,472)	1:79:B:PHE:HB3	1:76:B:PHE:HB3	4	0.74	0.31	0.76
(1,1010)	1:8:B:LEU:HD13	1:41:A:VAL:HA	4	0.72	0.71	0.38
(1,1010)	1:8:B:LEU:HD22	1:41:A:VAL:HA	4	0.72	0.71	0.38
(1,1010)	1:8:B:LEU:HD11	1:41:A:VAL:HA	4	0.72	0.71	0.38
(1,1009)	1:8:A:LEU:HD13	1:41:B:VAL:HA	4	0.72	0.72	0.38
(1,1009)	1:8:A:LEU:HD22	1:41:B:VAL:HA	4	0.72	0.72	0.38
(1,1009)	1:8:A:LEU:HD11	1:41:B:VAL:HA	4	0.72	0.72	0.38
(1,1643)	1:61:A:HIS:H	1:63:A:MET:HG3	4	0.62	0.3	0.65
(1,1643)	1:65:A:ASP:H	1:63:A:MET:HG3	4	0.62	0.3	0.65
(1,1643)	1:65:A:ASP:H	1:63:A:MET:HG2	4	0.62	0.3	0.65
(1,1644)	1:61:B:HIS:H	1:63:B:MET:HG3	4	0.61	0.3	0.64
(1,1644)	1:65:B:ASP:H	1:63:B:MET:HG3	4	0.61	0.3	0.64
(1,1644)	1:65:B:ASP:H	1:63:B:MET:HG2	4	0.61	0.3	0.64
(1,939)	1:5:A:MET:HB3	1:9:A:GLU:HA	4	0.61	0.09	0.62
(1,940)	1:5:B:MET:HB3	1:9:B:GLU:HA	4	0.61	0.09	0.62
(1,1579)	1:50:A:LYS:H	1:50:A:LYS:HG3	4	0.58	0.08	0.62
(1,1579)	1:50:A:LYS:H	1:51:A:LYS:HG3	4	0.58	0.08	0.62
(1,1580)	1:50:B:LYS:H	1:50:B:LYS:HG3	4	0.58	0.08	0.62
(1,1580)	1:50:B:LYS:H	1:51:B:LYS:HG3	4	0.58	0.08	0.62
(1,271)	1:12:A:ILE:H	1:8:A:LEU:HG	4	0.58	0.21	0.66
(1,271)	1:49:A:LEU:HG	1:51:A:LYS:H	4	0.58	0.21	0.66
(1,272)	1:12:B:ILE:H	1:8:B:LEU:HG	4	0.58	0.21	0.66
(1,272)	1:49:B:LEU:HG	1:51:B:LYS:H	4	0.58	0.21	0.66
(1,1054)	1:31:B:THR:HG22	1:71:B:ASP:HB2	4	0.58	0.44	0.53
(1,1054)	1:31:B:THR:HG21	1:71:B:ASP:HB2	4	0.58	0.44	0.53
(1,1054)	1:31:B:THR:HG21	1:71:B:ASP:HB3	4	0.58	0.44	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1053)	1:31:A:THR:HG22	1:71:A:ASP:HB2	4	0.58	0.44	0.52
(1,1053)	1:31:A:THR:HG21	1:71:A:ASP:HB2	4	0.58	0.44	0.52
(1,1053)	1:31:A:THR:HG21	1:71:A:ASP:HB3	4	0.58	0.44	0.52
(3,973)	1:5:A:MET:H	1:4:A:LYS:HB2	4	0.57	0.02	0.57
(3,973)	1:5:A:MET:H	1:4:A:LYS:HB3	4	0.57	0.02	0.57
(3,974)	1:5:B:MET:H	1:4:B:LYS:HB2	4	0.57	0.02	0.57
(3,974)	1:5:B:MET:H	1:4:B:LYS:HB3	4	0.57	0.02	0.57
(3,797)	1:107:A:PRO:HG3	1:108:A:GLY:HA3	4	0.51	0.08	0.53
(3,797)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	4	0.51	0.08	0.53
(3,798)	1:107:B:PRO:HG3	1:108:B:GLY:HA3	4	0.51	0.08	0.53
(3,798)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	4	0.51	0.08	0.53
(1,1175)	1:107:A:PRO:HG2	1:109:A:LEU:H	4	0.49	0.25	0.44
(1,1175)	1:107:A:PRO:HG3	1:105:A:HIS:H	4	0.49	0.25	0.44
(1,1776)	1:87:B:THR:H	1:16:A:ILE:HB	4	0.49	0.53	0.22
(1,1776)	1:87:B:THR:H	1:83:B:MET:HE1	4	0.49	0.53	0.22
(1,1776)	1:87:B:THR:H	1:83:B:MET:HE3	4	0.49	0.53	0.22
(1,1176)	1:107:B:PRO:HG2	1:109:B:LEU:H	4	0.49	0.25	0.43
(1,1176)	1:107:B:PRO:HG3	1:105:B:HIS:H	4	0.49	0.25	0.43
(1,1775)	1:87:A:THR:H	1:16:B:ILE:HB	4	0.49	0.52	0.22
(1,1775)	1:87:A:THR:H	1:83:A:MET:HE1	4	0.49	0.52	0.22
(1,1775)	1:87:A:THR:H	1:83:A:MET:HE3	4	0.49	0.52	0.22
(3,1088)	1:23:B:SER:H	1:40:B:LEU:HD22	4	0.46	0.2	0.4
(3,1088)	1:23:B:SER:H	1:40:B:LEU:HD21	4	0.46	0.2	0.4
(3,1088)	1:23:B:SER:H	1:40:B:LEU:HD23	4	0.46	0.2	0.4
(3,1087)	1:23:A:SER:H	1:40:A:LEU:HD22	4	0.46	0.21	0.4
(3,1087)	1:23:A:SER:H	1:40:A:LEU:HD21	4	0.46	0.21	0.4
(3,1087)	1:23:A:SER:H	1:40:A:LEU:HD23	4	0.46	0.21	0.4
(1,527)	1:49:A:LEU:HB3	1:50:A:LYS:HG2	4	0.45	0.15	0.4
(1,527)	1:49:A:LEU:HB2	1:50:A:LYS:HG2	4	0.45	0.15	0.4
(1,527)	1:49:A:LEU:HB3	1:51:A:LYS:HG3	4	0.45	0.15	0.4
(1,528)	1:49:B:LEU:HB3	1:50:B:LYS:HG2	4	0.45	0.15	0.4
(1,528)	1:49:B:LEU:HB2	1:50:B:LYS:HG2	4	0.45	0.15	0.4
(1,528)	1:49:B:LEU:HB3	1:51:B:LYS:HG3	4	0.45	0.15	0.4
(3,546)	1:33:B:ASN:HA	1:31:B:THR:HG22	4	0.42	0.34	0.26
(3,546)	1:33:B:ASN:HA	1:31:B:THR:HG21	4	0.42	0.34	0.26
(3,546)	1:33:B:ASN:HA	1:31:B:THR:HG23	4	0.42	0.34	0.26
(3,545)	1:33:A:ASN:HA	1:31:A:THR:HG22	4	0.42	0.33	0.26
(3,545)	1:33:A:ASN:HA	1:31:A:THR:HG21	4	0.42	0.33	0.26
(3,545)	1:33:A:ASN:HA	1:31:A:THR:HG23	4	0.42	0.33	0.26
(1,329)	1:78:A:GLU:H	1:66:A:LEU:HD22	4	0.41	0.22	0.4
(1,329)	1:66:A:LEU:HD13	1:84:A:ALA:H	4	0.41	0.22	0.4
(1,329)	1:66:A:LEU:HD12	1:84:A:ALA:H	4	0.41	0.22	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,329)	1:66:A:LEU:HD11	1:84:A:ALA:H	4	0.41	0.22	0.4
(1,330)	1:78:B:GLU:H	1:66:B:LEU:HD22	4	0.41	0.22	0.4
(1,330)	1:66:B:LEU:HD13	1:84:B:ALA:H	4	0.41	0.22	0.4
(1,330)	1:66:B:LEU:HD12	1:84:B:ALA:H	4	0.41	0.22	0.4
(1,330)	1:66:B:LEU:HD11	1:84:B:ALA:H	4	0.41	0.22	0.4
(1,1815)	1:110:A:GLY:H	1:48:A:PHE:HA	4	0.4	0.22	0.29
(1,1816)	1:110:B:GLY:H	1:48:B:PHE:HA	4	0.39	0.23	0.28
(1,507)	1:11:A:ASN:HB3	1:15:B:ILE:HG12	4	0.37	0.19	0.35
(1,507)	1:11:A:ASN:HB3	1:15:B:ILE:HG13	4	0.37	0.19	0.35
(1,507)	1:11:A:ASN:HB2	1:15:B:ILE:HG13	4	0.37	0.19	0.35
(1,508)	1:11:B:ASN:HB3	1:15:A:ILE:HG12	4	0.36	0.19	0.34
(1,508)	1:11:B:ASN:HB3	1:15:A:ILE:HG13	4	0.36	0.19	0.34
(1,508)	1:11:B:ASN:HB2	1:15:A:ILE:HG13	4	0.36	0.19	0.34
(3,503)	1:111:A:GLU:HA	1:107:A:PRO:HB2	4	0.36	0.13	0.36
(3,504)	1:111:B:GLU:HA	1:107:B:PRO:HB2	4	0.36	0.13	0.36
(3,1428)	1:86:B:LEU:H	1:86:B:LEU:HG	4	0.34	0.03	0.34
(3,1427)	1:86:A:LEU:H	1:86:A:LEU:HG	4	0.34	0.03	0.34
(3,980)	1:9:B:GLU:H	1:5:B:MET:HG2	4	0.32	0.13	0.32
(3,980)	1:9:B:GLU:H	1:5:B:MET:HG3	4	0.32	0.13	0.32
(3,979)	1:9:A:GLU:H	1:5:A:MET:HG2	4	0.32	0.13	0.32
(3,979)	1:9:A:GLU:H	1:5:A:MET:HG3	4	0.32	0.13	0.32
(1,596)	1:85:B:ARG:HG3	1:62:B:ILE:HG22	4	0.29	0.13	0.31
(1,596)	1:85:B:ARG:HG3	1:80:A:ILE:HG12	4	0.29	0.13	0.31
(3,225)	1:66:A:LEU:HD21	1:82:A:LEU:HA	4	0.29	0.16	0.26
(3,225)	1:66:A:LEU:HD13	1:82:A:LEU:HA	4	0.29	0.16	0.26
(3,225)	1:66:A:LEU:HD11	1:82:A:LEU:HA	4	0.29	0.16	0.26
(3,225)	1:66:A:LEU:HD12	1:82:A:LEU:HA	4	0.29	0.16	0.26
(3,839)	1:76:A:PHE:H	1:79:A:PHE:HB3	4	0.29	0.07	0.3
(3,840)	1:76:B:PHE:H	1:79:B:PHE:HB3	4	0.29	0.07	0.3
(1,595)	1:85:A:ARG:HG3	1:62:A:ILE:HG22	4	0.29	0.12	0.3
(1,595)	1:85:A:ARG:HG3	1:80:B:ILE:HG12	4	0.29	0.12	0.3
(3,329)	1:86:A:LEU:HD13	1:49:A:LEU:HG	4	0.26	0.08	0.27
(3,329)	1:86:A:LEU:HD11	1:49:A:LEU:HG	4	0.26	0.08	0.27
(3,329)	1:86:A:LEU:HD21	1:49:A:LEU:HG	4	0.26	0.08	0.27
(3,329)	1:86:A:LEU:HD23	1:49:A:LEU:HG	4	0.26	0.08	0.27
(1,1377)	1:18:A:THR:H	1:20:A:HIS:H	4	0.26	0.15	0.2
(3,330)	1:86:B:LEU:HD13	1:49:B:LEU:HG	4	0.26	0.09	0.28
(3,330)	1:86:B:LEU:HD11	1:49:B:LEU:HG	4	0.26	0.09	0.28
(3,330)	1:86:B:LEU:HD21	1:49:B:LEU:HG	4	0.26	0.09	0.28
(3,330)	1:86:B:LEU:HD23	1:49:B:LEU:HG	4	0.26	0.09	0.28
(1,1378)	1:18:B:THR:H	1:20:B:HIS:H	4	0.26	0.15	0.21
(1,1266)	1:77:B:GLU:H	1:84:A:ALA:HB1	4	0.25	0.12	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1266)	1:77:B:GLU:H	1:84:A:ALA:HB2	4	0.25	0.12	0.23
(1,1266)	1:77:B:GLU:H	1:84:A:ALA:HB3	4	0.25	0.12	0.23
(1,545)	1:107:A:PRO:HB3	1:108:A:GLY:H	4	0.23	0.07	0.23
(1,545)	1:107:A:PRO:HB2	1:108:A:GLY:H	4	0.23	0.07	0.23
(3,88)	1:34:B:GLN:HG2	1:38:B:LYS:HD2	4	0.23	0.1	0.2
(3,88)	1:34:B:GLN:HG3	1:38:B:LYS:HD3	4	0.23	0.1	0.2
(1,546)	1:68:B:THR:H	1:78:B:GLU:HB3	4	0.22	0.07	0.23
(1,546)	1:107:B:PRO:HB2	1:108:B:GLY:H	4	0.22	0.07	0.23
(1,546)	1:107:B:PRO:HB3	1:108:B:GLY:H	4	0.22	0.07	0.23
(3,87)	1:34:A:GLN:HG2	1:38:A:LYS:HD2	4	0.22	0.09	0.2
(3,87)	1:34:A:GLN:HG3	1:38:A:LYS:HD3	4	0.22	0.09	0.2
(3,1479)	1:100:A:GLY:H	1:99:A:GLU:HB3	4	0.22	0.11	0.18
(3,1479)	1:100:A:GLY:H	1:99:A:GLU:HB2	4	0.22	0.11	0.18
(3,187)	1:51:A:LYS:H	1:50:A:LYS:HG2	4	0.22	0.07	0.24
(3,187)	1:51:A:LYS:H	1:50:A:LYS:HG3	4	0.22	0.07	0.24
(3,188)	1:51:B:LYS:H	1:50:B:LYS:HG2	4	0.22	0.07	0.24
(3,188)	1:51:B:LYS:H	1:50:B:LYS:HG3	4	0.22	0.07	0.24
(3,1447)	1:88:A:TRP:H	1:77:B:GLU:HG3	4	0.22	0.1	0.22
(3,1447)	1:88:A:TRP:H	1:77:B:GLU:HG2	4	0.22	0.1	0.22
(4,259)	1:113:A:THR:H	1:107:A:PRO:HA	4	0.22	0.04	0.22
(4,260)	1:113:B:THR:H	1:107:B:PRO:HA	4	0.22	0.04	0.22
(1,1413)	1:21:A:GLN:H	1:29:A:PRO:HB2	4	0.22	0.06	0.22
(1,1413)	1:61:A:HIS:H	1:64:A:GLU:HB3	4	0.22	0.06	0.22
(1,1414)	1:21:B:GLN:H	1:29:B:PRO:HB2	4	0.22	0.06	0.22
(1,1414)	1:61:B:HIS:H	1:64:B:GLU:HB3	4	0.22	0.06	0.22
(3,1480)	1:100:B:GLY:H	1:99:B:GLU:HB3	4	0.21	0.12	0.17
(3,1480)	1:100:B:GLY:H	1:99:B:GLU:HB2	4	0.21	0.12	0.17
(1,629)	1:84:A:ALA:HA	1:86:A:LEU:HG	4	0.21	0.11	0.18
(1,630)	1:84:B:ALA:HA	1:86:B:LEU:HG	4	0.21	0.11	0.18
(1,1027)	1:84:A:ALA:HA	1:86:A:LEU:HG	4	0.21	0.11	0.18
(1,1028)	1:84:B:ALA:HA	1:86:B:LEU:HG	4	0.21	0.11	0.18
(1,1770)	1:87:B:THR:H	1:82:B:LEU:HD12	4	0.2	0.11	0.16
(1,1770)	1:87:B:THR:H	1:82:B:LEU:HD13	4	0.2	0.11	0.16
(1,980)	1:86:B:LEU:HD22	1:48:B:PHE:HB3	4	0.18	0.04	0.17
(1,980)	1:86:B:LEU:HD23	1:48:B:PHE:HB3	4	0.18	0.04	0.17
(1,980)	1:48:B:PHE:HB3	1:45:B:LEU:HD21	4	0.18	0.04	0.17
(1,980)	1:48:B:PHE:HB3	1:45:B:LEU:HD22	4	0.18	0.04	0.17
(1,979)	1:86:A:LEU:HD22	1:48:A:PHE:HB3	4	0.18	0.04	0.17
(1,979)	1:86:A:LEU:HD23	1:48:A:PHE:HB3	4	0.18	0.04	0.17
(1,979)	1:48:A:PHE:HB3	1:45:A:LEU:HD21	4	0.18	0.04	0.17
(1,979)	1:48:A:PHE:HB3	1:45:A:LEU:HD22	4	0.18	0.04	0.17
(3,200)	1:46:B:GLN:HB3	1:43:B:LYS:HA	4	0.18	0.08	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1275)	1:48:A:PHE:H	1:45:A:LEU:HG	4	0.17	0.06	0.16
(1,1276)	1:48:B:PHE:H	1:45:B:LEU:HG	4	0.17	0.05	0.16
(1,1495)	1:38:A:LYS:H	1:38:A:LYS:HD3	4	0.16	0.07	0.14
(1,1495)	1:38:A:LYS:H	1:38:A:LYS:HD2	4	0.16	0.07	0.14
(3,85)	1:7:A:GLN:HG3	1:7:A:GLN:HA	4	0.16	0.02	0.16
(3,86)	1:7:B:GLN:HG3	1:7:B:GLN:HA	4	0.16	0.02	0.16
(2,4)	1:74:A:LEU:N	1:32:A:LEU:O	4	0.16	0.06	0.14
(3,864)	1:74:B:LEU:H	1:31:B:THR:HB	4	0.16	0.02	0.16
(3,863)	1:74:A:LEU:H	1:31:A:THR:HB	4	0.16	0.02	0.16
(3,266)	1:42:B:ARG:HB2	1:43:B:LYS:H	4	0.15	0.01	0.16
(4,63)	1:32:A:LEU:HG	1:31:A:THR:HB	4	0.14	0.05	0.12
(4,64)	1:32:B:LEU:HG	1:31:B:THR:HB	4	0.14	0.05	0.12
(1,1539)	1:42:A:ARG:H	1:40:A:LEU:H	4	0.14	0.0	0.14
(3,79)	1:59:A:ILE:HB	1:38:A:LYS:HG2	4	0.14	0.02	0.14
(3,79)	1:59:A:ILE:HB	1:38:A:LYS:HG3	4	0.14	0.02	0.14
(3,80)	1:59:B:ILE:HB	1:38:B:LYS:HG2	4	0.14	0.02	0.14
(3,80)	1:59:B:ILE:HB	1:38:B:LYS:HG3	4	0.14	0.02	0.14
(1,1699)	1:71:A:ASP:H	1:72:A:LYS:HG3	4	0.13	0.02	0.13
(1,1700)	1:71:B:ASP:H	1:72:B:LYS:HG3	4	0.13	0.02	0.13
(3,590)	1:87:B:THR:HA	1:87:B:THR:HG22	4	0.12	0.01	0.12
(3,590)	1:87:B:THR:HA	1:87:B:THR:HG23	4	0.12	0.01	0.12
(1,1099)	1:24:A:VAL:HG11	1:22:A:TYR:HB2	4	0.12	0.02	0.12
(1,1099)	1:24:A:VAL:HG12	1:22:A:TYR:HB2	4	0.12	0.02	0.12
(1,1100)	1:24:B:VAL:HG11	1:22:B:TYR:HB2	4	0.12	0.02	0.12
(1,1100)	1:24:B:VAL:HG12	1:22:B:TYR:HB2	4	0.12	0.02	0.12
(3,589)	1:87:A:THR:HA	1:87:A:THR:HG22	4	0.12	0.01	0.12
(3,589)	1:87:A:THR:HA	1:87:A:THR:HG23	4	0.12	0.01	0.12
(1,1131)	1:54:A:LYS:HE2	1:53:A:ASN:HB3	3	1.42	0.79	1.13
(1,1131)	1:54:A:LYS:HE3	1:53:A:ASN:HB3	3	1.42	0.79	1.13
(1,1131)	1:72:A:LYS:HE2	1:63:A:MET:HG3	3	1.42	0.79	1.13
(1,1132)	1:54:B:LYS:HE2	1:53:B:ASN:HB3	3	1.41	0.8	1.12
(1,1132)	1:54:B:LYS:HE3	1:53:B:ASN:HB3	3	1.41	0.8	1.12
(1,1132)	1:72:B:LYS:HE2	1:63:B:MET:HG3	3	1.41	0.8	1.12
(3,815)	1:51:A:LYS:HG2	1:109:A:LEU:HD13	3	1.08	0.31	0.96
(3,815)	1:51:A:LYS:HG2	1:109:A:LEU:HD21	3	1.08	0.31	0.96
(3,816)	1:51:B:LYS:HG2	1:109:B:LEU:HD13	3	1.08	0.31	0.96
(3,816)	1:51:B:LYS:HG2	1:109:B:LEU:HD21	3	1.08	0.31	0.96
(1,17)	1:93:A:LYS:HA	1:109:A:LEU:HD12	3	0.95	0.27	0.93
(1,17)	1:92:A:GLU:HA	1:87:A:THR:HG21	3	0.95	0.27	0.93
(1,18)	1:93:B:LYS:HA	1:109:B:LEU:HD12	3	0.94	0.27	0.92
(1,18)	1:92:B:GLU:HA	1:87:B:THR:HG21	3	0.94	0.27	0.92
(1,144)	1:75:B:SER:HB3	1:79:B:PHE:HA	3	0.93	0.29	0.75

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,144)	1:75:B:SER:HB3	1:68:B:THR:HB	3	0.93	0.29	0.75
(1,143)	1:75:A:SER:HB3	1:79:A:PHE:HA	3	0.92	0.3	0.75
(1,143)	1:75:A:SER:HB3	1:68:A:THR:HB	3	0.92	0.3	0.75
(1,877)	1:34:A:GLN:HB2	1:72:A:LYS:HD3	3	0.87	0.26	0.92
(1,877)	1:34:A:GLN:HB2	1:72:A:LYS:HD2	3	0.87	0.26	0.92
(1,878)	1:34:B:GLN:HB2	1:72:B:LYS:HD3	3	0.87	0.25	0.91
(1,878)	1:34:B:GLN:HB2	1:72:B:LYS:HD2	3	0.87	0.25	0.91
(4,257)	1:108:A:GLY:H	1:111:A:GLU:HA	3	0.8	0.09	0.83
(4,258)	1:108:B:GLY:H	1:111:B:GLU:HA	3	0.8	0.09	0.83
(1,1204)	1:34:B:GLN:HB2	1:72:B:LYS:HD3	3	0.76	0.16	0.83
(1,1204)	1:60:B:GLU:HB2	1:62:B:ILE:HG13	3	0.76	0.16	0.83
(1,1204)	1:60:B:GLU:HB2	1:62:B:ILE:HG12	3	0.76	0.16	0.83
(1,1133)	1:51:A:LYS:HE2	1:53:A:ASN:HB3	3	0.76	0.35	0.62
(1,1133)	1:51:A:LYS:HE3	1:53:A:ASN:HB2	3	0.76	0.35	0.62
(1,1133)	1:72:A:LYS:HE2	1:63:A:MET:HG3	3	0.76	0.35	0.62
(1,1134)	1:51:B:LYS:HE2	1:53:B:ASN:HB3	3	0.75	0.35	0.61
(1,1134)	1:51:B:LYS:HE3	1:53:B:ASN:HB2	3	0.75	0.35	0.61
(1,1134)	1:72:B:LYS:HE2	1:63:B:MET:HG3	3	0.75	0.35	0.61
(1,1203)	1:34:A:GLN:HB2	1:72:A:LYS:HD3	3	0.75	0.15	0.82
(1,1203)	1:60:A:GLU:HB2	1:62:A:ILE:HG13	3	0.75	0.15	0.82
(1,1203)	1:60:A:GLU:HB2	1:62:A:ILE:HG12	3	0.75	0.15	0.82
(3,1474)	1:100:B:GLY:H	1:98:B:ASP:HA	3	0.68	0.5	0.41
(3,1473)	1:100:A:GLY:H	1:98:A:ASP:HA	3	0.68	0.49	0.4
(1,1159)	1:21:A:GLN:HG3	1:25:A:LYS:HD2	3	0.67	0.26	0.52
(1,1160)	1:21:B:GLN:HG3	1:25:B:LYS:HD2	3	0.67	0.26	0.52
(1,405)	1:42:A:ARG:HB3	1:53:A:ASN:HB2	3	0.65	0.18	0.59
(1,406)	1:42:B:ARG:HB3	1:53:B:ASN:HB2	3	0.65	0.18	0.59
(1,581)	1:42:A:ARG:HB3	1:53:A:ASN:HB2	3	0.65	0.18	0.59
(1,582)	1:42:B:ARG:HB3	1:53:B:ASN:HB2	3	0.65	0.18	0.59
(3,50)	1:78:B:GLU:HG2	1:77:B:GLU:H	3	0.65	0.34	0.86
(3,49)	1:78:A:GLU:HG2	1:77:A:GLU:H	3	0.64	0.35	0.86
(3,639)	1:8:A:LEU:HD12	1:83:B:MET:HG3	3	0.53	0.36	0.45
(3,639)	1:8:A:LEU:HD21	1:83:B:MET:HG2	3	0.53	0.36	0.45
(3,639)	1:8:A:LEU:HD13	1:83:B:MET:HG3	3	0.53	0.36	0.45
(3,640)	1:8:B:LEU:HD12	1:83:A:MET:HG3	3	0.52	0.34	0.44
(3,640)	1:8:B:LEU:HD21	1:83:A:MET:HG2	3	0.52	0.34	0.44
(3,640)	1:8:B:LEU:HD13	1:83:A:MET:HG3	3	0.52	0.34	0.44
(3,334)	1:86:B:LEU:HD13	1:48:B:PHE:HB3	3	0.48	0.26	0.6
(3,334)	1:86:B:LEU:HD23	1:48:B:PHE:HB3	3	0.48	0.26	0.6
(3,334)	1:86:B:LEU:HD22	1:48:B:PHE:HB3	3	0.48	0.26	0.6
(3,333)	1:86:A:LEU:HD13	1:48:A:PHE:HB3	3	0.47	0.26	0.6
(3,333)	1:86:A:LEU:HD23	1:48:A:PHE:HB3	3	0.47	0.26	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,333)	1:86:A:LEU:HD22	1:48:A:PHE:HB3	3	0.47	0.26	0.6
(1,651)	1:93:A:LYS:H	1:92:A:GLU:HB2	3	0.43	0.07	0.48
(1,651)	1:93:A:LYS:H	1:92:A:GLU:HB3	3	0.43	0.07	0.48
(1,652)	1:93:B:LYS:H	1:92:B:GLU:HB2	3	0.43	0.07	0.48
(1,652)	1:93:B:LYS:H	1:92:B:GLU:HB3	3	0.43	0.07	0.48
(1,1517)	1:40:A:LEU:H	1:25:A:LYS:HD3	3	0.41	0.17	0.43
(1,1517)	1:40:A:LEU:H	1:43:A:LYS:HD3	3	0.41	0.17	0.43
(1,1518)	1:40:B:LEU:H	1:25:B:LYS:HD3	3	0.41	0.17	0.44
(1,1518)	1:40:B:LEU:H	1:25:B:LYS:HD2	3	0.41	0.17	0.44
(1,1518)	1:40:B:LEU:H	1:43:B:LYS:HD3	3	0.41	0.17	0.44
(1,1635)	1:65:A:ASP:H	1:66:A:LEU:HG	3	0.39	0.04	0.4
(1,1635)	1:65:A:ASP:H	1:62:A:ILE:HG13	3	0.39	0.04	0.4
(1,1636)	1:65:B:ASP:H	1:66:B:LEU:HG	3	0.39	0.04	0.4
(1,1636)	1:65:B:ASP:H	1:62:B:ILE:HG13	3	0.39	0.04	0.4
(3,1366)	1:69:B:ASN:H	1:73:B:GLN:HB2	3	0.38	0.08	0.37
(1,1466)	1:35:B:GLY:H	1:72:B:LYS:HB3	3	0.37	0.13	0.37
(1,1466)	1:35:B:GLY:H	1:73:B:GLN:HG2	3	0.37	0.13	0.37
(1,1465)	1:35:A:GLY:H	1:72:A:LYS:HB3	3	0.37	0.13	0.38
(1,1465)	1:35:A:GLY:H	1:73:A:GLN:HG2	3	0.37	0.13	0.38
(3,1365)	1:69:A:ASN:H	1:73:A:GLN:HB2	3	0.37	0.08	0.37
(3,226)	1:66:B:LEU:HD13	1:82:B:LEU:HA	3	0.36	0.13	0.3
(3,226)	1:66:B:LEU:HD11	1:82:B:LEU:HA	3	0.36	0.13	0.3
(3,226)	1:66:B:LEU:HD12	1:82:B:LEU:HA	3	0.36	0.13	0.3
(3,637)	1:109:A:LEU:HD11	1:48:A:PHE:HA	3	0.35	0.15	0.36
(3,637)	1:109:A:LEU:HD12	1:48:A:PHE:HA	3	0.35	0.15	0.36
(3,637)	1:109:A:LEU:HD21	1:48:A:PHE:HA	3	0.35	0.15	0.36
(3,638)	1:109:B:LEU:HD11	1:48:B:PHE:HA	3	0.35	0.15	0.36
(3,638)	1:109:B:LEU:HD12	1:48:B:PHE:HA	3	0.35	0.15	0.36
(3,638)	1:109:B:LEU:HD21	1:48:B:PHE:HA	3	0.35	0.15	0.36
(3,1458)	1:89:B:ALA:H	1:16:A:ILE:HD13	3	0.35	0.17	0.29
(3,1458)	1:89:B:ALA:H	1:16:A:ILE:HD12	3	0.35	0.17	0.29
(3,1457)	1:89:A:ALA:H	1:16:B:ILE:HD13	3	0.35	0.16	0.3
(3,1457)	1:89:A:ALA:H	1:16:B:ILE:HD12	3	0.35	0.16	0.3
(1,1606)	1:80:B:ILE:H	1:78:B:GLU:HG3	3	0.34	0.1	0.39
(1,1606)	1:90:B:SER:H	1:13:A:GLU:HG2	3	0.34	0.1	0.39
(1,1605)	1:80:A:ILE:H	1:78:A:GLU:HG3	3	0.33	0.09	0.38
(1,1605)	1:90:A:SER:H	1:13:B:GLU:HG2	3	0.33	0.09	0.38
(3,208)	1:44:B:ASP:HA	1:9:A:GLU:HG3	3	0.31	0.1	0.38
(3,208)	1:44:B:ASP:HA	1:9:A:GLU:HG2	3	0.31	0.1	0.38
(3,179)	1:49:A:LEU:HG	1:48:A:PHE:HB3	3	0.3	0.08	0.34
(3,180)	1:49:B:LEU:HG	1:48:B:PHE:HB3	3	0.3	0.08	0.34
(3,207)	1:44:A:ASP:HA	1:9:B:GLU:HG3	3	0.3	0.1	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,207)	1:44:A:ASP:HA	1:9:B:GLU:HG2	3	0.3	0.1	0.33
(1,1265)	1:77:A:GLU:H	1:84:B:ALA:HB1	3	0.3	0.11	0.29
(1,1265)	1:77:A:GLU:H	1:84:B:ALA:HB2	3	0.3	0.11	0.29
(1,1265)	1:77:A:GLU:H	1:84:B:ALA:HB3	3	0.3	0.11	0.29
(3,881)	1:30:A:ASP:H	1:31:A:THR:HG23	3	0.3	0.05	0.31
(3,881)	1:30:A:ASP:H	1:31:A:THR:HG21	3	0.3	0.05	0.31
(3,53)	1:39:A:GLU:HG3	1:43:A:LYS:HD2	3	0.29	0.12	0.28
(3,53)	1:39:A:GLU:HG3	1:43:A:LYS:HD3	3	0.29	0.12	0.28
(3,54)	1:39:B:GLU:HG3	1:43:B:LYS:HD2	3	0.29	0.12	0.28
(3,54)	1:39:B:GLU:HG3	1:43:B:LYS:HD3	3	0.29	0.12	0.28
(3,882)	1:30:B:ASP:H	1:31:B:THR:HG23	3	0.29	0.05	0.3
(3,882)	1:30:B:ASP:H	1:31:B:THR:HG21	3	0.29	0.05	0.3
(3,671)	1:34:A:GLN:H	1:63:A:MET:HE3	3	0.29	0.03	0.3
(3,672)	1:34:B:GLN:H	1:63:B:MET:HE3	3	0.29	0.03	0.3
(3,539)	1:15:A:ILE:HA	1:8:B:LEU:HD11	3	0.28	0.06	0.26
(3,539)	1:15:A:ILE:HA	1:8:B:LEU:HD22	3	0.28	0.06	0.26
(3,539)	1:15:A:ILE:HA	1:8:B:LEU:HD23	3	0.28	0.06	0.26
(1,45)	1:39:A:GLU:HG2	1:44:A:ASP:H	3	0.28	0.11	0.35
(1,46)	1:39:B:GLU:HG2	1:44:B:ASP:H	3	0.28	0.11	0.35
(3,540)	1:15:B:ILE:HA	1:8:A:LEU:HD11	3	0.27	0.05	0.25
(3,540)	1:15:B:ILE:HA	1:8:A:LEU:HD22	3	0.27	0.05	0.25
(3,540)	1:15:B:ILE:HA	1:8:A:LEU:HD23	3	0.27	0.05	0.25
(1,297)	1:58:A:VAL:HG23	1:56:A:GLU:HB3	3	0.26	0.07	0.3
(1,297)	1:58:A:VAL:HG21	1:56:A:GLU:HB2	3	0.26	0.07	0.3
(1,297)	1:9:A:GLU:HB2	1:8:A:LEU:HD23	3	0.26	0.07	0.3
(3,1279)	1:57:A:LYS:H	1:57:A:LYS:HD3	3	0.26	0.17	0.18
(3,1280)	1:57:B:LYS:H	1:57:B:LYS:HD3	3	0.26	0.17	0.18
(1,298)	1:58:B:VAL:HG23	1:56:B:GLU:HB3	3	0.25	0.08	0.28
(1,298)	1:58:B:VAL:HG21	1:56:B:GLU:HB2	3	0.25	0.08	0.28
(1,298)	1:9:B:GLU:HB2	1:8:B:LEU:HD23	3	0.25	0.08	0.28
(1,293)	1:58:A:VAL:HG21	1:56:A:GLU:HB2	3	0.24	0.06	0.26
(1,293)	1:81:A:MET:HB2	1:80:A:ILE:HG13	3	0.24	0.06	0.26
(1,293)	1:81:A:MET:HB3	1:80:B:ILE:HG12	3	0.24	0.06	0.26
(1,294)	1:58:B:VAL:HG21	1:56:B:GLU:HB2	3	0.24	0.07	0.26
(1,294)	1:81:B:MET:HB2	1:80:B:ILE:HG13	3	0.24	0.07	0.26
(1,294)	1:81:B:MET:HB3	1:80:A:ILE:HG12	3	0.24	0.07	0.26
(1,1181)	1:58:A:VAL:HG21	1:56:A:GLU:HB2	3	0.24	0.06	0.26
(1,1181)	1:81:A:MET:HB2	1:80:A:ILE:HG13	3	0.24	0.06	0.26
(1,1181)	1:81:A:MET:HB3	1:80:B:ILE:HG12	3	0.24	0.06	0.26
(1,1182)	1:58:B:VAL:HG21	1:56:B:GLU:HB2	3	0.24	0.07	0.26
(1,1182)	1:81:B:MET:HB2	1:80:B:ILE:HG13	3	0.24	0.07	0.26
(1,1182)	1:81:B:MET:HB3	1:80:A:ILE:HG12	3	0.24	0.07	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,664)	1:63:B:MET:HE2	1:72:B:LYS:HA	3	0.24	0.08	0.28
(3,664)	1:63:B:MET:HE1	1:72:B:LYS:HA	3	0.24	0.08	0.28
(3,663)	1:63:A:MET:HE2	1:72:A:LYS:HA	3	0.23	0.08	0.28
(3,663)	1:63:A:MET:HE1	1:72:A:LYS:HA	3	0.23	0.08	0.28
(1,285)	1:51:A:LYS:H	1:50:A:LYS:HG2	3	0.22	0.08	0.22
(1,285)	1:51:A:LYS:H	1:50:A:LYS:HG3	3	0.22	0.08	0.22
(1,286)	1:51:B:LYS:H	1:50:B:LYS:HG2	3	0.22	0.08	0.22
(1,286)	1:51:B:LYS:H	1:50:B:LYS:HG3	3	0.22	0.08	0.22
(1,1374)	1:17:B:ASN:H	1:13:B:GLU:HA	3	0.22	0.02	0.23
(1,1384)	1:18:B:THR:H	1:16:B:ILE:HG13	3	0.22	0.1	0.19
(1,1373)	1:17:A:ASN:H	1:13:A:GLU:HA	3	0.21	0.02	0.22
(1,1383)	1:18:A:THR:H	1:16:A:ILE:HG13	3	0.21	0.1	0.18
(3,199)	1:46:A:GLN:HB3	1:43:A:LYS:HA	3	0.21	0.08	0.22
(1,1496)	1:38:B:LYS:H	1:38:B:LYS:HD2	3	0.19	0.06	0.17
(1,1496)	1:38:B:LYS:H	1:38:B:LYS:HD3	3	0.19	0.06	0.17
(1,579)	1:34:A:GLN:HG3	1:38:A:LYS:HD3	3	0.18	0.08	0.13
(1,579)	1:34:A:GLN:HG2	1:38:A:LYS:HD2	3	0.18	0.08	0.13
(1,580)	1:34:B:GLN:HG3	1:38:B:LYS:HD3	3	0.18	0.08	0.14
(1,580)	1:34:B:GLN:HG2	1:38:B:LYS:HD2	3	0.18	0.08	0.14
(2,86)	1:94:A:MET:H	1:90:A:SER:O	3	0.18	0.03	0.18
(3,1283)	1:57:A:LYS:H	1:58:A:VAL:HG23	3	0.17	0.03	0.17
(3,1283)	1:57:A:LYS:H	1:58:A:VAL:HG22	3	0.17	0.03	0.17
(3,1283)	1:57:A:LYS:H	1:58:A:VAL:HG21	3	0.17	0.03	0.17
(3,1284)	1:57:B:LYS:H	1:58:B:VAL:HG23	3	0.17	0.03	0.17
(3,1284)	1:57:B:LYS:H	1:58:B:VAL:HG22	3	0.17	0.03	0.17
(3,1284)	1:57:B:LYS:H	1:58:B:VAL:HG21	3	0.17	0.03	0.17
(1,682)	1:37:B:PHE:HB3	1:63:B:MET:H	3	0.16	0.01	0.17
(1,681)	1:37:A:PHE:HB3	1:63:A:MET:H	3	0.16	0.02	0.16
(1,1853)	1:5:A:MET:H	1:9:A:GLU:HG3	3	0.16	0.04	0.14
(1,1853)	1:109:A:LEU:H	1:13:B:GLU:HG3	3	0.16	0.04	0.14
(1,1853)	1:5:A:MET:H	1:9:A:GLU:HG2	3	0.16	0.04	0.14
(1,894)	1:78:B:GLU:HB3	1:74:B:LEU:HB3	3	0.15	0.01	0.15
(1,894)	1:78:B:GLU:HB2	1:74:B:LEU:HB3	3	0.15	0.01	0.15
(1,1854)	1:5:B:MET:H	1:9:B:GLU:HG3	3	0.15	0.03	0.14
(1,1854)	1:109:B:LEU:H	1:13:A:GLU:HG3	3	0.15	0.03	0.14
(1,1854)	1:5:B:MET:H	1:9:B:GLU:HG2	3	0.15	0.03	0.14
(2,79)	1:91:A:HIS:N	1:87:A:THR:O	3	0.15	0.02	0.14
(3,564)	1:78:B:GLU:HB3	1:74:B:LEU:HB3	3	0.15	0.01	0.15
(3,564)	1:78:B:GLU:HB2	1:74:B:LEU:HB3	3	0.15	0.01	0.15
(1,893)	1:78:A:GLU:HB3	1:74:A:LEU:HB3	3	0.15	0.01	0.15
(1,893)	1:78:A:GLU:HB2	1:74:A:LEU:HB3	3	0.15	0.01	0.15
(3,563)	1:78:A:GLU:HB3	1:74:A:LEU:HB3	3	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,563)	1:78:A:GLU:HB2	1:74:A:LEU:HB3	3	0.15	0.01	0.15
(3,156)	1:34:B:GLN:HA	1:34:B:GLN:HG3	3	0.15	0.03	0.16
(3,155)	1:34:A:GLN:HA	1:34:A:GLN:HG3	3	0.15	0.03	0.15
(3,679)	1:85:A:ARG:HG2	1:85:A:ARG:HA	3	0.14	0.02	0.14
(3,680)	1:85:B:ARG:HG2	1:85:B:ARG:HA	3	0.14	0.01	0.14
(4,111)	1:76:A:PHE:H	1:31:A:THR:H	3	0.13	0.03	0.12
(4,112)	1:76:B:PHE:H	1:31:B:THR:H	3	0.13	0.03	0.11
(2,21)	1:20:A:HIS:N	1:16:A:ILE:O	3	0.12	0.01	0.12
(4,235)	1:81:A:MET:H	1:81:B:MET:H	3	0.12	0.02	0.11
(4,236)	1:81:B:MET:H	1:81:A:MET:H	3	0.12	0.02	0.11
(3,1343)	1:66:A:LEU:H	1:66:A:LEU:HG	3	0.11	0.01	0.11
(3,942)	1:48:B:PHE:H	1:50:B:LYS:H	3	0.1	0.0	0.1
(3,941)	1:48:A:PHE:H	1:50:A:LYS:H	3	0.1	0.0	0.1
(3,738)	1:24:B:VAL:HG21	1:29:B:PRO:HB2	2	2.45	0.53	2.45
(3,737)	1:24:A:VAL:HG21	1:29:A:PRO:HB2	2	2.44	0.52	2.44
(3,534)	1:24:B:VAL:HA	1:29:B:PRO:HA	2	2.39	0.34	2.39
(3,533)	1:24:A:VAL:HA	1:29:A:PRO:HA	2	2.37	0.32	2.37
(1,142)	1:80:B:ILE:HD11	1:83:A:MET:HE3	2	1.72	0.72	1.72
(1,142)	1:80:B:ILE:HD12	1:83:B:MET:HE1	2	1.72	0.72	1.72
(1,141)	1:80:A:ILE:HD11	1:83:B:MET:HE3	2	1.7	0.73	1.7
(1,141)	1:80:A:ILE:HD12	1:83:A:MET:HE1	2	1.7	0.73	1.7
(1,1129)	1:30:A:ASP:HB3	1:76:A:PHE:HA	2	1.08	0.52	1.08
(1,1129)	1:4:A:LYS:HE3	1:6:A:SER:HB3	2	1.08	0.52	1.08
(1,1130)	1:30:B:ASP:HB3	1:76:B:PHE:HA	2	1.08	0.52	1.08
(1,1130)	1:4:B:LYS:HE3	1:6:B:SER:HB3	2	1.08	0.52	1.08
(3,643)	1:8:A:LEU:HD21	1:40:B:LEU:HD22	2	1.06	0.31	1.06
(3,643)	1:8:A:LEU:HD13	1:40:B:LEU:HD21	2	1.06	0.31	1.06
(3,644)	1:8:B:LEU:HD21	1:40:A:LEU:HD22	2	1.04	0.31	1.04
(3,644)	1:8:B:LEU:HD13	1:40:A:LEU:HD21	2	1.04	0.31	1.04
(3,332)	1:86:B:LEU:HD12	1:9:A:GLU:HG2	2	0.82	0.38	0.82
(3,331)	1:86:A:LEU:HD12	1:9:B:GLU:HG2	2	0.82	0.38	0.82
(3,239)	1:77:A:GLU:HB2	1:78:A:GLU:HG2	2	0.73	0.05	0.73
(3,240)	1:77:B:GLU:HB2	1:78:B:GLU:HG2	2	0.73	0.05	0.73
(1,315)	1:109:A:LEU:HB3	1:111:A:GLU:HB2	2	0.7	0.01	0.7
(1,316)	1:109:B:LEU:HB3	1:111:B:GLU:HB2	2	0.7	0.01	0.7
(3,383)	1:51:A:LYS:HD3	1:109:A:LEU:HD23	2	0.7	0.21	0.7
(3,383)	1:51:A:LYS:HD3	1:109:A:LEU:HD21	2	0.7	0.21	0.7
(3,384)	1:51:B:LYS:HD3	1:109:B:LEU:HD23	2	0.7	0.22	0.7
(3,384)	1:51:B:LYS:HD3	1:109:B:LEU:HD21	2	0.7	0.22	0.7
(1,799)	1:111:A:GLU:HA	1:50:A:LYS:HE2	2	0.68	0.11	0.68
(1,799)	1:111:A:GLU:HA	1:93:A:LYS:HE3	2	0.68	0.11	0.68
(1,800)	1:111:B:GLU:HA	1:50:B:LYS:HE2	2	0.68	0.11	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,800)	1:111:B:GLU:HA	1:93:B:LYS:HE3	2	0.68	0.11	0.68
(1,661)	1:49:A:LEU:HG	1:52:A:GLU:HG2	2	0.66	0.24	0.66
(1,661)	1:49:A:LEU:HG	1:52:A:GLU:HG3	2	0.66	0.24	0.66
(1,1737)	1:36:A:GLU:H	1:33:A:ASN:HB3	2	0.66	0.09	0.66
(1,1737)	1:36:A:GLU:H	1:33:A:ASN:HB2	2	0.66	0.09	0.66
(1,1738)	1:36:B:GLU:H	1:33:B:ASN:HB3	2	0.66	0.09	0.66
(1,1738)	1:36:B:GLU:H	1:33:B:ASN:HB2	2	0.66	0.09	0.66
(1,662)	1:49:B:LEU:HG	1:52:B:GLU:HG2	2	0.66	0.25	0.66
(1,662)	1:49:B:LEU:HG	1:52:B:GLU:HG3	2	0.66	0.25	0.66
(3,35)	1:58:A:VAL:HG23	1:57:A:LYS:HE3	2	0.59	0.08	0.59
(3,35)	1:58:A:VAL:HG23	1:57:A:LYS:HE2	2	0.59	0.08	0.59
(3,36)	1:58:B:VAL:HG23	1:57:B:LYS:HE3	2	0.58	0.08	0.58
(3,36)	1:58:B:VAL:HG23	1:57:B:LYS:HE2	2	0.58	0.08	0.58
(1,745)	1:111:A:GLU:HG2	1:109:A:LEU:HB3	2	0.55	0.32	0.55
(3,479)	1:111:A:GLU:HG2	1:109:A:LEU:HB3	2	0.55	0.32	0.55
(1,746)	1:111:B:GLU:HG2	1:109:B:LEU:HB3	2	0.55	0.32	0.55
(3,480)	1:111:B:GLU:HG2	1:109:B:LEU:HB3	2	0.55	0.32	0.55
(1,1852)	1:5:B:MET:H	1:5:B:MET:HG3	2	0.55	0.26	0.55
(1,1851)	1:5:A:MET:H	1:5:A:MET:HG3	2	0.54	0.25	0.54
(1,249)	1:36:A:GLU:HB3	1:25:A:LYS:HE2	2	0.53	0.16	0.53
(1,250)	1:36:B:GLU:HB3	1:25:B:LYS:HE2	2	0.53	0.17	0.53
(3,787)	1:67:A:ASP:HB2	1:78:A:GLU:HB2	2	0.52	0.06	0.52
(3,787)	1:67:A:ASP:HB2	1:78:A:GLU:HB3	2	0.52	0.06	0.52
(3,788)	1:67:B:ASP:HB2	1:78:B:GLU:HB2	2	0.52	0.06	0.52
(3,788)	1:67:B:ASP:HB2	1:78:B:GLU:HB3	2	0.52	0.06	0.52
(1,787)	1:32:A:LEU:HG	1:40:A:LEU:HB2	2	0.5	0.01	0.5
(1,788)	1:32:B:LEU:HG	1:40:B:LEU:HB2	2	0.5	0.01	0.5
(1,1007)	1:8:A:LEU:HD22	1:40:B:LEU:HA	2	0.5	0.08	0.5
(1,1007)	1:8:A:LEU:HD11	1:83:B:MET:HA	2	0.5	0.08	0.5
(1,1008)	1:8:B:LEU:HD22	1:40:A:LEU:HA	2	0.5	0.07	0.5
(1,1008)	1:8:B:LEU:HD11	1:83:A:MET:HA	2	0.5	0.07	0.5
(1,217)	1:12:A:ILE:HG23	1:48:B:PHE:HB2	2	0.49	0.2	0.49
(1,217)	1:12:A:ILE:HG23	1:48:B:PHE:HB3	2	0.49	0.2	0.49
(1,218)	1:12:B:ILE:HG23	1:48:A:PHE:HB2	2	0.48	0.21	0.48
(1,218)	1:12:B:ILE:HG23	1:48:A:PHE:HB3	2	0.48	0.21	0.48
(1,1161)	1:21:A:GLN:HG2	1:19:A:PHE:HB2	2	0.48	0.06	0.48
(1,1162)	1:21:B:GLN:HG2	1:19:B:PHE:HB2	2	0.48	0.06	0.48
(3,866)	1:52:B:GLU:H	1:51:B:LYS:HG3	2	0.48	0.2	0.48
(3,865)	1:52:A:GLU:H	1:51:A:LYS:HG3	2	0.48	0.19	0.48
(1,1291)	1:7:A:GLN:H	1:7:A:GLN:HG3	2	0.46	0.18	0.46
(1,1291)	1:5:A:MET:H	1:5:A:MET:HG3	2	0.46	0.18	0.46
(1,1292)	1:7:B:GLN:H	1:7:B:GLN:HG3	2	0.46	0.18	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1292)	1:5:B:MET:H	1:5:B:MET:HG3	2	0.46	0.18	0.46
(3,771)	1:14:A:THR:HG21	1:17:A:ASN:HB3	2	0.46	0.14	0.46
(3,771)	1:14:A:THR:HG23	1:17:A:ASN:HB3	2	0.46	0.14	0.46
(3,772)	1:14:B:THR:HG21	1:17:B:ASN:HB3	2	0.46	0.14	0.46
(3,772)	1:14:B:THR:HG23	1:17:B:ASN:HB3	2	0.46	0.14	0.46
(3,149)	1:77:A:GLU:HA	1:81:B:MET:HE2	2	0.45	0.05	0.45
(3,149)	1:77:A:GLU:HA	1:81:B:MET:HE3	2	0.45	0.05	0.45
(1,903)	1:86:A:LEU:HB3	1:109:A:LEU:HG	2	0.44	0.01	0.44
(1,903)	1:82:A:LEU:HB3	1:80:A:ILE:HB	2	0.44	0.01	0.44
(1,904)	1:86:B:LEU:HB3	1:109:B:LEU:HG	2	0.44	0.01	0.44
(1,904)	1:82:B:LEU:HB3	1:80:B:ILE:HB	2	0.44	0.01	0.44
(3,150)	1:77:B:GLU:HA	1:81:A:MET:HE2	2	0.44	0.04	0.44
(3,150)	1:77:B:GLU:HA	1:81:A:MET:HE3	2	0.44	0.04	0.44
(3,617)	1:57:A:LYS:HA	1:57:A:LYS:HG2	2	0.44	0.01	0.44
(3,618)	1:57:B:LYS:HA	1:57:B:LYS:HG2	2	0.44	0.01	0.44
(3,106)	1:38:B:LYS:HG2	1:34:B:GLN:HA	2	0.44	0.23	0.44
(3,106)	1:38:B:LYS:HG3	1:34:B:GLN:HA	2	0.44	0.23	0.44
(3,105)	1:38:A:LYS:HG2	1:34:A:GLN:HA	2	0.43	0.22	0.43
(3,105)	1:38:A:LYS:HG3	1:34:A:GLN:HA	2	0.43	0.22	0.43
(1,591)	1:85:A:ARG:HG3	1:66:A:LEU:HG	2	0.34	0.19	0.34
(1,592)	1:85:B:ARG:HG3	1:66:B:LEU:HG	2	0.34	0.19	0.34
(3,500)	1:32:B:LEU:HG	1:23:B:SER:HB3	2	0.32	0.06	0.32
(3,499)	1:32:A:LEU:HG	1:23:A:SER:HB3	2	0.32	0.06	0.32
(1,1561)	1:44:A:ASP:H	1:40:A:LEU:HD23	2	0.31	0.08	0.31
(1,1561)	1:44:A:ASP:H	1:40:A:LEU:HD22	2	0.31	0.08	0.31
(1,1562)	1:44:B:ASP:H	1:40:B:LEU:HD23	2	0.31	0.09	0.31
(1,1562)	1:44:B:ASP:H	1:40:B:LEU:HD22	2	0.31	0.09	0.31
(1,1499)	1:44:A:ASP:H	1:40:A:LEU:HD23	2	0.3	0.08	0.3
(1,1499)	1:44:A:ASP:H	1:40:A:LEU:HD22	2	0.3	0.08	0.3
(1,1500)	1:44:B:ASP:H	1:40:B:LEU:HD23	2	0.3	0.08	0.3
(1,1500)	1:44:B:ASP:H	1:40:B:LEU:HD22	2	0.3	0.08	0.3
(3,147)	1:60:A:GLU:HG3	1:56:A:GLU:H	2	0.3	0.19	0.3
(3,147)	1:60:A:GLU:HG2	1:56:A:GLU:H	2	0.3	0.19	0.3
(3,1167)	1:38:A:LYS:H	1:38:A:LYS:HG3	2	0.28	0.08	0.28
(3,1168)	1:38:B:LYS:H	1:38:B:LYS:HG3	2	0.28	0.08	0.28
(3,669)	1:74:A:LEU:H	1:63:A:MET:HE2	2	0.26	0.04	0.26
(3,669)	1:74:A:LEU:H	1:63:A:MET:HE1	2	0.26	0.04	0.26
(3,670)	1:74:B:LEU:H	1:63:B:MET:HE2	2	0.26	0.04	0.26
(3,670)	1:74:B:LEU:H	1:63:B:MET:HE1	2	0.26	0.04	0.26
(3,711)	1:11:A:ASN:HB2	1:8:A:LEU:HA	2	0.26	0.16	0.26
(3,711)	1:11:A:ASN:HB3	1:8:A:LEU:HA	2	0.26	0.16	0.26
(3,712)	1:11:B:ASN:HB2	1:8:B:LEU:HA	2	0.26	0.16	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,712)	1:11:B:ASN:HB3	1:8:B:LEU:HA	2	0.26	0.16	0.26
(3,777)	1:21:A:GLN:HG2	1:32:A:LEU:HD23	2	0.26	0.16	0.26
(3,777)	1:21:A:GLN:HG2	1:32:A:LEU:HD21	2	0.26	0.16	0.26
(1,1723)	1:81:A:MET:H	1:78:A:GLU:HG2	2	0.26	0.09	0.26
(1,1723)	1:81:A:MET:H	1:83:A:MET:HG2	2	0.26	0.09	0.26
(1,1724)	1:81:B:MET:H	1:78:B:GLU:HG2	2	0.26	0.09	0.26
(1,1724)	1:81:B:MET:H	1:83:B:MET:HG2	2	0.26	0.09	0.26
(1,626)	1:96:B:GLU:HG2	1:97:B:GLY:H	2	0.26	0.04	0.26
(1,626)	1:99:B:GLU:H	1:99:B:GLU:HG3	2	0.26	0.04	0.26
(1,625)	1:96:A:GLU:HG2	1:97:A:GLY:H	2	0.25	0.05	0.25
(1,625)	1:99:A:GLU:H	1:99:A:GLU:HG3	2	0.25	0.05	0.25
(1,735)	1:5:A:MET:HA	1:10:A:ARG:HA	2	0.25	0.05	0.25
(1,736)	1:5:B:MET:HA	1:10:B:ARG:HA	2	0.24	0.04	0.24
(1,1155)	1:32:A:LEU:HG	1:76:A:PHE:HA	2	0.24	0.08	0.24
(1,1156)	1:32:B:LEU:HG	1:76:B:PHE:HA	2	0.24	0.08	0.24
(1,1557)	1:46:A:GLN:H	1:49:A:LEU:HD13	2	0.24	0.05	0.24
(1,1557)	1:46:A:GLN:H	1:49:A:LEU:HD12	2	0.24	0.05	0.24
(1,1558)	1:46:B:GLN:H	1:49:B:LEU:HD13	2	0.24	0.05	0.24
(1,1558)	1:46:B:GLN:H	1:49:B:LEU:HD12	2	0.24	0.05	0.24
(3,552)	1:25:B:LYS:HD2	1:24:B:VAL:HG12	2	0.24	0.04	0.24
(3,552)	1:25:B:LYS:HD2	1:24:B:VAL:HG11	2	0.24	0.04	0.24
(3,1489)	1:103:A:HIS:H	1:101:A:PRO:HB3	2	0.24	0.12	0.24
(3,1489)	1:103:A:HIS:H	1:101:A:PRO:HB2	2	0.24	0.12	0.24
(3,1490)	1:103:B:HIS:H	1:101:B:PRO:HB3	2	0.24	0.12	0.24
(3,1490)	1:103:B:HIS:H	1:101:B:PRO:HB2	2	0.24	0.12	0.24
(1,73)	1:48:A:PHE:HB3	1:86:A:LEU:HG	2	0.24	0.03	0.24
(1,74)	1:48:B:PHE:HB3	1:86:B:LEU:HG	2	0.24	0.03	0.24
(1,1039)	1:85:A:ARG:HA	1:89:A:ALA:HB1	2	0.24	0.09	0.24
(1,1040)	1:85:B:ARG:HA	1:89:B:ALA:HB1	2	0.24	0.09	0.24
(3,551)	1:25:A:LYS:HD2	1:24:A:VAL:HG12	2	0.24	0.04	0.24
(3,551)	1:25:A:LYS:HD2	1:24:A:VAL:HG11	2	0.24	0.04	0.24
(1,715)	1:46:A:GLN:HG2	1:45:A:LEU:HD23	2	0.23	0.13	0.23
(1,715)	1:21:A:GLN:HG2	1:32:A:LEU:HD21	2	0.23	0.13	0.23
(1,1193)	1:47:A:ASN:HB3	1:111:A:GLU:HB3	2	0.22	0.04	0.22
(1,1193)	1:47:A:ASN:HB2	1:111:A:GLU:HB3	2	0.22	0.04	0.22
(1,1194)	1:47:B:ASN:HB3	1:111:B:GLU:HB3	2	0.22	0.04	0.22
(1,1194)	1:47:B:ASN:HB2	1:111:B:GLU:HB3	2	0.22	0.04	0.22
(1,1651)	1:62:A:ILE:H	1:62:A:ILE:HD11	2	0.22	0.08	0.22
(1,1651)	1:62:A:ILE:H	1:62:A:ILE:HD13	2	0.22	0.08	0.22
(1,1652)	1:62:B:ILE:H	1:62:B:ILE:HD11	2	0.22	0.08	0.22
(1,1652)	1:62:B:ILE:H	1:62:B:ILE:HD13	2	0.22	0.08	0.22
(1,1576)	1:49:B:LEU:H	1:49:B:LEU:HD23	2	0.21	0.02	0.21

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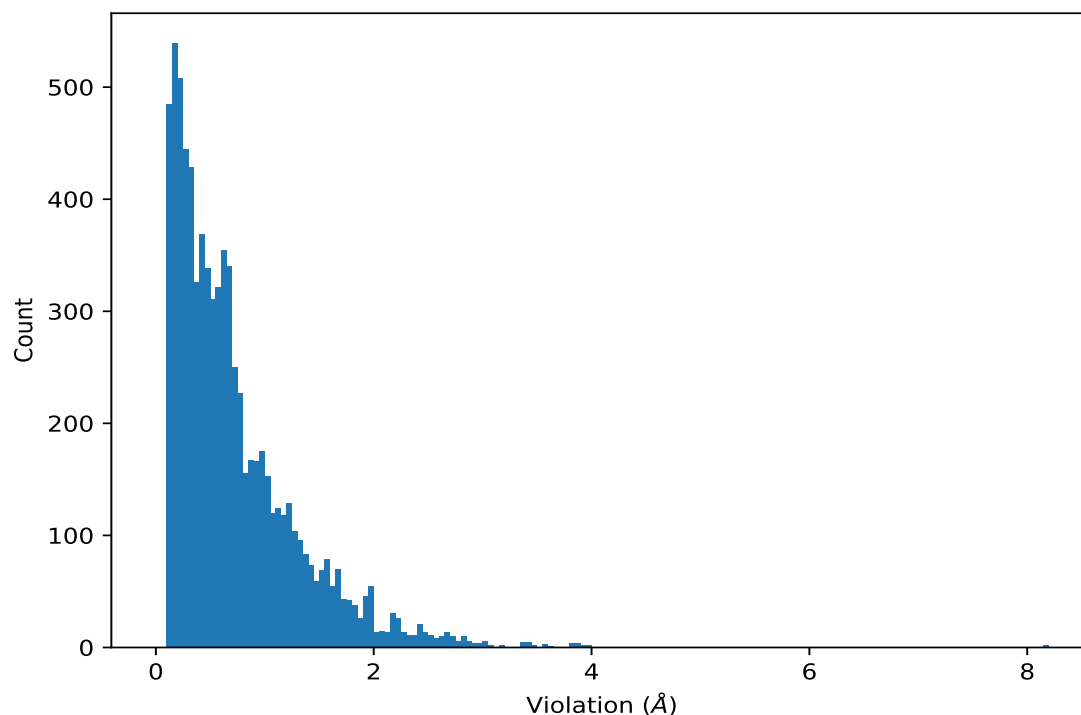
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1576)	1:49:B:LEU:H	1:49:B:LEU:HD22	2	0.21	0.02	0.21
(3,51)	1:39:A:GLU:HG3	1:43:A:LYS:HE2	2	0.21	0.04	0.21
(3,51)	1:39:A:GLU:HG3	1:43:A:LYS:HE3	2	0.21	0.04	0.21
(3,206)	1:44:B:ASP:HA	1:6:A:SER:HB3	2	0.21	0.06	0.21
(3,859)	1:74:A:LEU:H	1:74:A:LEU:HD22	2	0.21	0.02	0.21
(3,860)	1:74:B:LEU:H	1:74:B:LEU:HD22	2	0.21	0.02	0.21
(3,903)	1:72:A:LYS:H	1:72:A:LYS:HD3	2	0.21	0.04	0.21
(3,903)	1:72:A:LYS:H	1:72:A:LYS:HD2	2	0.21	0.04	0.21
(3,904)	1:72:B:LYS:H	1:72:B:LYS:HD3	2	0.21	0.04	0.21
(3,904)	1:72:B:LYS:H	1:72:B:LYS:HD2	2	0.21	0.04	0.21
(3,52)	1:39:B:GLU:HG3	1:43:B:LYS:HE2	2	0.21	0.03	0.21
(3,52)	1:39:B:GLU:HG3	1:43:B:LYS:HE3	2	0.21	0.03	0.21
(1,1575)	1:49:A:LEU:H	1:49:A:LEU:HD23	2	0.2	0.03	0.2
(1,1575)	1:49:A:LEU:H	1:49:A:LEU:HD22	2	0.2	0.03	0.2
(3,205)	1:44:A:ASP:HA	1:6:B:SER:HB3	2	0.2	0.06	0.2
(1,821)	1:46:A:GLN:HG3	1:50:A:LYS:HE2	2	0.18	0.03	0.18
(1,821)	1:46:A:GLN:HG3	1:50:A:LYS:HE3	2	0.18	0.03	0.18
(1,822)	1:46:B:GLN:HG3	1:50:B:LYS:HE2	2	0.17	0.02	0.17
(1,822)	1:46:B:GLN:HG3	1:50:B:LYS:HE3	2	0.17	0.02	0.17
(1,1757)	1:84:A:ALA:H	1:86:A:LEU:H	2	0.16	0.01	0.16
(1,1757)	1:22:A:TYR:H	1:24:A:VAL:H	2	0.16	0.01	0.16
(3,1363)	1:69:A:ASN:H	1:68:A:THR:HB	2	0.16	0.03	0.16
(1,1758)	1:84:B:ALA:H	1:86:B:LEU:H	2	0.16	0.02	0.16
(1,1758)	1:22:B:TYR:H	1:24:B:VAL:H	2	0.16	0.02	0.16
(3,1364)	1:69:B:ASN:H	1:68:B:THR:HB	2	0.16	0.04	0.16
(1,1529)	1:42:A:ARG:H	1:59:A:ILE:HD12	2	0.15	0.03	0.15
(1,1529)	1:42:A:ARG:H	1:49:A:LEU:HD12	2	0.15	0.03	0.15
(1,1530)	1:42:B:ARG:H	1:59:B:ILE:HD12	2	0.15	0.03	0.15
(1,1530)	1:42:B:ARG:H	1:49:B:LEU:HD12	2	0.15	0.03	0.15
(2,62)	1:81:A:MET:H	1:77:A:GLU:O	2	0.15	0.02	0.15
(1,1833)	1:94:A:MET:H	1:90:A:SER:H	2	0.14	0.02	0.14
(1,1834)	1:94:B:MET:H	1:90:B:SER:H	2	0.14	0.02	0.14
(1,759)	1:99:A:GLU:HG3	1:99:A:GLU:HA	2	0.13	0.01	0.13
(1,760)	1:99:B:GLU:HG3	1:99:B:GLU:HA	2	0.13	0.0	0.13
(3,1344)	1:66:B:LEU:H	1:66:B:LEU:HG	2	0.12	0.01	0.12
(2,76)	1:89:A:ALA:H	1:85:A:ARG:O	2	0.12	0.02	0.12
(2,84)	1:93:A:LYS:H	1:89:A:ALA:O	2	0.12	0.0	0.12
(4,231)	1:79:A:PHE:H	1:80:A:ILE:HB	2	0.12	0.0	0.12
(4,232)	1:79:B:PHE:H	1:80:B:ILE:HB	2	0.12	0.0	0.12

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)
(3,794)	1:107:B:PRO:HG2	1:93:B:LYS:HG3	3	8.2
(3,793)	1:107:A:PRO:HG2	1:93:A:LYS:HG3	3	8.2
(1,1202)	1:34:B:GLN:HB3	1:32:B:LEU:HD23	10	3.99
(1,1201)	1:34:A:GLN:HB3	1:32:A:LEU:HD23	10	3.99
(1,1201)	1:34:A:GLN:HB3	1:32:A:LEU:HD23	5	3.92
(1,1202)	1:34:B:GLN:HB3	1:32:B:LEU:HD23	5	3.91
(1,1202)	1:34:B:GLN:HB3	1:32:B:LEU:HD23	4	3.89
(1,1202)	1:34:B:GLN:HB2	1:32:B:LEU:HD11	2	3.88
(1,1201)	1:34:A:GLN:HB3	1:32:A:LEU:HD23	4	3.88
(1,1201)	1:34:A:GLN:HB2	1:32:A:LEU:HD11	2	3.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1202)	1:34:B:GLN:HB3	1:32:B:LEU:HD21	9	3.83
(1,1201)	1:34:A:GLN:HB3	1:32:A:LEU:HD23	6	3.83
(1,1202)	1:34:B:GLN:HB3	1:32:B:LEU:HD23	6	3.82
(1,1201)	1:34:A:GLN:HB3	1:32:A:LEU:HD21	9	3.82
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	5	3.6
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	5	3.59
(1,1202)	1:60:B:GLU:HB2	1:66:B:LEU:HD11	7	3.57
(1,1201)	1:60:A:GLU:HB2	1:66:A:LEU:HD11	7	3.57
(1,1202)	1:34:B:GLN:HB2	1:32:B:LEU:HD12	3	3.49
(1,1201)	1:34:A:GLN:HB2	1:32:A:LEU:HD12	3	3.48
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	1	3.42
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	1	3.42
(1,1078)	1:31:B:THR:HG22	1:25:B:LYS:HG3	5	3.41
(1,1077)	1:31:A:THR:HG22	1:25:A:LYS:HG3	5	3.41
(1,401)	1:38:A:LYS:HD2	1:57:A:LYS:HE3	8	3.4
(1,402)	1:38:B:LYS:HD2	1:57:B:LYS:HE3	8	3.39
(1,1202)	1:60:B:GLU:HB3	1:66:B:LEU:HD12	1	3.37
(1,1201)	1:60:A:GLU:HB3	1:66:A:LEU:HD12	1	3.35
(1,1078)	1:31:B:THR:HG23	1:25:B:LYS:HG3	4	3.35
(1,1077)	1:31:A:THR:HG23	1:25:A:LYS:HG3	4	3.35
(1,208)	1:13:B:GLU:HB2	1:8:B:LEU:HD13	5	3.16
(1,207)	1:13:A:GLU:HB2	1:8:A:LEU:HD13	5	3.16
(1,914)	1:66:B:LEU:HD21	1:64:B:GLU:HG2	9	3.06
(1,913)	1:66:A:LEU:HD21	1:64:A:GLU:HG2	9	3.05
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	6	3.04
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	6	3.04
(1,914)	1:66:B:LEU:HD23	1:64:B:GLU:HG2	6	3.03
(1,1078)	1:31:B:THR:HG22	1:25:B:LYS:HG3	2	3.02
(1,913)	1:66:A:LEU:HD23	1:64:A:GLU:HG2	6	3.02
(1,1077)	1:31:A:THR:HG22	1:25:A:LYS:HG3	2	3.01
(3,738)	1:24:B:VAL:HG21	1:29:B:PRO:HB2	9	2.98
(1,1202)	1:34:B:GLN:HB3	1:32:B:LEU:HD21	8	2.97
(1,1201)	1:34:A:GLN:HB3	1:32:A:LEU:HD21	8	2.97
(3,737)	1:24:A:VAL:HG21	1:29:A:PRO:HB2	9	2.96
(1,836)	1:76:B:PHE:HB2	1:81:B:MET:HB2	9	2.92
(1,835)	1:76:A:PHE:HB2	1:81:A:MET:HB2	9	2.92
(1,402)	1:85:B:ARG:HB3	1:51:B:LYS:HE3	10	2.91
(1,401)	1:85:A:ARG:HB3	1:51:A:LYS:HE3	10	2.91
(1,340)	1:66:B:LEU:HD11	1:76:B:PHE:HA	2	2.88
(1,340)	1:66:B:LEU:HD23	1:76:B:PHE:HA	1	2.86
(1,339)	1:66:A:LEU:HD23	1:76:A:PHE:HA	1	2.86
(1,339)	1:41:A:VAL:HG12	1:6:B:SER:HB3	2	2.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:70:B:ALA:HB3	1:74:B:LEU:HD23	3	2.85
(1,1037)	1:70:A:ALA:HB3	1:74:A:LEU:HD23	3	2.85
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD13	10	2.84
(1,108)	1:7:B:GLN:HG2	1:12:B:ILE:HD13	6	2.84
(1,107)	1:7:A:GLN:HG2	1:12:A:ILE:HD13	6	2.84
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD13	10	2.83
(1,1077)	1:31:A:THR:HG23	1:66:A:LEU:HB3	9	2.82
(1,401)	1:85:A:ARG:HB2	1:51:A:LYS:HE3	7	2.82
(1,1078)	1:31:B:THR:HG23	1:66:B:LEU:HB3	9	2.81
(1,402)	1:85:B:ARG:HB2	1:51:B:LYS:HE3	7	2.81
(1,207)	1:13:A:GLU:HB3	1:8:B:LEU:HD12	2	2.81
(1,208)	1:13:B:GLU:HB3	1:8:A:LEU:HD12	2	2.8
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	3	2.77
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	3	2.77
(1,914)	1:66:B:LEU:HD21	1:64:B:GLU:HG2	2	2.77
(1,913)	1:66:A:LEU:HD21	1:64:A:GLU:HG2	2	2.77
(1,232)	1:12:B:ILE:HG23	1:80:B:ILE:HG21	10	2.77
(1,231)	1:12:A:ILE:HG23	1:80:A:ILE:HG21	10	2.77
(1,138)	1:16:B:ILE:HD13	1:11:B:ASN:HB3	10	2.74
(1,137)	1:16:A:ILE:HD13	1:11:A:ASN:HB3	10	2.74
(3,534)	1:24:B:VAL:HA	1:29:B:PRO:HA	9	2.73
(1,914)	1:66:B:LEU:HD23	1:64:B:GLU:HG2	4	2.73
(1,913)	1:66:A:LEU:HD23	1:64:A:GLU:HG2	4	2.73
(1,1078)	1:31:B:THR:HG21	1:25:B:LYS:HG3	10	2.7
(1,1077)	1:31:A:THR:HG21	1:25:A:LYS:HG3	10	2.7
(1,1038)	1:70:B:ALA:HB1	1:74:B:LEU:HD22	1	2.7
(1,1037)	1:70:A:ALA:HB1	1:74:A:LEU:HD22	1	2.7
(1,56)	1:13:B:GLU:HG3	1:109:A:LEU:HD21	7	2.7
(3,533)	1:24:A:VAL:HA	1:29:A:PRO:HA	9	2.69
(1,55)	1:13:A:GLU:HG3	1:109:B:LEU:HD21	7	2.69
(1,455)	1:7:A:GLN:HB3	1:21:B:GLN:HG2	6	2.68
(1,340)	1:41:B:VAL:HG13	1:6:A:SER:HB3	3	2.68
(1,456)	1:7:B:GLN:HB3	1:21:A:GLN:HG2	6	2.67
(1,339)	1:41:A:VAL:HG13	1:6:B:SER:HB3	3	2.67
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG21	4	2.67
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG21	4	2.67
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD12	3	2.67
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD12	3	2.67
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	4	2.66
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	4	2.65
(1,456)	1:7:B:GLN:HB3	1:46:A:GLN:HG2	4	2.65
(1,207)	1:13:A:GLU:HB2	1:8:A:LEU:HD13	4	2.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:13:B:GLU:HB3	1:8:A:LEU:HD23	1	2.64
(1,208)	1:13:B:GLU:HB2	1:8:B:LEU:HD13	4	2.64
(1,455)	1:7:A:GLN:HB3	1:46:B:GLN:HG2	4	2.63
(1,207)	1:13:A:GLU:HB3	1:8:B:LEU:HD23	1	2.62
(1,1038)	1:70:B:ALA:HB1	1:74:B:LEU:HD21	9	2.61
(1,220)	1:12:B:ILE:HG23	1:19:B:PHE:HB3	8	2.61
(1,219)	1:12:A:ILE:HG23	1:19:A:PHE:HB3	8	2.61
(1,1038)	1:70:B:ALA:HB3	1:74:B:LEU:HD23	6	2.6
(1,1037)	1:70:A:ALA:HB3	1:74:A:LEU:HD23	6	2.6
(1,1037)	1:70:A:ALA:HB1	1:74:A:LEU:HD21	9	2.6
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD11	7	2.59
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD11	7	2.58
(1,208)	1:13:B:GLU:HB2	1:8:B:LEU:HD22	10	2.58
(1,207)	1:13:A:GLU:HB2	1:8:A:LEU:HD22	10	2.58
(1,138)	1:16:B:ILE:HD13	1:11:B:ASN:HB2	3	2.57
(1,137)	1:16:A:ILE:HD13	1:11:A:ASN:HB2	3	2.57
(1,914)	1:66:B:LEU:HD13	1:52:B:GLU:HG2	3	2.55
(1,913)	1:66:A:LEU:HD13	1:52:A:GLU:HG2	3	2.55
(1,914)	1:66:B:LEU:HD12	1:52:B:GLU:HG2	5	2.53
(1,913)	1:66:A:LEU:HD12	1:52:A:GLU:HG2	5	2.53
(1,464)	1:79:B:PHE:HB2	1:22:B:TYR:HB2	8	2.53
(1,463)	1:79:A:PHE:HB2	1:22:A:TYR:HB2	8	2.53
(1,722)	1:77:B:GLU:HB3	1:66:B:LEU:HD23	3	2.51
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD23	7	2.5
(1,1132)	1:54:B:LYS:HE2	1:53:B:ASN:HB3	1	2.5
(1,1131)	1:54:A:LYS:HE2	1:53:A:ASN:HB3	1	2.5
(1,914)	1:66:B:LEU:HD21	1:64:B:GLU:HG2	10	2.5
(1,913)	1:66:A:LEU:HD21	1:64:A:GLU:HG2	10	2.5
(1,721)	1:77:A:GLU:HB3	1:66:A:LEU:HD23	3	2.5
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD23	7	2.49
(1,1038)	1:70:B:ALA:HB1	1:74:B:LEU:HD22	10	2.48
(1,1037)	1:70:A:ALA:HB1	1:74:A:LEU:HD22	10	2.48
(1,208)	1:13:B:GLU:HB2	1:87:A:THR:HG23	9	2.48
(1,207)	1:13:A:GLU:HB2	1:87:B:THR:HG23	9	2.48
(1,108)	1:7:B:GLN:HG3	1:12:B:ILE:HD13	7	2.48
(1,107)	1:7:A:GLN:HG3	1:12:A:ILE:HD13	7	2.48
(1,24)	1:65:B:ASP:HA	1:72:B:LYS:HA	9	2.47
(1,23)	1:65:A:ASP:HA	1:72:A:LYS:HA	9	2.47
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	8	2.46
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	8	2.46
(1,402)	1:92:B:GLU:HB3	1:30:A:ASP:HB2	3	2.46
(1,232)	1:12:B:ILE:HG23	1:80:B:ILE:HG22	1	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:12:A:ILE:HG23	1:80:A:ILE:HG22	1	2.46
(1,1037)	1:70:A:ALA:HB2	1:74:A:LEU:HD23	4	2.44
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG21	9	2.44
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG21	9	2.44
(1,401)	1:92:A:GLU:HB3	1:30:B:ASP:HB2	3	2.44
(1,142)	1:80:B:ILE:HD12	1:83:B:MET:HE1	7	2.44
(1,1038)	1:70:B:ALA:HB2	1:74:B:LEU:HD23	4	2.43
(1,1037)	1:70:A:ALA:HB2	1:74:A:LEU:HD22	2	2.43
(1,141)	1:80:A:ILE:HD12	1:83:A:MET:HE1	7	2.43
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG22	9	2.42
(1,1038)	1:70:B:ALA:HB2	1:74:B:LEU:HD22	2	2.42
(1,1038)	1:70:B:ALA:HB2	1:74:B:LEU:HD22	5	2.41
(1,1037)	1:70:A:ALA:HB2	1:74:A:LEU:HD22	5	2.41
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG22	9	2.4
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG11	1	2.4
(1,340)	1:66:B:LEU:HD11	1:76:B:PHE:HA	9	2.4
(1,339)	1:66:A:LEU:HD11	1:76:A:PHE:HA	9	2.4
(1,232)	1:12:B:ILE:HG22	1:80:B:ILE:HG21	5	2.4
(1,231)	1:12:A:ILE:HG22	1:80:A:ILE:HG21	5	2.4
(1,207)	1:13:A:GLU:HB2	1:87:B:THR:HG23	7	2.4
(1,138)	1:16:B:ILE:HD12	1:11:B:ASN:HB2	2	2.4
(1,137)	1:16:A:ILE:HD12	1:11:A:ASN:HB2	2	2.4
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG11	1	2.39
(1,455)	1:7:A:GLN:HB3	1:46:B:GLN:HG2	7	2.39
(1,208)	1:13:B:GLU:HB2	1:87:A:THR:HG23	7	2.38
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD23	4	2.37
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD23	4	2.37
(1,456)	1:7:B:GLN:HB3	1:46:A:GLN:HG2	7	2.37
(1,1386)	1:18:B:THR:H	1:12:B:ILE:HG23	8	2.36
(1,1385)	1:18:A:THR:H	1:12:A:ILE:HG23	8	2.36
(1,220)	1:12:B:ILE:HG22	1:19:B:PHE:HB2	6	2.36
(1,219)	1:12:A:ILE:HG22	1:19:A:PHE:HB2	6	2.36
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG22	9	2.35
(1,402)	1:42:B:ARG:HB3	1:4:A:LYS:HE2	6	2.34
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG22	9	2.34
(1,108)	1:7:B:GLN:HG2	1:12:B:ILE:HD11	4	2.34
(1,108)	1:34:B:GLN:HG2	1:59:B:ILE:HD11	10	2.34
(1,107)	1:7:A:GLN:HG2	1:12:A:ILE:HD11	4	2.34
(1,107)	1:34:A:GLN:HG2	1:59:A:ILE:HD11	10	2.34
(1,401)	1:42:A:ARG:HB3	1:4:B:LYS:HE2	6	2.31
(1,340)	1:66:B:LEU:HD21	1:76:B:PHE:HA	7	2.31
(1,339)	1:66:A:LEU:HD21	1:76:A:PHE:HA	7	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG23	2	2.3
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG23	2	2.3
(1,402)	1:85:B:ARG:HB3	1:51:B:LYS:HE3	4	2.29
(1,107)	1:34:A:GLN:HG3	1:59:A:ILE:HD11	3	2.29
(1,401)	1:85:A:ARG:HB3	1:51:A:LYS:HE3	4	2.28
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD21	7	2.28
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD21	7	2.28
(1,108)	1:34:B:GLN:HG3	1:59:B:ILE:HD11	3	2.28
(1,1038)	1:70:B:ALA:HB2	1:74:B:LEU:HD21	8	2.27
(1,1037)	1:70:A:ALA:HB2	1:74:A:LEU:HD21	8	2.26
(1,340)	1:66:B:LEU:HD13	1:76:B:PHE:HA	5	2.26
(1,339)	1:66:A:LEU:HD13	1:76:A:PHE:HA	5	2.26
(1,208)	1:13:B:GLU:HB2	1:87:A:THR:HG23	3	2.26
(1,207)	1:13:A:GLU:HB2	1:87:B:THR:HG23	3	2.26
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG22	1	2.25
(1,754)	1:111:B:GLU:HG2	1:4:A:LYS:HE3	2	2.25
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG22	2	2.24
(1,1036)	1:63:B:MET:HE1	1:41:B:VAL:HG22	8	2.24
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG23	1	2.24
(1,1035)	1:63:A:MET:HE1	1:41:A:VAL:HG22	8	2.24
(1,753)	1:111:A:GLU:HG2	1:4:B:LYS:HE3	2	2.24
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG11	6	2.24
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG11	6	2.24
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG13	10	2.23
(1,1078)	1:31:B:THR:HG22	1:25:B:LYS:HG3	1	2.23
(1,1077)	1:31:A:THR:HG22	1:25:A:LYS:HG3	1	2.23
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG23	1	2.23
(1,220)	1:12:B:ILE:HG21	1:19:B:PHE:HB2	10	2.23
(1,219)	1:12:A:ILE:HG21	1:19:A:PHE:HB2	10	2.23
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD22	9	2.23
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG13	10	2.22
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG22	2	2.22
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG21	2	2.22
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG21	2	2.22
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD22	9	2.22
(1,108)	1:34:B:GLN:HG2	1:59:B:ILE:HD12	1	2.22
(1,107)	1:34:A:GLN:HG2	1:59:A:ILE:HD12	1	2.22
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG22	1	2.21
(1,220)	1:12:B:ILE:HG22	1:19:B:PHE:HB2	2	2.21
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG23	3	2.2
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG23	3	2.2
(1,219)	1:12:A:ILE:HG22	1:19:A:PHE:HB2	2	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1386)	1:18:B:THR:H	1:12:B:ILE:HG23	5	2.19
(1,1385)	1:18:A:THR:H	1:12:A:ILE:HG23	5	2.19
(1,753)	1:111:A:GLU:HG3	1:51:A:LYS:HE2	6	2.19
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG12	2	2.19
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG12	2	2.19
(1,340)	1:66:B:LEU:HD12	1:76:B:PHE:HA	10	2.19
(1,339)	1:66:A:LEU:HD12	1:76:A:PHE:HA	10	2.19
(1,207)	1:13:A:GLU:HB3	1:87:B:THR:HG22	8	2.19
(1,138)	1:16:B:ILE:HD11	1:11:B:ASN:HB3	9	2.19
(1,137)	1:16:A:ILE:HD11	1:11:A:ASN:HB3	9	2.19
(1,108)	1:7:B:GLN:HG3	1:12:B:ILE:HD13	2	2.19
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG22	3	2.18
(1,754)	1:92:B:GLU:HG2	1:30:A:ASP:HB2	3	2.18
(1,754)	1:111:B:GLU:HG3	1:51:B:LYS:HE2	6	2.18
(1,208)	1:13:B:GLU:HB3	1:87:A:THR:HG22	8	2.18
(1,107)	1:7:A:GLN:HG3	1:12:A:ILE:HD13	2	2.18
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG22	3	2.17
(1,914)	1:66:B:LEU:HD11	1:64:B:GLU:HG2	8	2.17
(1,913)	1:66:A:LEU:HD11	1:64:A:GLU:HG2	8	2.17
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	6	2.17
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	6	2.17
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD23	2	2.16
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD23	2	2.16
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	6	2.16
(1,464)	1:79:B:PHE:HB2	1:22:B:TYR:HB2	4	2.16
(1,463)	1:79:A:PHE:HB2	1:22:A:TYR:HB2	4	2.16
(1,340)	1:66:B:LEU:HD12	1:76:B:PHE:HA	4	2.16
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	6	2.16
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG22	6	2.15
(1,753)	1:92:A:GLU:HG2	1:30:B:ASP:HB2	3	2.15
(1,339)	1:66:A:LEU:HD12	1:76:A:PHE:HA	4	2.15
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG22	6	2.13
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD13	5	2.12
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD13	5	2.12
(1,1385)	1:18:A:THR:H	1:12:A:ILE:HG21	10	2.11
(1,1077)	1:31:A:THR:HG22	1:68:A:THR:HG22	3	2.11
(1,908)	1:86:B:LEU:HB2	1:9:A:GLU:HG2	1	2.11
(1,907)	1:86:A:LEU:HB2	1:9:B:GLU:HG2	1	2.11
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD12	3	2.11
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD12	3	2.11
(1,1386)	1:18:B:THR:H	1:12:B:ILE:HG21	10	2.1
(1,1078)	1:31:B:THR:HG22	1:68:B:THR:HG22	3	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD12	3	2.1
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD12	3	2.1
(1,107)	1:7:A:GLN:HG2	1:12:A:ILE:HD13	9	2.1
(1,908)	1:86:B:LEU:HB2	1:9:A:GLU:HG3	10	2.09
(1,401)	1:92:A:GLU:HB2	1:51:A:LYS:HE3	9	2.09
(1,108)	1:7:B:GLN:HG2	1:12:B:ILE:HD13	9	2.09
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG13	7	2.08
(1,907)	1:86:A:LEU:HB2	1:9:B:GLU:HG3	10	2.08
(1,402)	1:92:B:GLU:HB2	1:51:B:LYS:HE3	9	2.08
(1,108)	1:7:B:GLN:HG2	1:12:B:ILE:HD13	5	2.08
(1,107)	1:7:A:GLN:HG2	1:12:A:ILE:HD13	5	2.08
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG13	7	2.07
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG23	1	2.06
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG21	10	2.06
(3,534)	1:24:B:VAL:HA	1:29:B:PRO:HA	6	2.05
(3,533)	1:24:A:VAL:HA	1:29:A:PRO:HA	6	2.05
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG21	10	2.05
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD12	4	2.05
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG11	1	2.04
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG11	1	2.04
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD12	4	2.04
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG23	1	2.03
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG11	5	2.02
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG11	5	2.02
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD11	10	2.01
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD11	10	2.01
(1,1214)	1:50:B:LYS:HE2	1:49:B:LEU:HB2	2	2.0
(1,1213)	1:50:A:LYS:HE2	1:49:A:LEU:HB2	2	2.0
(1,464)	1:79:B:PHE:HB2	1:67:B:ASP:HB2	9	2.0
(1,220)	1:12:B:ILE:HG21	1:19:B:PHE:HB2	1	2.0
(1,220)	1:12:B:ILE:HG22	1:19:B:PHE:HB2	9	2.0
(1,219)	1:12:A:ILE:HG21	1:19:A:PHE:HB2	1	2.0
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HG21	6	1.99
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD11	4	1.99
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HG21	6	1.99
(1,1207)	1:34:A:GLN:HB2	1:71:A:ASP:HA	3	1.99
(1,1038)	1:70:B:ALA:HB3	1:74:B:LEU:HD22	7	1.99
(1,1037)	1:70:A:ALA:HB3	1:74:A:LEU:HD22	7	1.99
(1,914)	1:66:B:LEU:HD13	1:64:B:GLU:HG2	1	1.99
(1,913)	1:66:A:LEU:HD13	1:64:A:GLU:HG2	1	1.99
(1,463)	1:79:A:PHE:HB2	1:67:A:ASP:HB2	9	1.99
(1,402)	1:92:B:GLU:HB2	1:51:B:LYS:HE3	2	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:12:A:ILE:HG22	1:19:A:PHE:HB2	9	1.99
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD11	4	1.98
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG23	4	1.98
(1,1208)	1:34:B:GLN:HB2	1:71:B:ASP:HA	3	1.98
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	10	1.98
(1,401)	1:92:A:GLU:HB2	1:51:A:LYS:HE3	2	1.98
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	10	1.98
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB2	6	1.97
(1,1804)	1:109:B:LEU:H	1:49:B:LEU:H	9	1.97
(1,1803)	1:109:A:LEU:H	1:49:A:LEU:H	9	1.97
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG23	4	1.97
(1,1006)	1:109:B:LEU:HD22	1:86:B:LEU:H	5	1.97
(1,1005)	1:109:A:LEU:HD22	1:86:A:LEU:H	5	1.97
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD13	6	1.97
(1,722)	1:77:B:GLU:HB3	1:66:A:LEU:HD22	4	1.97
(1,721)	1:77:A:GLU:HB3	1:66:B:LEU:HD22	4	1.97
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	10	1.97
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD22	2	1.97
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	10	1.97
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB2	6	1.96
(1,1214)	1:50:B:LYS:HE3	1:49:B:LEU:HB2	8	1.96
(1,1213)	1:50:A:LYS:HE3	1:49:A:LEU:HB2	8	1.96
(1,1208)	1:39:B:GLU:HB3	1:32:B:LEU:HA	4	1.96
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD13	6	1.96
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD12	4	1.96
(1,464)	1:79:B:PHE:HB2	1:22:B:TYR:HB2	3	1.96
(1,463)	1:79:A:PHE:HB2	1:22:A:TYR:HB2	3	1.96
(1,400)	1:63:B:MET:HB3	1:72:B:LYS:HE2	9	1.96
(1,399)	1:63:A:MET:HB3	1:72:A:LYS:HE2	9	1.96
(1,340)	1:66:B:LEU:HD13	1:76:B:PHE:HA	6	1.96
(1,339)	1:66:A:LEU:HD13	1:76:A:PHE:HA	6	1.96
(1,220)	1:12:B:ILE:HG22	1:19:B:PHE:HB2	7	1.96
(1,219)	1:12:A:ILE:HG22	1:19:A:PHE:HB2	7	1.96
(1,207)	1:13:A:GLU:HB2	1:8:A:LEU:HD12	6	1.96
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD22	2	1.96
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD12	4	1.96
(1,1207)	1:39:A:GLU:HB3	1:32:A:LEU:HA	4	1.95
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG22	3	1.95
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG22	3	1.95
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD12	4	1.95
(1,455)	1:7:A:GLN:HB3	1:21:B:GLN:HG2	1	1.95
(1,208)	1:13:B:GLU:HB2	1:8:B:LEU:HD12	6	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD21	6	1.95
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD21	6	1.95
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD12	4	1.95
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD13	7	1.94
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD13	7	1.94
(1,1009)	1:8:A:LEU:HD22	1:41:B:VAL:HA	2	1.94
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD13	1	1.94
(1,872)	1:34:B:GLN:HB2	1:64:B:GLU:HG3	8	1.94
(1,871)	1:34:A:GLN:HB2	1:64:A:GLU:HG3	8	1.94
(1,835)	1:76:A:PHE:HB2	1:81:B:MET:HE3	6	1.94
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	2	1.94
(1,220)	1:12:B:ILE:HG22	1:19:B:PHE:HB2	4	1.94
(1,219)	1:12:A:ILE:HG22	1:19:A:PHE:HB2	4	1.94
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	2	1.94
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD13	1	1.93
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD13	1	1.93
(3,738)	1:24:B:VAL:HG21	1:29:B:PRO:HB2	6	1.92
(3,737)	1:24:A:VAL:HG21	1:29:A:PRO:HB2	6	1.92
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG11	4	1.92
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG11	6	1.92
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG11	4	1.92
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG11	6	1.92
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG23	6	1.92
(1,1214)	1:50:B:LYS:HE3	1:49:B:LEU:HB2	4	1.92
(1,1213)	1:50:A:LYS:HE3	1:49:A:LEU:HB2	4	1.92
(1,1010)	1:8:B:LEU:HD22	1:41:A:VAL:HA	2	1.92
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD11	8	1.92
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD11	8	1.92
(1,836)	1:76:B:PHE:HB2	1:81:A:MET:HE3	6	1.92
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	2	1.92
(1,220)	1:12:B:ILE:HG23	1:19:B:PHE:HB3	5	1.92
(1,219)	1:12:A:ILE:HG23	1:19:A:PHE:HB3	5	1.92
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD23	1	1.92
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD23	1	1.92
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	2	1.92
(1,456)	1:7:B:GLN:HB3	1:21:A:GLN:HG2	1	1.91
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG23	6	1.91
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG23	6	1.9
(1,1214)	1:50:B:LYS:HE3	1:49:B:LEU:HB2	1	1.9
(1,1213)	1:50:A:LYS:HE3	1:49:A:LEU:HB2	1	1.9
(1,992)	1:8:B:LEU:HD11	1:20:A:HIS:HB3	2	1.9
(1,991)	1:8:A:LEU:HD11	1:20:B:HIS:HB3	2	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD13	1	1.9
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD21	5	1.9
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG23	6	1.9
(1,220)	1:12:B:ILE:HG22	1:19:B:PHE:HB3	3	1.9
(1,219)	1:12:A:ILE:HG22	1:19:A:PHE:HB3	3	1.9
(1,108)	1:34:B:GLN:HG2	1:59:B:ILE:HD13	8	1.9
(1,107)	1:34:A:GLN:HG2	1:59:A:ILE:HD13	8	1.9
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG12	1	1.89
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG12	1	1.89
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD12	3	1.89
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD12	3	1.89
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG21	5	1.89
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD12	9	1.89
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD12	9	1.89
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD23	8	1.88
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG21	5	1.88
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD21	5	1.88
(1,872)	1:34:B:GLN:HB2	1:71:B:ASP:HB3	4	1.88
(1,871)	1:34:A:GLN:HB2	1:71:A:ASP:HB3	4	1.88
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG22	7	1.88
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD12	9	1.88
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD12	9	1.88
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG23	3	1.87
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD23	8	1.87
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG22	7	1.87
(1,402)	1:85:B:ARG:HB3	1:51:B:LYS:HE3	5	1.87
(1,401)	1:85:A:ARG:HB3	1:51:A:LYS:HE3	5	1.87
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG23	3	1.86
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD11	9	1.86
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD13	10	1.86
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD11	9	1.86
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD13	10	1.86
(1,353)	1:58:A:VAL:HG22	1:54:A:LYS:HA	7	1.85
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG22	5	1.84
(1,1036)	1:63:B:MET:HE2	1:41:B:VAL:HG21	6	1.84
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG22	5	1.84
(1,1035)	1:63:A:MET:HE2	1:41:A:VAL:HG21	6	1.84
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD12	9	1.84
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD12	9	1.84
(1,354)	1:58:B:VAL:HG22	1:54:B:LYS:HA	7	1.84
(3,256)	1:33:B:ASN:HB3	1:31:B:THR:HG21	6	1.83
(1,1056)	1:33:B:ASN:HB3	1:31:B:THR:HG21	6	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:51:B:LYS:HE3	1:41:B:VAL:HG11	5	1.83
(1,513)	1:51:A:LYS:HE3	1:41:A:VAL:HG11	5	1.83
(3,255)	1:33:A:ASN:HB3	1:31:A:THR:HG21	6	1.82
(1,1208)	1:39:B:GLU:HB3	1:32:B:LEU:HA	8	1.82
(1,1207)	1:39:A:GLU:HB3	1:32:A:LEU:HA	8	1.82
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD12	2	1.82
(1,1055)	1:33:A:ASN:HB3	1:31:A:THR:HG21	6	1.82
(1,1005)	1:8:A:LEU:HD21	1:22:B:TYR:H	3	1.82
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG21	2	1.82
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG21	2	1.82
(1,464)	1:79:B:PHE:HB2	1:22:B:TYR:HB2	6	1.82
(1,463)	1:79:A:PHE:HB2	1:22:A:TYR:HB2	6	1.82
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	9	1.82
(3,190)	1:93:B:LYS:HG3	1:109:B:LEU:HD22	3	1.81
(3,189)	1:93:A:LYS:HG3	1:109:A:LEU:HD22	3	1.81
(1,1213)	1:50:A:LYS:HE3	1:49:A:LEU:HB2	6	1.81
(1,514)	1:51:B:LYS:HE3	1:41:B:VAL:HG13	3	1.81
(1,513)	1:51:A:LYS:HE3	1:41:A:VAL:HG13	3	1.81
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	9	1.81
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD21	8	1.8
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD21	8	1.8
(1,1214)	1:50:B:LYS:HE3	1:49:B:LEU:HB2	6	1.8
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG22	4	1.8
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD12	2	1.8
(1,1006)	1:8:B:LEU:HD21	1:22:A:TYR:H	3	1.8
(1,835)	1:76:A:PHE:HB2	1:81:B:MET:HB2	1	1.8
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	1	1.8
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD13	1	1.8
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD13	9	1.8
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG22	4	1.79
(1,770)	1:37:B:PHE:HB3	1:59:B:ILE:HD13	7	1.79
(1,769)	1:37:A:PHE:HB3	1:59:A:ILE:HD13	7	1.79
(1,522)	1:49:B:LEU:HB2	1:86:B:LEU:HG	7	1.79
(1,521)	1:49:A:LEU:HB2	1:86:A:LEU:HG	7	1.79
(1,488)	1:85:B:ARG:HG3	1:80:A:ILE:HD11	5	1.79
(1,120)	1:85:B:ARG:HG3	1:80:A:ILE:HD11	5	1.79
(1,104)	1:7:B:GLN:HG2	1:15:A:ILE:HG21	4	1.79
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD13	9	1.79
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG23	9	1.78
(1,836)	1:76:B:PHE:HB2	1:81:A:MET:HB2	1	1.78
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	1	1.78
(1,487)	1:85:A:ARG:HG3	1:80:B:ILE:HD11	5	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG3	1	1.78
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG3	1	1.78
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD13	1	1.78
(1,119)	1:85:A:ARG:HG3	1:80:B:ILE:HD11	5	1.78
(3,494)	1:59:B:ILE:HD11	1:38:B:LYS:HE2	3	1.77
(3,493)	1:59:A:ILE:HD11	1:38:A:LYS:HE2	3	1.77
(1,103)	1:7:A:GLN:HG2	1:15:B:ILE:HG21	4	1.77
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG23	9	1.76
(1,1148)	1:32:B:LEU:HG	1:24:B:VAL:HG12	8	1.76
(1,1147)	1:32:A:LEU:HG	1:24:A:VAL:HG12	8	1.76
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD12	7	1.76
(1,1078)	1:31:B:THR:HG22	1:25:B:LYS:HG3	7	1.76
(1,1077)	1:31:A:THR:HG22	1:25:A:LYS:HG3	7	1.76
(1,722)	1:77:B:GLU:HB3	1:66:B:LEU:HD22	5	1.76
(1,462)	1:32:B:LEU:HG	1:24:B:VAL:HG12	8	1.76
(1,461)	1:32:A:LEU:HG	1:24:A:VAL:HG12	8	1.76
(1,276)	1:19:B:PHE:HB2	1:13:B:GLU:HA	10	1.76
(1,275)	1:19:A:PHE:HB2	1:13:A:GLU:HA	10	1.76
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD12	10	1.76
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD12	10	1.76
(1,105)	1:7:A:GLN:HG3	1:15:B:ILE:HD13	7	1.76
(1,1386)	1:18:B:THR:H	1:87:A:THR:HG23	7	1.75
(1,1385)	1:18:A:THR:H	1:87:B:THR:HG23	7	1.75
(1,1208)	1:39:B:GLU:HB3	1:32:B:LEU:HA	1	1.75
(1,1207)	1:39:A:GLU:HB3	1:32:A:LEU:HA	1	1.75
(1,721)	1:77:A:GLU:HB3	1:66:A:LEU:HD22	5	1.75
(1,522)	1:49:B:LEU:HB3	1:82:B:LEU:HG	3	1.75
(1,106)	1:7:B:GLN:HG3	1:15:A:ILE:HD13	7	1.75
(1,56)	1:13:B:GLU:HG2	1:86:A:LEU:HD13	9	1.75
(1,521)	1:49:A:LEU:HB3	1:82:A:LEU:HG	3	1.74
(1,402)	1:92:B:GLU:HB2	1:51:B:LYS:HE3	1	1.74
(1,401)	1:92:A:GLU:HB2	1:51:A:LYS:HE3	1	1.74
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD12	8	1.74
(1,55)	1:13:A:GLU:HG2	1:86:B:LEU:HD13	9	1.74
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD12	1	1.73
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD12	1	1.73
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD22	5	1.73
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD22	5	1.73
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD12	7	1.73
(1,722)	1:77:B:GLU:HB2	1:74:B:LEU:HD22	9	1.73
(1,721)	1:77:A:GLU:HB2	1:74:A:LEU:HD22	9	1.73
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG12	9	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG12	9	1.73
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD12	8	1.73
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD22	2	1.72
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD22	2	1.72
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG13	9	1.72
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG13	9	1.72
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD11	1	1.72
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD11	1	1.72
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD11	4	1.72
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD12	7	1.72
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD11	4	1.72
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD12	7	1.72
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD22	6	1.71
(1,913)	1:66:A:LEU:HD12	1:64:A:GLU:HG2	7	1.71
(1,522)	1:49:B:LEU:HB2	1:86:B:LEU:HG	4	1.71
(1,521)	1:49:A:LEU:HB2	1:86:A:LEU:HG	4	1.71
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	7	1.71
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	7	1.71
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD22	6	1.7
(1,1214)	1:50:B:LYS:HE3	1:49:B:LEU:HB2	5	1.7
(1,1213)	1:50:A:LYS:HE3	1:49:A:LEU:HB2	5	1.7
(1,1208)	1:34:B:GLN:HB2	1:71:B:ASP:HA	7	1.7
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD13	6	1.7
(1,914)	1:66:B:LEU:HD12	1:64:B:GLU:HG2	7	1.7
(1,464)	1:79:B:PHE:HB3	1:67:B:ASP:HB2	10	1.7
(1,463)	1:79:A:PHE:HB3	1:67:A:ASP:HB2	10	1.7
(1,276)	1:19:B:PHE:HB2	1:13:B:GLU:HA	2	1.7
(1,275)	1:19:A:PHE:HB2	1:13:A:GLU:HA	2	1.7
(1,42)	1:78:B:GLU:HG2	1:76:B:PHE:HA	3	1.7
(1,41)	1:78:A:GLU:HG2	1:76:A:PHE:HA	3	1.7
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD13	9	1.69
(1,1207)	1:34:A:GLN:HB2	1:71:A:ASP:HA	7	1.69
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD13	6	1.69
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD23	1	1.69
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD21	10	1.69
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD23	1	1.69
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD21	10	1.69
(1,871)	1:34:A:GLN:HB2	1:71:A:ASP:HB3	10	1.69
(1,522)	1:49:B:LEU:HB3	1:82:B:LEU:HG	1	1.69
(1,521)	1:49:A:LEU:HB3	1:82:A:LEU:HG	1	1.69
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG12	2	1.68
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG12	2	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD13	9	1.68
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	10	1.68
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	10	1.68
(1,1208)	1:34:B:GLN:HB2	1:71:B:ASP:HA	2	1.68
(1,1207)	1:34:A:GLN:HB2	1:71:A:ASP:HA	5	1.68
(1,872)	1:34:B:GLN:HB2	1:71:B:ASP:HB3	10	1.68
(1,722)	1:77:B:GLU:HB2	1:74:B:LEU:HD22	8	1.68
(1,721)	1:77:A:GLU:HB2	1:74:A:LEU:HD22	8	1.68
(1,624)	1:19:B:PHE:HB2	1:21:B:GLN:HA	6	1.68
(1,623)	1:19:A:PHE:HB2	1:21:A:GLN:HA	6	1.68
(1,462)	1:10:B:ARG:HG2	1:12:B:ILE:HD12	6	1.68
(1,276)	1:19:B:PHE:HB2	1:21:B:GLN:HA	6	1.68
(1,276)	1:19:B:PHE:HB2	1:21:B:GLN:HA	9	1.68
(1,275)	1:19:A:PHE:HB2	1:21:A:GLN:HA	6	1.68
(1,275)	1:19:A:PHE:HB2	1:21:A:GLN:HA	9	1.68
(1,226)	1:12:B:ILE:HG21	1:45:A:LEU:HG	8	1.68
(1,225)	1:12:A:ILE:HG21	1:45:B:LEU:HG	8	1.68
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG11	8	1.67
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG11	8	1.67
(1,1208)	1:34:B:GLN:HB2	1:71:B:ASP:HA	5	1.67
(1,1207)	1:34:A:GLN:HB2	1:71:A:ASP:HA	2	1.67
(1,722)	1:77:B:GLU:HB2	1:74:B:LEU:HD23	7	1.67
(1,721)	1:77:A:GLU:HB2	1:74:A:LEU:HD23	7	1.67
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD12	5	1.67
(1,461)	1:10:A:ARG:HG2	1:12:A:ILE:HD12	6	1.67
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD13	2	1.67
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD13	2	1.67
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD11	6	1.67
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD11	6	1.67
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD12	5	1.66
(1,354)	1:58:B:VAL:HG23	1:54:B:LYS:HA	1	1.66
(1,354)	1:58:B:VAL:HG21	1:54:B:LYS:HA	5	1.66
(1,353)	1:58:A:VAL:HG23	1:54:A:LYS:HA	1	1.66
(1,353)	1:58:A:VAL:HG21	1:54:A:LYS:HA	5	1.66
(1,276)	1:19:B:PHE:HB3	1:13:B:GLU:HA	3	1.66
(1,275)	1:19:A:PHE:HB3	1:13:A:GLU:HA	3	1.66
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD22	5	1.66
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD22	5	1.66
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD22	8	1.66
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD22	8	1.66
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD13	5	1.66
(1,4)	1:73:B:GLN:HG2	1:75:B:SER:HB2	8	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:94:B:MET:H	1:89:B:ALA:HB2	7	1.65
(1,1819)	1:94:A:MET:H	1:89:A:ALA:HB2	7	1.65
(1,1804)	1:93:B:LYS:H	1:88:B:TRP:H	6	1.65
(1,1214)	1:50:B:LYS:HE3	1:49:B:LEU:HB2	3	1.65
(1,1213)	1:50:A:LYS:HE3	1:49:A:LEU:HB2	3	1.65
(1,872)	1:34:B:GLN:HB2	1:64:B:GLU:HG3	5	1.65
(1,871)	1:34:A:GLN:HB2	1:64:A:GLU:HG3	5	1.65
(1,442)	1:10:B:ARG:HG2	1:4:B:LYS:HG3	8	1.65
(1,441)	1:10:A:ARG:HG2	1:4:A:LYS:HG3	8	1.65
(1,354)	1:58:B:VAL:HG21	1:54:B:LYS:HA	4	1.65
(1,354)	1:58:B:VAL:HG22	1:54:B:LYS:HA	8	1.65
(1,353)	1:58:A:VAL:HG21	1:54:A:LYS:HA	4	1.65
(1,353)	1:58:A:VAL:HG22	1:54:A:LYS:HA	8	1.65
(1,226)	1:12:B:ILE:HG23	1:45:A:LEU:HG	2	1.65
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD13	5	1.65
(1,3)	1:73:A:GLN:HG2	1:75:A:SER:HB2	8	1.65
(1,1803)	1:93:A:LYS:H	1:88:A:TRP:H	6	1.64
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD12	2	1.64
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD12	2	1.64
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG3	1	1.64
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG3	1	1.64
(1,354)	1:58:B:VAL:HG23	1:54:B:LYS:HA	6	1.64
(1,353)	1:58:A:VAL:HG23	1:54:A:LYS:HA	6	1.64
(1,276)	1:19:B:PHE:HB3	1:40:B:LEU:HA	1	1.64
(1,275)	1:19:A:PHE:HB3	1:40:A:LEU:HA	1	1.64
(1,225)	1:12:A:ILE:HG23	1:45:B:LEU:HG	2	1.64
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD11	5	1.64
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD12	4	1.63
(1,990)	1:48:B:PHE:HB3	1:13:A:GLU:H	10	1.63
(1,989)	1:48:A:PHE:HB3	1:13:B:GLU:H	10	1.63
(1,862)	1:25:B:LYS:HD3	1:33:B:ASN:HB3	1	1.63
(1,861)	1:25:A:LYS:HD3	1:33:A:ASN:HB3	1	1.63
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG3	3	1.63
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG3	3	1.63
(1,288)	1:9:B:GLU:HB3	1:11:B:ASN:HA	1	1.63
(1,287)	1:9:A:GLU:HB3	1:11:A:ASN:HA	1	1.63
(1,226)	1:12:B:ILE:HG23	1:45:A:LEU:HG	9	1.63
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD12	4	1.63
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD11	5	1.63
(1,68)	1:48:B:PHE:HB3	1:13:A:GLU:H	10	1.63
(1,67)	1:48:A:PHE:HB3	1:13:B:GLU:H	10	1.63
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD12	4	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:11:B:ASN:HB2	1:5:B:MET:HG2	2	1.62
(1,463)	1:11:A:ASN:HB2	1:5:A:MET:HG2	2	1.62
(1,225)	1:12:A:ILE:HG23	1:45:B:LEU:HG	9	1.62
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD12	4	1.62
(1,104)	1:7:B:GLN:HG2	1:15:A:ILE:HG22	10	1.62
(1,103)	1:7:A:GLN:HG2	1:15:B:ILE:HG22	10	1.62
(1,42)	1:78:B:GLU:HG3	1:76:B:PHE:HA	2	1.62
(1,41)	1:78:A:GLU:HG3	1:76:A:PHE:HA	2	1.62
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG13	3	1.61
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD12	10	1.61
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD21	6	1.61
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD21	6	1.61
(1,514)	1:51:B:LYS:HE3	1:41:B:VAL:HG11	8	1.61
(1,513)	1:51:A:LYS:HE3	1:41:A:VAL:HG11	8	1.61
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG3	9	1.61
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG3	9	1.61
(1,226)	1:12:B:ILE:HG21	1:45:A:LEU:HG	5	1.61
(1,225)	1:12:A:ILE:HG21	1:45:B:LEU:HG	5	1.61
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG13	3	1.6
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD12	10	1.6
(1,1129)	1:30:A:ASP:HB3	1:76:A:PHE:HA	10	1.6
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	9	1.6
(1,955)	1:21:A:GLN:HB2	1:32:A:LEU:HD22	8	1.6
(1,399)	1:63:A:MET:HB3	1:72:A:LYS:HE2	1	1.6
(1,390)	1:16:B:ILE:HD13	1:10:B:ARG:HA	8	1.6
(1,389)	1:16:A:ILE:HD13	1:10:A:ARG:HA	8	1.6
(1,192)	1:77:B:GLU:HA	1:66:B:LEU:HD22	8	1.6
(1,191)	1:77:A:GLU:HA	1:66:A:LEU:HD22	8	1.6
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	9	1.6
(1,1130)	1:30:B:ASP:HB3	1:76:B:PHE:HA	10	1.59
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	9	1.59
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD13	2	1.59
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD13	2	1.59
(1,956)	1:21:B:GLN:HB2	1:32:B:LEU:HD22	8	1.59
(1,562)	1:16:B:ILE:HB	1:12:B:ILE:HG12	5	1.59
(1,561)	1:16:A:ILE:HB	1:12:A:ILE:HG12	5	1.59
(1,512)	1:51:B:LYS:HE2	1:58:B:VAL:HG22	2	1.59
(1,511)	1:51:A:LYS:HE2	1:58:A:VAL:HG22	2	1.59
(1,400)	1:63:B:MET:HB3	1:72:B:LYS:HE2	1	1.59
(1,354)	1:58:B:VAL:HG22	1:54:B:LYS:HA	10	1.59
(1,353)	1:58:A:VAL:HG22	1:54:A:LYS:HA	10	1.59
(1,226)	1:12:B:ILE:HG21	1:80:B:ILE:HB	3	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:12:A:ILE:HG21	1:80:A:ILE:HB	3	1.59
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	9	1.59
(1,24)	1:65:B:ASP:HA	1:72:B:LYS:HA	1	1.59
(1,23)	1:65:A:ASP:HA	1:72:A:LYS:HA	1	1.59
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD21	9	1.58
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD21	9	1.58
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG13	5	1.58
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG13	5	1.58
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD12	8	1.58
(1,720)	1:77:B:GLU:HB2	1:68:B:THR:HG22	7	1.58
(1,719)	1:77:A:GLU:HB2	1:68:A:THR:HG22	7	1.58
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD13	3	1.58
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD13	3	1.58
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	7	1.58
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	9	1.58
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	7	1.58
(1,354)	1:58:B:VAL:HG23	1:54:B:LYS:HA	9	1.58
(1,353)	1:58:A:VAL:HG23	1:54:A:LYS:HA	9	1.58
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD13	3	1.58
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD13	3	1.58
(1,1804)	1:16:B:ILE:H	1:87:A:THR:H	7	1.57
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD12	3	1.57
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD12	3	1.57
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HG22	2	1.57
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD12	8	1.57
(1,722)	1:77:B:GLU:HB3	1:66:B:LEU:HD22	10	1.57
(1,721)	1:77:A:GLU:HB3	1:66:A:LEU:HD22	10	1.57
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD13	4	1.57
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD13	4	1.57
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	9	1.57
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD13	4	1.57
(1,1803)	1:16:A:ILE:H	1:87:B:THR:H	7	1.56
(1,1586)	1:51:B:LYS:H	1:41:B:VAL:HG12	9	1.56
(1,1585)	1:51:A:LYS:H	1:41:A:VAL:HG12	9	1.56
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HG22	2	1.56
(1,1213)	1:49:A:LEU:HB2	1:54:A:LYS:HE3	10	1.56
(1,1208)	1:39:B:GLU:HB3	1:32:B:LEU:HA	9	1.56
(1,1207)	1:39:A:GLU:HB3	1:32:A:LEU:HA	9	1.56
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD13	3	1.56
(1,984)	1:48:B:PHE:HB3	1:40:B:LEU:HD11	7	1.56
(1,983)	1:48:A:PHE:HB3	1:40:A:LEU:HD11	7	1.56
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD21	4	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD21	4	1.56
(1,514)	1:51:B:LYS:HE3	1:41:B:VAL:HG13	7	1.56
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD13	4	1.56
(1,276)	1:19:B:PHE:HB3	1:13:B:GLU:HA	8	1.56
(1,275)	1:19:A:PHE:HB3	1:13:A:GLU:HA	8	1.56
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD11	10	1.56
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD11	10	1.56
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD13	2	1.55
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD13	2	1.55
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HG21	9	1.55
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HG21	9	1.55
(1,1214)	1:49:B:LEU:HB2	1:54:B:LYS:HE3	10	1.55
(1,1006)	1:8:B:LEU:HD21	1:22:A:TYR:H	4	1.55
(1,1005)	1:8:A:LEU:HD21	1:22:B:TYR:H	4	1.55
(1,984)	1:48:B:PHE:HB2	1:16:A:ILE:HD12	4	1.55
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD13	3	1.55
(1,754)	1:92:B:GLU:HG3	1:51:B:LYS:HE3	10	1.55
(1,753)	1:92:A:GLU:HG3	1:51:A:LYS:HE3	10	1.55
(1,722)	1:77:B:GLU:HB2	1:74:B:LEU:HD23	1	1.55
(1,721)	1:77:A:GLU:HB2	1:74:A:LEU:HD23	1	1.55
(1,513)	1:51:A:LYS:HE3	1:41:A:VAL:HG13	7	1.55
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG3	5	1.55
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG3	5	1.55
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG3	7	1.55
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	4	1.54
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	4	1.54
(1,1208)	1:34:B:GLN:HB2	1:71:B:ASP:HA	10	1.54
(1,1036)	1:63:B:MET:HE1	1:41:B:VAL:HG23	4	1.54
(1,1035)	1:63:A:MET:HE1	1:41:A:VAL:HG23	4	1.54
(1,983)	1:48:A:PHE:HB2	1:16:B:ILE:HD12	4	1.54
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD22	9	1.54
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD22	9	1.54
(1,360)	1:77:B:GLU:HB2	1:31:B:THR:HG22	3	1.54
(1,359)	1:77:A:GLU:HB2	1:31:A:THR:HG22	3	1.54
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG3	7	1.54
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD13	2	1.54
(1,226)	1:62:B:ILE:HG22	1:32:B:LEU:HB2	10	1.54
(1,225)	1:62:A:ILE:HG22	1:32:A:LEU:HB2	10	1.54
(1,106)	1:7:B:GLN:HG3	1:15:A:ILE:HD13	8	1.54
(1,105)	1:7:A:GLN:HG3	1:15:B:ILE:HD13	8	1.54
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD12	2	1.53
(1,1207)	1:34:A:GLN:HB2	1:71:A:ASP:HA	10	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG23	9	1.53
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG22	7	1.53
(1,722)	1:77:B:GLU:HB2	1:66:B:LEU:HD21	6	1.53
(1,721)	1:77:A:GLU:HB2	1:66:A:LEU:HD21	6	1.53
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG21	10	1.53
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG21	10	1.53
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG13	8	1.53
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG13	8	1.53
(1,226)	1:62:B:ILE:HG23	1:32:B:LEU:HB2	6	1.53
(1,225)	1:62:A:ILE:HG23	1:32:A:LEU:HB2	6	1.53
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD11	9	1.52
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD12	2	1.52
(1,1208)	1:34:B:GLN:HB2	1:71:B:ASP:HA	6	1.52
(1,1207)	1:34:A:GLN:HB2	1:71:A:ASP:HA	6	1.52
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG22	7	1.52
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG23	9	1.52
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG21	5	1.52
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG21	5	1.52
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD13	5	1.52
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD13	2	1.52
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD13	9	1.52
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD13	9	1.52
(1,42)	1:78:B:GLU:HG2	1:76:B:PHE:HA	6	1.52
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD12	7	1.51
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD12	7	1.51
(3,816)	1:51:B:LYS:HG2	1:109:B:LEU:HD21	10	1.51
(3,815)	1:51:A:LYS:HG2	1:109:A:LEU:HD21	10	1.51
(1,1804)	1:109:B:LEU:H	1:113:B:THR:H	8	1.51
(1,1803)	1:109:A:LEU:H	1:113:A:THR:H	8	1.51
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG23	6	1.51
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG23	6	1.51
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD11	9	1.51
(1,1214)	1:50:B:LYS:HE2	1:49:B:LEU:HB2	9	1.51
(1,1213)	1:50:A:LYS:HE2	1:49:A:LEU:HB2	9	1.51
(1,988)	1:48:B:PHE:HB3	1:109:B:LEU:H	8	1.51
(1,987)	1:48:A:PHE:HB3	1:109:A:LEU:H	8	1.51
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD22	7	1.51
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD22	7	1.51
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG13	10	1.51
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	5	1.51
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	5	1.51
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD13	5	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG2	8	1.51
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG2	8	1.51
(1,41)	1:78:A:GLU:HG2	1:76:A:PHE:HA	6	1.51
(1,1097)	1:59:A:ILE:HG22	1:42:A:ARG:HD2	9	1.5
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD22	3	1.5
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD22	3	1.5
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG13	10	1.5
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG3	4	1.5
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG3	4	1.5
(1,1803)	1:109:A:LEU:H	1:5:B:MET:H	1	1.49
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG22	4	1.49
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG22	4	1.49
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD13	3	1.49
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD13	3	1.49
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD13	6	1.49
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD13	6	1.49
(1,1098)	1:59:B:ILE:HG22	1:42:B:ARG:HD2	9	1.49
(1,956)	1:21:B:GLN:HB3	1:32:B:LEU:HD21	5	1.49
(1,955)	1:21:A:GLN:HB3	1:32:A:LEU:HD21	5	1.49
(1,796)	1:111:B:GLU:HA	1:10:A:ARG:HG2	2	1.49
(1,795)	1:111:A:GLU:HA	1:10:B:ARG:HG2	2	1.49
(1,458)	1:111:B:GLU:HA	1:10:A:ARG:HG2	2	1.49
(1,457)	1:111:A:GLU:HA	1:10:B:ARG:HG2	2	1.49
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG3	10	1.49
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD12	5	1.48
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD12	5	1.48
(1,758)	1:96:B:GLU:HG2	1:107:B:PRO:HD2	10	1.48
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG3	7	1.48
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG3	7	1.48
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG3	10	1.48
(1,288)	1:9:B:GLU:HB2	1:11:B:ASN:HA	2	1.48
(1,287)	1:9:A:GLU:HB2	1:11:A:ASN:HA	2	1.48
(1,276)	1:19:B:PHE:HB2	1:21:B:GLN:HA	4	1.48
(1,275)	1:19:A:PHE:HB2	1:21:A:GLN:HA	4	1.48
(1,103)	1:7:A:GLN:HG2	1:15:B:ILE:HG23	1	1.48
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG12	7	1.47
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG12	7	1.47
(1,1098)	1:59:B:ILE:HG22	1:42:B:ARG:HD2	4	1.47
(1,1097)	1:59:A:ILE:HG22	1:42:A:ARG:HD2	4	1.47
(1,757)	1:96:A:GLU:HG2	1:107:A:PRO:HD2	10	1.47
(1,600)	1:18:B:THR:HG22	1:11:A:ASN:HB2	5	1.47
(1,599)	1:18:A:THR:HG22	1:11:B:ASN:HB2	5	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:7:B:GLN:HG2	1:15:A:ILE:HG23	1	1.47
(3,186)	1:19:B:PHE:HB3	1:83:B:MET:HG3	9	1.46
(3,185)	1:19:A:PHE:HB3	1:83:A:MET:HG3	9	1.46
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD22	3	1.46
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD12	5	1.46
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	6	1.46
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD22	2	1.46
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD22	2	1.46
(1,118)	1:66:B:LEU:HG	1:62:B:ILE:HD12	7	1.46
(1,117)	1:66:A:LEU:HG	1:62:A:ILE:HD12	7	1.46
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	6	1.46
(3,255)	1:33:A:ASN:HB3	1:31:A:THR:HG22	8	1.45
(3,186)	1:19:B:PHE:HB3	1:83:B:MET:HG2	4	1.45
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	8	1.45
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD12	5	1.45
(1,1055)	1:33:A:ASN:HB3	1:31:A:THR:HG22	8	1.45
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	6	1.45
(1,360)	1:46:B:GLN:HB3	1:59:B:ILE:HD13	1	1.45
(1,359)	1:46:A:GLN:HB3	1:59:A:ILE:HD13	1	1.45
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG2	3	1.45
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG2	3	1.45
(1,230)	1:12:B:ILE:HG21	1:15:B:ILE:HG23	4	1.45
(1,229)	1:12:A:ILE:HG21	1:15:A:ILE:HG23	4	1.45
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	6	1.45
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	6	1.45
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	6	1.45
(3,256)	1:33:B:ASN:HB3	1:31:B:THR:HG22	8	1.44
(3,185)	1:19:A:PHE:HB3	1:83:A:MET:HG2	4	1.44
(1,1804)	1:109:B:LEU:H	1:5:A:MET:H	1	1.44
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD22	3	1.44
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	8	1.44
(1,1097)	1:59:A:ILE:HG22	1:42:A:ARG:HD2	1	1.44
(1,1056)	1:33:B:ASN:HB3	1:31:B:THR:HG22	8	1.44
(1,106)	1:7:B:GLN:HG3	1:15:A:ILE:HD11	3	1.44
(1,105)	1:7:A:GLN:HG3	1:15:B:ILE:HD11	3	1.44
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG3	2	1.43
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG3	2	1.43
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD13	10	1.43
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD13	10	1.43
(1,1098)	1:59:B:ILE:HG22	1:42:B:ARG:HD2	1	1.43
(1,835)	1:76:A:PHE:HB2	1:29:A:PRO:HB2	8	1.43
(1,522)	1:49:B:LEU:HB2	1:86:B:LEU:HG	2	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	1:49:A:LEU:HB2	1:86:A:LEU:HG	2	1.43
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG2	7	1.42
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG2	7	1.42
(3,84)	1:87:B:THR:HG23	1:92:B:GLU:HG2	8	1.42
(3,83)	1:87:A:THR:HG23	1:92:A:GLU:HG2	8	1.42
(1,1035)	1:63:A:MET:HE3	1:41:A:VAL:HG21	7	1.42
(1,836)	1:76:B:PHE:HB2	1:29:B:PRO:HB2	8	1.42
(1,744)	1:87:B:THR:HG23	1:92:B:GLU:HG2	8	1.42
(1,743)	1:87:A:THR:HG23	1:92:A:GLU:HG2	8	1.42
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	6	1.42
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	7	1.42
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	6	1.42
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	7	1.42
(1,522)	1:49:B:LEU:HB2	1:86:B:LEU:HG	8	1.42
(1,521)	1:49:A:LEU:HB2	1:86:A:LEU:HG	8	1.42
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD13	6	1.42
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD13	6	1.42
(1,230)	1:12:B:ILE:HG23	1:80:B:ILE:HD12	10	1.42
(1,229)	1:12:A:ILE:HG23	1:80:A:ILE:HD12	10	1.42
(1,70)	1:48:B:PHE:HB3	1:53:B:ASN:HB2	3	1.42
(1,69)	1:48:A:PHE:HB3	1:53:A:ASN:HB2	3	1.42
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	1	1.42
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	1	1.42
(1,1776)	1:87:B:THR:H	1:16:A:ILE:HB	1	1.41
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD11	4	1.41
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD11	4	1.41
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD13	10	1.41
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD13	10	1.41
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD13	5	1.41
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD13	5	1.41
(1,1218)	1:87:B:THR:HG21	1:83:B:MET:HB3	5	1.41
(1,1217)	1:87:A:THR:HG21	1:83:A:MET:HB3	5	1.41
(1,1036)	1:63:B:MET:HE3	1:41:B:VAL:HG21	7	1.41
(1,988)	1:48:B:PHE:HB2	1:5:A:MET:H	5	1.41
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	8	1.41
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	8	1.41
(1,464)	1:79:B:PHE:HB3	1:81:B:MET:HG2	5	1.41
(1,340)	1:66:B:LEU:HD22	1:76:B:PHE:HA	8	1.41
(1,339)	1:66:A:LEU:HD22	1:76:A:PHE:HA	8	1.41
(1,288)	1:9:B:GLU:HB2	1:11:B:ASN:HA	3	1.41
(1,106)	1:7:B:GLN:HG2	1:15:A:ILE:HD11	1	1.41
(1,105)	1:7:A:GLN:HG2	1:15:B:ILE:HD11	1	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG22	2	1.4
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG22	2	1.4
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	7	1.4
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	7	1.4
(1,993)	1:109:A:LEU:HD21	1:47:A:ASN:HB3	5	1.4
(1,987)	1:48:A:PHE:HB2	1:5:B:MET:H	5	1.4
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD13	5	1.4
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD13	5	1.4
(1,872)	1:34:B:GLN:HB2	1:64:B:GLU:HG3	2	1.4
(1,756)	1:96:B:GLU:HG2	1:97:B:GLY:HA3	8	1.4
(1,522)	1:49:B:LEU:HB3	1:82:B:LEU:HG	9	1.4
(1,521)	1:49:A:LEU:HB3	1:82:A:LEU:HG	9	1.4
(1,463)	1:79:A:PHE:HB3	1:81:A:MET:HG2	5	1.4
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG2	9	1.4
(1,287)	1:9:A:GLU:HB2	1:11:A:ASN:HA	3	1.4
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG2	9	1.4
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG3	10	1.39
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG3	10	1.39
(1,1244)	1:52:B:GLU:H	1:86:B:LEU:HD11	3	1.39
(1,1243)	1:52:A:GLU:H	1:86:A:LEU:HD11	3	1.39
(1,994)	1:109:B:LEU:HD21	1:47:B:ASN:HB3	5	1.39
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG21	5	1.39
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG21	5	1.39
(1,871)	1:34:A:GLN:HB2	1:64:A:GLU:HG3	2	1.39
(1,836)	1:76:B:PHE:HB3	1:29:B:PRO:HB2	3	1.39
(1,835)	1:76:A:PHE:HB3	1:29:A:PRO:HB2	3	1.39
(1,755)	1:96:A:GLU:HG2	1:97:A:GLY:HA3	8	1.39
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG22	4	1.39
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG22	4	1.39
(1,562)	1:16:B:ILE:HB	1:12:B:ILE:HG12	10	1.39
(1,561)	1:16:A:ILE:HB	1:12:A:ILE:HG12	10	1.39
(1,513)	1:51:A:LYS:HE2	1:41:A:VAL:HG11	4	1.39
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG2	9	1.39
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	3	1.39
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	3	1.39
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD12	5	1.39
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD12	5	1.39
(1,288)	1:9:B:GLU:HB2	1:11:B:ASN:HA	9	1.39
(1,287)	1:9:A:GLU:HB2	1:11:A:ASN:HA	9	1.39
(1,230)	1:62:B:ILE:HG23	1:41:B:VAL:HG23	7	1.39
(1,229)	1:62:A:ILE:HG23	1:41:A:VAL:HG23	7	1.39
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG2	9	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1474)	1:100:B:GLY:H	1:98:B:ASP:HA	10	1.38
(3,802)	1:29:B:PRO:HD3	1:30:B:ASP:HB2	9	1.38
(3,220)	1:66:B:LEU:HD12	1:74:B:LEU:HA	3	1.38
(3,219)	1:66:A:LEU:HD12	1:74:A:LEU:HA	3	1.38
(3,84)	1:87:B:THR:HG21	1:92:B:GLU:HG3	3	1.38
(3,83)	1:87:A:THR:HG21	1:92:A:GLU:HG3	3	1.38
(1,1775)	1:87:A:THR:H	1:16:B:ILE:HB	1	1.38
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD11	5	1.38
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD11	5	1.38
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD13	7	1.38
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD13	7	1.38
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD23	4	1.38
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD23	4	1.38
(1,744)	1:87:B:THR:HG21	1:92:B:GLU:HG3	3	1.38
(1,743)	1:87:A:THR:HG21	1:92:A:GLU:HG3	3	1.38
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	9	1.38
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	9	1.38
(1,561)	1:16:A:ILE:HB	1:93:B:LYS:HB3	4	1.38
(1,514)	1:51:B:LYS:HE2	1:41:B:VAL:HG11	4	1.38
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD22	6	1.38
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	8	1.38
(3,1473)	1:100:A:GLY:H	1:98:A:ASP:HA	10	1.37
(3,643)	1:8:A:LEU:HD21	1:40:B:LEU:HD22	2	1.37
(1,1820)	1:94:B:MET:H	1:89:B:ALA:HB2	5	1.37
(1,1819)	1:94:A:MET:H	1:89:A:ALA:HB2	5	1.37
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HD11	10	1.37
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HD11	10	1.37
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD23	3	1.37
(1,872)	1:34:B:GLN:HB2	1:64:B:GLU:HG3	6	1.37
(1,835)	1:76:A:PHE:HB2	1:81:B:MET:HE3	5	1.37
(1,562)	1:16:B:ILE:HB	1:12:B:ILE:HG12	2	1.37
(1,562)	1:16:B:ILE:HB	1:93:A:LYS:HB3	4	1.37
(1,561)	1:16:A:ILE:HB	1:12:A:ILE:HG12	2	1.37
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD22	6	1.37
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	8	1.37
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD12	1	1.36
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD12	1	1.36
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD23	3	1.36
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG21	2	1.36
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG21	2	1.36
(1,871)	1:34:A:GLN:HB2	1:64:A:GLU:HG3	6	1.36
(1,836)	1:76:B:PHE:HB2	1:81:A:MET:HE3	5	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:49:B:LEU:HB2	1:86:B:LEU:HG	6	1.36
(1,521)	1:49:A:LEU:HB2	1:86:A:LEU:HG	6	1.36
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	8	1.36
(3,644)	1:8:B:LEU:HD21	1:40:A:LEU:HD22	2	1.35
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	3	1.35
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	3	1.35
(1,1820)	1:21:B:GLN:H	1:40:B:LEU:HG	10	1.35
(1,1819)	1:21:A:GLN:H	1:40:A:LEU:HG	10	1.35
(1,1524)	1:41:B:VAL:H	1:62:B:ILE:HG21	8	1.35
(1,1523)	1:41:A:VAL:H	1:62:A:ILE:HG21	8	1.35
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD12	10	1.35
(1,1006)	1:8:B:LEU:HD12	1:22:A:TYR:H	10	1.35
(1,771)	1:58:A:VAL:HA	1:59:A:ILE:HD11	10	1.35
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	8	1.35
(1,143)	1:75:A:SER:HB3	1:79:A:PHE:HA	1	1.35
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD12	10	1.34
(1,1297)	1:8:A:LEU:H	1:15:B:ILE:HG23	6	1.34
(1,1005)	1:8:A:LEU:HD12	1:22:B:TYR:H	10	1.34
(1,912)	1:66:B:LEU:HD13	1:64:B:GLU:HA	4	1.34
(1,911)	1:66:A:LEU:HD13	1:64:A:GLU:HA	4	1.34
(1,836)	1:76:B:PHE:HB3	1:29:B:PRO:HB2	2	1.34
(1,835)	1:76:A:PHE:HB3	1:29:A:PRO:HB2	2	1.34
(1,772)	1:58:B:VAL:HA	1:59:B:ILE:HD11	10	1.34
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD13	7	1.34
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD22	1	1.34
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD22	1	1.34
(1,144)	1:75:B:SER:HB3	1:79:B:PHE:HA	1	1.34
(1,1388)	1:18:B:THR:H	1:15:B:ILE:HD13	4	1.33
(1,1387)	1:18:A:THR:H	1:15:A:ILE:HD13	4	1.33
(1,1298)	1:8:B:LEU:H	1:15:A:ILE:HG23	6	1.33
(1,1005)	1:109:A:LEU:HD12	1:86:A:LEU:H	2	1.33
(1,758)	1:96:B:GLU:HG2	1:107:B:PRO:HD2	2	1.33
(1,757)	1:96:A:GLU:HG2	1:107:A:PRO:HD2	2	1.33
(1,521)	1:49:A:LEU:HB3	1:82:A:LEU:HG	10	1.33
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG11	3	1.33
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG11	3	1.33
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	4	1.33
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	2	1.33
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	2	1.33
(1,226)	1:12:B:ILE:HG23	1:45:A:LEU:HG	4	1.33
(1,225)	1:12:A:ILE:HG23	1:45:B:LEU:HG	4	1.33
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	5	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:21:B:GLN:H	1:40:B:LEU:HG	6	1.32
(1,1782)	1:89:B:ALA:H	1:85:B:ARG:HG2	1	1.32
(1,1781)	1:89:A:ALA:H	1:85:A:ARG:HG2	1	1.32
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD12	2	1.32
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD12	2	1.32
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD13	8	1.32
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD13	8	1.32
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	3	1.32
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	3	1.32
(1,1006)	1:109:B:LEU:HD12	1:86:B:LEU:H	2	1.32
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD13	10	1.32
(1,770)	1:37:B:PHE:HB3	1:59:B:ILE:HD13	4	1.32
(1,769)	1:37:A:PHE:HB3	1:59:A:ILE:HD13	4	1.32
(1,624)	1:42:B:ARG:HA	1:44:B:ASP:HB2	1	1.32
(1,623)	1:42:A:ARG:HA	1:44:A:ASP:HB2	1	1.32
(1,522)	1:49:B:LEU:HB3	1:82:B:LEU:HG	10	1.32
(1,462)	1:10:B:ARG:HG3	1:12:B:ILE:HD13	10	1.32
(1,461)	1:10:A:ARG:HG3	1:12:A:ILE:HD13	10	1.32
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	4	1.32
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD11	1	1.32
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD13	7	1.32
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	10	1.32
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	5	1.32
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	10	1.32
(3,84)	1:87:B:THR:HG23	1:92:B:GLU:HG2	5	1.31
(3,83)	1:87:A:THR:HG23	1:92:A:GLU:HG2	5	1.31
(1,1819)	1:21:A:GLN:H	1:40:A:LEU:HG	6	1.31
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD21	8	1.31
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD21	8	1.31
(1,1036)	1:63:B:MET:HE1	1:41:B:VAL:HG21	10	1.31
(1,1035)	1:63:A:MET:HE1	1:41:A:VAL:HG21	10	1.31
(1,994)	1:8:B:LEU:HD22	1:22:A:TYR:HB2	9	1.31
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD13	10	1.31
(1,907)	1:86:A:LEU:HB2	1:9:B:GLU:HG2	9	1.31
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG21	3	1.31
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG21	3	1.31
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	9	1.31
(1,772)	1:58:B:VAL:HA	1:59:B:ILE:HD13	8	1.31
(1,771)	1:58:A:VAL:HA	1:59:A:ILE:HD13	8	1.31
(1,744)	1:87:B:THR:HG23	1:92:B:GLU:HG2	5	1.31
(1,743)	1:87:A:THR:HG23	1:92:A:GLU:HG2	5	1.31
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	9	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	4	1.31
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	4	1.31
(1,348)	1:5:B:MET:HG3	1:4:B:LYS:HE3	2	1.31
(1,347)	1:5:A:MET:HG3	1:4:A:LYS:HE3	2	1.31
(1,287)	1:9:A:GLU:HB2	1:11:A:ASN:HA	5	1.31
(3,801)	1:29:A:PRO:HD3	1:30:A:ASP:HB2	9	1.3
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD11	9	1.3
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD11	9	1.3
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD13	5	1.3
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD13	5	1.3
(1,993)	1:8:A:LEU:HD22	1:22:B:TYR:HB2	9	1.3
(1,991)	1:8:A:LEU:HD23	1:80:B:ILE:HA	7	1.3
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD21	8	1.3
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD21	8	1.3
(1,908)	1:86:B:LEU:HB2	1:9:A:GLU:HG2	9	1.3
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	9	1.3
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	9	1.3
(1,562)	1:16:B:ILE:HB	1:12:B:ILE:HG12	3	1.3
(1,561)	1:16:A:ILE:HB	1:12:A:ILE:HG12	3	1.3
(1,358)	1:46:B:GLN:HB3	1:39:B:GLU:HA	4	1.3
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	9	1.3
(1,357)	1:46:A:GLN:HB3	1:39:A:GLU:HA	4	1.3
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	9	1.3
(1,308)	1:44:B:ASP:HA	1:12:A:ILE:HD12	9	1.3
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD11	1	1.3
(1,307)	1:44:A:ASP:HA	1:12:B:ILE:HD12	9	1.3
(1,288)	1:9:B:GLU:HB2	1:11:B:ASN:HA	5	1.3
(1,1301)	1:9:A:GLU:H	1:15:B:ILE:HG23	6	1.29
(1,992)	1:8:B:LEU:HD23	1:80:A:ILE:HA	7	1.29
(1,988)	1:48:B:PHE:HB2	1:5:A:MET:H	3	1.29
(1,987)	1:48:A:PHE:HB2	1:5:B:MET:H	3	1.29
(1,836)	1:76:B:PHE:HB3	1:29:B:PRO:HB2	10	1.29
(1,835)	1:76:A:PHE:HB3	1:29:A:PRO:HB2	10	1.29
(1,624)	1:42:B:ARG:HA	1:44:B:ASP:HB2	5	1.29
(1,354)	1:92:B:GLU:HA	1:87:B:THR:HG21	3	1.29
(1,353)	1:92:A:GLU:HA	1:87:A:THR:HG21	3	1.29
(1,288)	1:9:B:GLU:HB3	1:11:B:ASN:HA	6	1.29
(1,287)	1:9:A:GLU:HB3	1:11:A:ASN:HA	6	1.29
(1,276)	1:19:B:PHE:HB2	1:13:B:GLU:HA	7	1.29
(1,275)	1:19:A:PHE:HB2	1:13:A:GLU:HA	7	1.29
(1,18)	1:92:B:GLU:HA	1:87:B:THR:HG21	3	1.29
(1,17)	1:92:A:GLU:HA	1:87:A:THR:HG21	3	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:9:B:GLU:H	1:15:A:ILE:HG23	6	1.28
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD22	3	1.28
(1,796)	1:111:B:GLU:HA	1:50:B:LYS:HB2	10	1.28
(1,795)	1:111:A:GLU:HA	1:50:A:LYS:HB2	10	1.28
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	5	1.28
(1,623)	1:42:A:ARG:HA	1:44:A:ASP:HB2	5	1.28
(1,458)	1:111:B:GLU:HA	1:50:B:LYS:HB2	10	1.28
(1,457)	1:111:A:GLU:HA	1:50:A:LYS:HB2	10	1.28
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD13	10	1.28
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD13	10	1.28
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD13	7	1.28
(1,24)	1:96:B:GLU:HA	1:107:B:PRO:HD3	6	1.28
(1,23)	1:96:A:GLU:HA	1:107:A:PRO:HD3	6	1.28
(3,752)	1:59:B:ILE:HG21	1:61:B:HIS:HB3	9	1.27
(3,751)	1:59:A:ILE:HG21	1:61:A:HIS:HB3	9	1.27
(3,494)	1:59:B:ILE:HD13	1:38:B:LYS:HE3	7	1.27
(3,493)	1:59:A:ILE:HD13	1:38:A:LYS:HE3	7	1.27
(3,256)	1:33:B:ASN:HB2	1:31:B:THR:HG21	9	1.27
(1,1820)	1:94:B:MET:H	1:89:B:ALA:HB2	2	1.27
(1,1819)	1:94:A:MET:H	1:89:A:ALA:HB2	2	1.27
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG22	1	1.27
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG12	10	1.27
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG22	1	1.27
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG12	10	1.27
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD22	3	1.27
(1,1056)	1:33:B:ASN:HB2	1:31:B:THR:HG21	9	1.27
(1,911)	1:66:A:LEU:HD22	1:64:A:GLU:HA	3	1.27
(1,722)	1:77:B:GLU:HB3	1:66:A:LEU:HD22	2	1.27
(1,721)	1:77:A:GLU:HB3	1:66:B:LEU:HD22	2	1.27
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	5	1.27
(1,225)	1:12:A:ILE:HG22	1:45:B:LEU:HG	1	1.27
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD13	7	1.27
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG23	8	1.26
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG23	8	1.26
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD22	6	1.26
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD22	6	1.26
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD23	1	1.26
(3,83)	1:87:A:THR:HG23	1:92:A:GLU:HG2	10	1.26
(1,1820)	1:94:B:MET:H	1:89:B:ALA:HB3	9	1.26
(1,1819)	1:94:A:MET:H	1:89:A:ALA:HB3	9	1.26
(1,1224)	1:42:B:ARG:HA	1:45:B:LEU:HA	7	1.26
(1,1223)	1:42:A:ARG:HA	1:45:A:LEU:HA	7	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:66:B:LEU:HD22	1:64:B:GLU:HA	3	1.26
(1,912)	1:66:B:LEU:HD13	1:64:B:GLU:HA	10	1.26
(1,911)	1:66:A:LEU:HD13	1:64:A:GLU:HA	10	1.26
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	5	1.26
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	5	1.26
(1,743)	1:87:A:THR:HG23	1:92:A:GLU:HG2	10	1.26
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	10	1.26
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	10	1.26
(1,456)	1:7:B:GLN:HB3	1:9:B:GLU:HG3	10	1.26
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	7	1.26
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	8	1.26
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	10	1.26
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	7	1.26
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	8	1.26
(1,288)	1:9:B:GLU:HB2	1:11:B:ASN:HA	8	1.26
(1,287)	1:9:A:GLU:HB2	1:11:A:ASN:HA	8	1.26
(3,752)	1:59:B:ILE:HG23	1:61:B:HIS:HB3	6	1.25
(3,751)	1:59:A:ILE:HG23	1:61:A:HIS:HB3	6	1.25
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	1	1.25
(3,255)	1:33:A:ASN:HB2	1:31:A:THR:HG21	9	1.25
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD23	1	1.25
(3,84)	1:87:B:THR:HG23	1:92:B:GLU:HG2	10	1.25
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	8	1.25
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	8	1.25
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD12	7	1.25
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD13	9	1.25
(1,1218)	1:87:B:THR:HG22	1:83:B:MET:HB3	4	1.25
(1,1217)	1:87:A:THR:HG22	1:83:A:MET:HB3	4	1.25
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG22	7	1.25
(1,1136)	1:57:B:LYS:HE3	1:60:B:GLU:HG3	2	1.25
(1,1135)	1:57:A:LYS:HE3	1:60:A:GLU:HG3	2	1.25
(1,1055)	1:33:A:ASN:HB2	1:31:A:THR:HG21	9	1.25
(1,988)	1:48:B:PHE:HB2	1:109:B:LEU:H	2	1.25
(1,987)	1:48:A:PHE:HB2	1:109:A:LEU:H	2	1.25
(1,987)	1:48:A:PHE:HB2	1:5:B:MET:H	4	1.25
(1,772)	1:58:B:VAL:HA	1:59:B:ILE:HD12	1	1.25
(1,771)	1:58:A:VAL:HA	1:59:A:ILE:HD12	1	1.25
(1,744)	1:87:B:THR:HG23	1:92:B:GLU:HG2	10	1.25
(1,462)	1:32:B:LEU:HG	1:87:A:THR:HG22	7	1.25
(1,455)	1:7:A:GLN:HB3	1:9:A:GLU:HG3	10	1.25
(1,390)	1:16:B:ILE:HD12	1:10:B:ARG:HA	1	1.25
(1,389)	1:16:A:ILE:HD12	1:10:A:ARG:HA	1	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	10	1.25
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	3	1.25
(1,82)	1:46:B:GLN:HG2	1:8:A:LEU:H	5	1.25
(1,81)	1:46:A:GLN:HG2	1:8:B:LEU:H	5	1.25
(1,55)	1:13:A:GLU:HG2	1:86:B:LEU:HD13	3	1.25
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD13	2	1.24
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD13	2	1.24
(3,752)	1:59:B:ILE:HG22	1:61:B:HIS:HB2	3	1.24
(3,752)	1:59:B:ILE:HG22	1:61:B:HIS:HB3	5	1.24
(3,751)	1:59:A:ILE:HG22	1:61:A:HIS:HB2	3	1.24
(3,751)	1:59:A:ILE:HG22	1:61:A:HIS:HB3	5	1.24
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	1	1.24
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD12	7	1.24
(1,1387)	1:18:A:THR:H	1:16:A:ILE:HD13	6	1.24
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD13	9	1.24
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD13	3	1.24
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD13	3	1.24
(1,1134)	1:51:B:LYS:HE2	1:53:B:ASN:HB3	1	1.24
(1,1133)	1:51:A:LYS:HE2	1:53:A:ASN:HB3	1	1.24
(1,990)	1:48:B:PHE:HB2	1:12:A:ILE:H	8	1.24
(1,988)	1:48:B:PHE:HB2	1:5:A:MET:H	4	1.24
(1,988)	1:48:B:PHE:HB3	1:109:B:LEU:H	10	1.24
(1,987)	1:48:A:PHE:HB3	1:109:A:LEU:H	10	1.24
(1,772)	1:58:B:VAL:HA	1:59:B:ILE:HD12	9	1.24
(1,771)	1:58:A:VAL:HA	1:59:A:ILE:HD12	9	1.24
(1,690)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	5	1.24
(1,689)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	5	1.24
(1,360)	1:77:B:GLU:HB2	1:87:A:THR:HG21	8	1.24
(1,288)	1:9:B:GLU:HB3	1:11:B:ASN:HA	4	1.24
(1,287)	1:9:A:GLU:HB3	1:11:A:ASN:HA	4	1.24
(1,276)	1:19:B:PHE:HB3	1:13:B:GLU:HA	5	1.24
(1,275)	1:19:A:PHE:HB3	1:13:A:GLU:HA	5	1.24
(1,226)	1:12:B:ILE:HG22	1:45:A:LEU:HG	1	1.24
(1,56)	1:13:B:GLU:HG2	1:86:A:LEU:HD13	3	1.24
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	4	1.23
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD22	8	1.23
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD22	8	1.23
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG21	3	1.23
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG21	3	1.23
(1,1388)	1:18:B:THR:H	1:16:B:ILE:HD13	6	1.23
(1,1196)	1:98:B:ASP:HA	1:95:B:HIS:HB3	9	1.23
(1,1195)	1:98:A:ASP:HA	1:95:A:HIS:HB3	9	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:32:B:LEU:HG	1:87:A:THR:HG21	2	1.23
(1,989)	1:48:A:PHE:HB2	1:12:B:ILE:H	8	1.23
(1,912)	1:66:B:LEU:HD11	1:64:B:GLU:HA	6	1.23
(1,911)	1:66:A:LEU:HD11	1:64:A:GLU:HA	6	1.23
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	2	1.23
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	2	1.23
(1,561)	1:16:A:ILE:HB	1:93:B:LYS:HB3	1	1.23
(1,462)	1:32:B:LEU:HG	1:87:A:THR:HG21	2	1.23
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	6	1.23
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	3	1.23
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	10	1.22
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	10	1.22
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	10	1.22
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	10	1.22
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG21	2	1.22
(1,1147)	1:32:A:LEU:HG	1:87:B:THR:HG22	7	1.22
(1,991)	1:8:A:LEU:HD22	1:20:B:HIS:HB2	1	1.22
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	2	1.22
(1,796)	1:111:B:GLU:HA	1:10:A:ARG:HG2	7	1.22
(1,795)	1:111:A:GLU:HA	1:10:B:ARG:HG2	7	1.22
(1,770)	1:37:B:PHE:HB3	1:59:B:ILE:HD13	5	1.22
(1,769)	1:37:A:PHE:HB3	1:59:A:ILE:HD13	5	1.22
(1,562)	1:16:B:ILE:HB	1:93:A:LYS:HB2	8	1.22
(1,562)	1:16:B:ILE:HB	1:12:B:ILE:HG12	9	1.22
(1,561)	1:16:A:ILE:HB	1:93:B:LYS:HB2	8	1.22
(1,561)	1:16:A:ILE:HB	1:12:A:ILE:HG12	9	1.22
(1,461)	1:32:A:LEU:HG	1:87:B:THR:HG21	2	1.22
(1,461)	1:32:A:LEU:HG	1:87:B:THR:HG22	7	1.22
(1,458)	1:111:B:GLU:HA	1:10:A:ARG:HG2	7	1.22
(1,457)	1:111:A:GLU:HA	1:10:B:ARG:HG2	7	1.22
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	10	1.22
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	10	1.22
(1,359)	1:77:A:GLU:HB2	1:87:B:THR:HG21	8	1.22
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	2	1.22
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	3	1.22
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG21	9	1.21
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	4	1.21
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	3	1.21
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	3	1.21
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD22	4	1.21
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD22	4	1.21
(3,83)	1:87:A:THR:HG21	1:92:A:GLU:HG2	6	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:21:B:GLN:H	1:40:B:LEU:HG	1	1.21
(1,1819)	1:21:A:GLN:H	1:40:A:LEU:HG	1	1.21
(1,1574)	1:48:B:PHE:H	1:41:B:VAL:HA	9	1.21
(1,1573)	1:48:A:PHE:H	1:41:A:VAL:HA	9	1.21
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD21	5	1.21
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD21	5	1.21
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD21	1	1.21
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD21	1	1.21
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD11	8	1.21
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD11	8	1.21
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	2	1.21
(1,743)	1:87:A:THR:HG21	1:92:A:GLU:HG2	6	1.21
(1,479)	1:63:A:MET:HB2	1:59:A:ILE:HD12	8	1.21
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	6	1.21
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	5	1.21
(1,358)	1:46:B:GLN:HB3	1:40:B:LEU:HA	6	1.21
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	5	1.21
(1,357)	1:46:A:GLN:HB3	1:40:A:LEU:HA	6	1.21
(1,224)	1:62:B:ILE:HG21	1:66:B:LEU:HG	7	1.21
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	2	1.21
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	2	1.21
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	3	1.21
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	2	1.21
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG21	9	1.2
(3,332)	1:86:B:LEU:HD12	1:9:A:GLU:HG2	8	1.2
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	6	1.2
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	6	1.2
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD23	7	1.2
(3,84)	1:87:B:THR:HG21	1:92:B:GLU:HG2	6	1.2
(1,1582)	1:50:B:LYS:H	1:45:B:LEU:HD23	7	1.2
(1,1581)	1:50:A:LYS:H	1:45:A:LEU:HD23	7	1.2
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD12	3	1.2
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD12	3	1.2
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD13	7	1.2
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD13	7	1.2
(1,1184)	1:96:B:GLU:HB2	1:93:B:LYS:HD2	1	1.2
(1,1138)	1:14:B:THR:HG21	1:12:B:ILE:HA	6	1.2
(1,1137)	1:14:A:THR:HG21	1:12:A:ILE:HA	6	1.2
(1,862)	1:25:B:LYS:HD2	1:33:B:ASN:HB3	10	1.2
(1,753)	1:111:A:GLU:HG3	1:4:B:LYS:HE3	4	1.2
(1,744)	1:87:B:THR:HG21	1:92:B:GLU:HG2	6	1.2
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	4	1.2
(1,689)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	4	1.2
(1,562)	1:16:B:ILE:HB	1:93:A:LYS:HB3	1	1.2
(1,480)	1:63:B:MET:HB2	1:59:B:ILE:HD12	8	1.2
(1,348)	1:5:B:MET:HG3	1:4:B:LYS:HE3	10	1.2
(1,223)	1:62:A:ILE:HG21	1:66:A:LEU:HG	7	1.2
(1,42)	1:78:B:GLU:HG2	1:76:B:PHE:HA	5	1.2
(1,41)	1:78:A:GLU:HG2	1:76:A:PHE:HA	5	1.2
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG22	7	1.19
(3,752)	1:59:B:ILE:HG23	1:61:B:HIS:HB3	2	1.19
(3,751)	1:59:A:ILE:HG23	1:61:A:HIS:HB3	2	1.19
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD13	1	1.19
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD23	4	1.19
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD13	1	1.19
(3,331)	1:86:A:LEU:HD12	1:9:B:GLU:HG2	8	1.19
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	9	1.19
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD23	7	1.19
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG2	8	1.19
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG2	8	1.19
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	3	1.19
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	3	1.19
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD11	2	1.19
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	2	1.19
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	2	1.19
(1,1183)	1:96:A:GLU:HB2	1:93:A:LYS:HD2	1	1.19
(1,992)	1:8:B:LEU:HD22	1:20:A:HIS:HB2	1	1.19
(1,938)	1:46:B:GLN:HG2	1:8:A:LEU:HD21	9	1.19
(1,937)	1:46:A:GLN:HG2	1:8:B:LEU:HD21	9	1.19
(1,861)	1:25:A:LYS:HD2	1:33:A:ASN:HB3	10	1.19
(1,754)	1:111:B:GLU:HG3	1:4:A:LYS:HE3	4	1.19
(1,754)	1:111:B:GLU:HG3	1:4:A:LYS:HE2	7	1.19
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	1	1.19
(1,694)	1:74:B:LEU:HG	1:78:B:GLU:HG2	4	1.19
(1,693)	1:74:A:LEU:HG	1:78:A:GLU:HG2	4	1.19
(1,562)	1:16:B:ILE:HB	1:93:A:LYS:HB3	7	1.19
(1,347)	1:5:A:MET:HG3	1:4:A:LYS:HE3	10	1.19
(1,230)	1:12:B:ILE:HG23	1:80:B:ILE:HD12	1	1.19
(1,229)	1:12:A:ILE:HG23	1:80:A:ILE:HD12	1	1.19
(1,212)	1:12:B:ILE:HG22	1:11:B:ASN:HA	9	1.19
(1,211)	1:12:A:ILE:HG22	1:11:A:ASN:HA	9	1.19
(1,24)	1:96:B:GLU:HA	1:107:B:PRO:HD2	2	1.19
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG22	7	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD23	4	1.18
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	5	1.18
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	8	1.18
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	9	1.18
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	5	1.18
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	8	1.18
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD22	10	1.18
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD22	10	1.18
(1,1546)	1:43:B:LYS:H	1:59:B:ILE:HD11	9	1.18
(1,1545)	1:43:A:LYS:H	1:59:A:ILE:HD11	9	1.18
(1,1224)	1:42:B:ARG:HA	1:45:B:LEU:HA	6	1.18
(1,1216)	1:49:B:LEU:HB2	1:9:A:GLU:HB2	1	1.18
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	7	1.18
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	9	1.18
(1,561)	1:16:A:ILE:HB	1:93:B:LYS:HB3	7	1.18
(1,358)	1:46:B:GLN:HB3	1:39:B:GLU:HA	1	1.18
(1,357)	1:46:A:GLN:HB3	1:39:A:GLU:HA	1	1.18
(1,23)	1:96:A:GLU:HA	1:107:A:PRO:HD2	2	1.18
(1,1781)	1:89:A:ALA:H	1:85:A:ARG:HG2	4	1.17
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG13	3	1.17
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG13	3	1.17
(1,1545)	1:43:A:LYS:H	1:49:A:LEU:HD11	6	1.17
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD11	2	1.17
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD12	8	1.17
(1,1223)	1:42:A:ARG:HA	1:45:A:LEU:HA	6	1.17
(1,1215)	1:49:A:LEU:HB2	1:9:B:GLU:HB2	1	1.17
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB3	4	1.17
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB3	4	1.17
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	7	1.17
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	9	1.17
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG12	5	1.17
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG12	5	1.17
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD13	4	1.17
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG3	9	1.17
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG3	9	1.17
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	6	1.17
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	6	1.17
(1,212)	1:12:B:ILE:HG22	1:11:B:ASN:HA	2	1.17
(3,84)	1:87:B:THR:HG21	1:92:B:GLU:HG2	1	1.16
(3,83)	1:87:A:THR:HG21	1:92:A:GLU:HG2	1	1.16
(1,1782)	1:89:B:ALA:H	1:85:B:ARG:HG2	4	1.16
(1,1582)	1:50:B:LYS:H	1:45:B:LEU:HD22	4	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:50:A:LYS:H	1:45:A:LEU:HD22	4	1.16
(1,1546)	1:43:B:LYS:H	1:49:B:LEU:HD11	6	1.16
(1,1546)	1:43:B:LYS:H	1:59:B:ILE:HD13	10	1.16
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD11	9	1.16
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB3	2	1.16
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB3	2	1.16
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD12	8	1.16
(1,1098)	1:59:B:ILE:HG22	1:42:B:ARG:HD2	7	1.16
(1,1097)	1:59:A:ILE:HG22	1:42:A:ARG:HD2	7	1.16
(1,1068)	1:11:B:ASN:HB3	1:12:B:ILE:HD13	7	1.16
(1,1067)	1:11:A:ASN:HB3	1:12:A:ILE:HD13	7	1.16
(1,1054)	1:31:B:THR:HG22	1:71:B:ASP:HB2	8	1.16
(1,1053)	1:31:A:THR:HG22	1:71:A:ASP:HB2	8	1.16
(1,877)	1:34:A:GLN:HB2	1:72:A:LYS:HD2	1	1.16
(1,744)	1:87:B:THR:HG21	1:92:B:GLU:HG2	1	1.16
(1,743)	1:87:A:THR:HG21	1:92:A:GLU:HG2	1	1.16
(1,694)	1:74:B:LEU:HG	1:64:B:GLU:HG3	9	1.16
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD13	4	1.16
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	2	1.16
(1,212)	1:12:B:ILE:HG21	1:11:B:ASN:HA	1	1.16
(1,212)	1:12:B:ILE:HG22	1:11:B:ASN:HA	4	1.16
(1,212)	1:12:B:ILE:HG21	1:11:B:ASN:HA	10	1.16
(1,211)	1:12:A:ILE:HG21	1:11:A:ASN:HA	1	1.16
(1,211)	1:12:A:ILE:HG22	1:11:A:ASN:HA	2	1.16
(1,211)	1:12:A:ILE:HG22	1:11:A:ASN:HA	4	1.16
(1,211)	1:12:A:ILE:HG21	1:11:A:ASN:HA	10	1.16
(3,752)	1:59:B:ILE:HG21	1:61:B:HIS:HB3	7	1.15
(3,751)	1:59:A:ILE:HG21	1:61:A:HIS:HB3	7	1.15
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD23	6	1.15
(1,1545)	1:43:A:LYS:H	1:59:A:ILE:HD12	8	1.15
(1,1545)	1:43:A:LYS:H	1:59:A:ILE:HD13	10	1.15
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD11	9	1.15
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD22	5	1.15
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	8	1.15
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	8	1.15
(1,878)	1:34:B:GLN:HB2	1:72:B:LYS:HD2	1	1.15
(1,770)	1:37:B:PHE:HB3	1:59:B:ILE:HD11	3	1.15
(1,769)	1:37:A:PHE:HB3	1:59:A:ILE:HD11	3	1.15
(1,693)	1:74:A:LEU:HG	1:64:A:GLU:HG3	9	1.15
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	2	1.15
(1,212)	1:12:B:ILE:HG21	1:11:B:ASN:HA	6	1.15
(1,211)	1:12:A:ILE:HG21	1:11:A:ASN:HA	6	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG21	6	1.14
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD23	3	1.14
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD23	3	1.14
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD23	6	1.14
(1,1546)	1:43:B:LYS:H	1:59:B:ILE:HD12	8	1.14
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD22	5	1.14
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD21	9	1.14
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD21	9	1.14
(1,1006)	1:8:B:LEU:HD13	1:22:A:TYR:H	7	1.14
(1,753)	1:111:A:GLU:HG3	1:4:B:LYS:HE2	7	1.14
(1,624)	1:42:B:ARG:HA	1:44:B:ASP:HB2	2	1.14
(1,624)	1:42:B:ARG:HA	1:44:B:ASP:HB2	7	1.14
(1,623)	1:42:A:ARG:HA	1:44:A:ASP:HB2	2	1.14
(1,623)	1:42:A:ARG:HA	1:44:A:ASP:HB2	7	1.14
(1,212)	1:12:B:ILE:HG23	1:11:B:ASN:HA	8	1.14
(1,211)	1:12:A:ILE:HG23	1:11:A:ASN:HA	8	1.14
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG21	6	1.13
(3,494)	1:59:B:ILE:HD12	1:38:B:LYS:HE2	6	1.13
(3,493)	1:59:A:ILE:HD12	1:38:A:LYS:HE2	6	1.13
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD21	5	1.13
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD21	5	1.13
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	1	1.13
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	7	1.13
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	1	1.13
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	7	1.13
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD23	2	1.13
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD22	8	1.13
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD23	2	1.13
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD22	8	1.13
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG21	8	1.13
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG21	8	1.13
(1,1131)	1:54:A:LYS:HE3	1:53:A:ASN:HB3	3	1.13
(1,1005)	1:8:A:LEU:HD13	1:22:B:TYR:H	7	1.13
(1,993)	1:8:A:LEU:HD21	1:22:B:TYR:HB2	3	1.13
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB3	8	1.13
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB3	8	1.13
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	3	1.13
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	3	1.13
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	3	1.13
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	3	1.13
(1,464)	1:79:B:PHE:HB3	1:81:B:MET:HG3	7	1.13
(1,463)	1:79:A:PHE:HB3	1:81:A:MET:HG3	7	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:12:B:ILE:HG22	1:11:B:ASN:HA	3	1.13
(1,211)	1:12:A:ILE:HG22	1:11:A:ASN:HA	3	1.13
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD23	2	1.12
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD22	10	1.12
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD22	10	1.12
(3,220)	1:66:B:LEU:HD21	1:74:B:LEU:HA	7	1.12
(3,219)	1:66:A:LEU:HD21	1:74:A:LEU:HA	7	1.12
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD23	7	1.12
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD22	10	1.12
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD23	7	1.12
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD22	10	1.12
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD21	1	1.12
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD11	1	1.12
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD11	1	1.12
(1,1196)	1:98:B:ASP:HA	1:95:B:HIS:HB3	10	1.12
(1,1132)	1:54:B:LYS:HE3	1:53:B:ASN:HB3	3	1.12
(1,994)	1:8:B:LEU:HD21	1:22:A:TYR:HB2	3	1.12
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD11	6	1.12
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG2	8	1.12
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG2	8	1.12
(1,212)	1:12:B:ILE:HG22	1:11:B:ASN:HA	7	1.12
(1,211)	1:12:A:ILE:HG22	1:11:A:ASN:HA	7	1.12
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG12	4	1.11
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG12	4	1.11
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG22	4	1.11
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG22	4	1.11
(3,794)	1:107:B:PRO:HG3	1:93:B:LYS:HG2	9	1.11
(3,793)	1:107:A:PRO:HG3	1:93:A:LYS:HG2	9	1.11
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD22	5	1.11
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD23	2	1.11
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD22	5	1.11
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	6	1.11
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	6	1.11
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD21	4	1.11
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD21	4	1.11
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD23	6	1.11
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD23	6	1.11
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD11	1	1.11
(1,1195)	1:98:A:ASP:HA	1:95:A:HIS:HB3	10	1.11
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	1	1.11
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD11	6	1.11
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB3	5	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	5	1.11
(1,698)	1:107:B:PRO:HG3	1:93:B:LYS:HG2	9	1.11
(1,697)	1:107:A:PRO:HG3	1:93:A:LYS:HG2	9	1.11
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG22	3	1.11
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG22	1	1.11
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG22	3	1.11
(1,472)	1:79:B:PHE:HB3	1:76:B:PHE:HB3	2	1.11
(1,471)	1:79:A:PHE:HB3	1:76:A:PHE:HB3	2	1.11
(1,212)	1:12:B:ILE:HG23	1:11:B:ASN:HA	5	1.11
(1,211)	1:12:A:ILE:HG23	1:11:A:ASN:HA	5	1.11
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	1	1.11
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG22	1	1.1
(3,279)	1:72:A:LYS:HG3	1:73:A:GLN:HB2	4	1.1
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG2	1	1.1
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG2	1	1.1
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG13	4	1.1
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG13	4	1.1
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD21	9	1.1
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD21	9	1.1
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD22	4	1.1
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD22	4	1.1
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	1	1.1
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	1	1.1
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD11	1	1.1
(1,1218)	1:87:B:THR:HG21	1:83:B:MET:HB3	10	1.1
(1,1217)	1:87:A:THR:HG21	1:83:A:MET:HB3	10	1.1
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	3	1.1
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	4	1.1
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	3	1.1
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	4	1.1
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB3	5	1.1
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	5	1.1
(1,872)	1:34:B:GLN:HB2	1:64:B:GLU:HG3	7	1.1
(1,871)	1:34:A:GLN:HB2	1:64:A:GLU:HG3	7	1.1
(1,770)	1:37:B:PHE:HB3	1:59:B:ILE:HD12	6	1.1
(1,769)	1:37:A:PHE:HB3	1:59:A:ILE:HD12	6	1.1
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG22	1	1.1
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	3	1.1
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	3	1.1
(1,359)	1:46:A:GLN:HB3	1:49:A:LEU:HD11	6	1.1
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG12	6	1.09
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG12	6	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,752)	1:59:B:ILE:HG21	1:61:B:HIS:HB3	4	1.09
(3,751)	1:59:A:ILE:HG21	1:61:A:HIS:HB3	4	1.09
(3,280)	1:72:B:LYS:HG3	1:73:B:GLN:HB2	4	1.09
(3,219)	1:66:A:LEU:HD22	1:74:A:LEU:HA	8	1.09
(3,164)	1:13:B:GLU:HB2	1:14:B:THR:HG21	8	1.09
(3,163)	1:13:A:GLU:HB2	1:14:A:THR:HG21	8	1.09
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG13	10	1.09
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG13	1	1.09
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG13	10	1.09
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD21	1	1.09
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	5	1.09
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	5	1.09
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	2	1.09
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	4	1.09
(1,698)	1:74:B:LEU:HG	1:40:B:LEU:HB3	3	1.09
(1,697)	1:74:A:LEU:HG	1:40:A:LEU:HB3	3	1.09
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG2	6	1.09
(1,360)	1:46:B:GLN:HB3	1:49:B:LEU:HD11	6	1.09
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	8	1.09
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	4	1.09
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	4	1.09
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG2	6	1.09
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG13	1	1.08
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG11	7	1.08
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG13	1	1.08
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG11	7	1.08
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD23	9	1.08
(3,220)	1:66:B:LEU:HD22	1:74:B:LEU:HA	8	1.08
(3,84)	1:87:B:THR:HG21	1:92:B:GLU:HG2	4	1.08
(3,83)	1:87:A:THR:HG21	1:92:A:GLU:HG2	4	1.08
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG13	1	1.08
(1,1574)	1:48:B:PHE:H	1:41:B:VAL:HA	4	1.08
(1,1573)	1:48:A:PHE:H	1:41:A:VAL:HA	4	1.08
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	2	1.08
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	1	1.08
(1,988)	1:48:B:PHE:HB2	1:109:B:LEU:H	7	1.08
(1,987)	1:48:A:PHE:HB2	1:109:A:LEU:H	7	1.08
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB1	3	1.08
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	4	1.08
(1,744)	1:87:B:THR:HG21	1:92:B:GLU:HG2	4	1.08
(1,743)	1:87:A:THR:HG21	1:92:A:GLU:HG2	4	1.08
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	1	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	1	1.08
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG2	6	1.08
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	4	1.08
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	4	1.08
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	8	1.08
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG2	6	1.08
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	1	1.08
(1,20)	1:93:B:LYS:HA	1:109:B:LEU:HG	3	1.08
(1,19)	1:93:A:LYS:HA	1:109:A:LEU:HG	3	1.08
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD12	8	1.07
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD12	8	1.07
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG22	1	1.07
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD23	9	1.07
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG11	9	1.07
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG11	9	1.07
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	9	1.07
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	9	1.07
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	10	1.07
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	10	1.07
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG23	7	1.07
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG23	7	1.07
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB3	2	1.07
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB1	3	1.07
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB3	2	1.07
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG2	9	1.07
(1,262)	1:49:B:LEU:HG	1:89:B:ALA:HB3	8	1.07
(1,261)	1:49:A:LEU:HG	1:89:A:ALA:HB3	8	1.07
(1,230)	1:62:B:ILE:HG21	1:41:B:VAL:HG23	9	1.07
(1,229)	1:62:A:ILE:HG21	1:41:A:VAL:HG23	9	1.07
(1,4)	1:73:B:GLN:HG3	1:70:B:ALA:HA	4	1.07
(1,3)	1:73:A:GLN:HG3	1:70:A:ALA:HA	4	1.07
(3,1466)	1:110:B:GLY:H	1:108:B:GLY:HA3	6	1.06
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD22	10	1.06
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD22	10	1.06
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD11	7	1.06
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB3	1	1.06
(1,1270)	1:48:B:PHE:H	1:51:B:LYS:HE2	6	1.06
(1,1269)	1:48:A:PHE:H	1:51:A:LYS:HE2	6	1.06
(1,1224)	1:50:B:LYS:HA	1:45:B:LEU:HA	3	1.06
(1,1223)	1:50:A:LYS:HA	1:45:A:LEU:HA	3	1.06
(1,1218)	1:87:B:THR:HG22	1:15:A:ILE:HB	2	1.06
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	1	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG2	9	1.06
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG3	3	1.06
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG3	3	1.06
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	10	1.06
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	10	1.06
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD13	2	1.06
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD13	2	1.06
(3,1465)	1:110:A:GLY:H	1:108:A:GLY:HA3	6	1.05
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG13	2	1.05
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG23	5	1.05
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG23	5	1.05
(3,586)	1:66:B:LEU:HD12	1:79:B:PHE:HB2	3	1.05
(3,585)	1:66:A:LEU:HD12	1:79:A:PHE:HB2	3	1.05
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD21	10	1.05
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG3	6	1.05
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG3	6	1.05
(3,84)	1:87:B:THR:HG23	1:92:B:GLU:HG2	2	1.05
(3,83)	1:87:A:THR:HG23	1:92:A:GLU:HG2	2	1.05
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD22	5	1.05
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD22	5	1.05
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD11	7	1.05
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	1	1.05
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE1	1	1.05
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE1	1	1.05
(1,744)	1:87:B:THR:HG23	1:92:B:GLU:HG2	2	1.05
(1,743)	1:87:A:THR:HG23	1:92:A:GLU:HG2	2	1.05
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD22	10	1.05
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD22	10	1.05
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG3	1	1.05
(1,280)	1:19:B:PHE:HB2	1:32:B:LEU:HB2	3	1.05
(1,279)	1:19:A:PHE:HB2	1:32:A:LEU:HB2	3	1.05
(1,138)	1:16:B:ILE:HD13	1:93:A:LYS:HE2	7	1.05
(1,137)	1:16:A:ILE:HD13	1:93:B:LYS:HE2	7	1.05
(1,82)	1:46:B:GLN:HG2	1:8:A:LEU:H	8	1.05
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG13	2	1.04
(3,752)	1:59:B:ILE:HG21	1:61:B:HIS:HB3	1	1.04
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	5	1.04
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	5	1.04
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD21	10	1.04
(3,90)	1:7:B:GLN:HG2	1:44:A:ASP:HB2	4	1.04
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG13	2	1.04
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG13	2	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1574)	1:48:B:PHE:H	1:41:B:VAL:HA	1	1.04
(1,1573)	1:48:A:PHE:H	1:41:A:VAL:HA	1	1.04
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD21	2	1.04
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD21	2	1.04
(1,1509)	1:39:A:GLU:H	1:38:A:LYS:HD3	1	1.04
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD12	5	1.04
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD23	9	1.04
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD13	4	1.04
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD12	6	1.04
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD12	6	1.04
(1,1218)	1:87:B:THR:HG22	1:83:B:MET:HB3	6	1.04
(1,1217)	1:87:A:THR:HG22	1:15:B:ILE:HB	2	1.04
(1,1217)	1:87:A:THR:HG22	1:83:A:MET:HB3	6	1.04
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	5	1.04
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	5	1.04
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG23	6	1.04
(1,992)	1:8:B:LEU:HD23	1:48:A:PHE:HB3	4	1.04
(1,991)	1:8:A:LEU:HD23	1:48:B:PHE:HB3	4	1.04
(1,974)	1:7:B:GLN:HG2	1:44:A:ASP:HB2	4	1.04
(1,912)	1:66:B:LEU:HD12	1:64:B:GLU:HA	2	1.04
(1,911)	1:66:A:LEU:HD12	1:64:A:GLU:HA	2	1.04
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG2	6	1.04
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG2	6	1.04
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	7	1.04
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	7	1.04
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG2	5	1.04
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG3	1	1.04
(1,81)	1:46:A:GLN:HG2	1:8:B:LEU:H	8	1.04
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG2	5	1.04
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG22	2	1.03
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG22	2	1.03
(3,802)	1:29:B:PRO:HD2	1:30:B:ASP:HB2	6	1.03
(3,751)	1:59:A:ILE:HG21	1:61:A:HIS:HB3	1	1.03
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD23	3	1.03
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD23	3	1.03
(1,1548)	1:43:B:LYS:H	1:40:B:LEU:HG	9	1.03
(1,1547)	1:43:A:LYS:H	1:40:A:LEU:HG	9	1.03
(1,1510)	1:39:B:GLU:H	1:38:B:LYS:HD3	1	1.03
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD12	5	1.03
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD23	9	1.03
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD13	4	1.03
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB3	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1160)	1:21:B:GLN:HG3	1:25:B:LYS:HD2	8	1.03
(1,1159)	1:21:A:GLN:HG3	1:25:A:LYS:HD2	8	1.03
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD13	8	1.03
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD13	8	1.03
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG23	6	1.03
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD13	8	1.03
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD13	8	1.03
(1,693)	1:74:A:LEU:HG	1:78:A:GLU:HG3	1	1.03
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD22	2	1.03
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD22	2	1.03
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG2	5	1.03
(1,336)	1:41:B:VAL:HG11	1:48:B:PHE:H	8	1.03
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG2	5	1.03
(3,801)	1:29:A:PRO:HD2	1:30:A:ASP:HB2	6	1.02
(3,89)	1:7:A:GLN:HG2	1:44:B:ASP:HB2	4	1.02
(3,84)	1:87:B:THR:HG21	1:92:B:GLU:HG2	7	1.02
(3,83)	1:87:A:THR:HG21	1:92:A:GLU:HG2	7	1.02
(1,1782)	1:89:B:ALA:H	1:93:B:LYS:HB2	8	1.02
(1,1782)	1:89:B:ALA:H	1:85:B:ARG:HG2	9	1.02
(1,1781)	1:89:A:ALA:H	1:93:A:LYS:HB2	8	1.02
(1,1781)	1:89:A:ALA:H	1:85:A:ARG:HG2	9	1.02
(1,1548)	1:43:B:LYS:H	1:40:B:LEU:HG	7	1.02
(1,1547)	1:43:A:LYS:H	1:40:A:LEU:HG	7	1.02
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD23	1	1.02
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD23	1	1.02
(1,1224)	1:42:B:ARG:HA	1:45:B:LEU:HA	2	1.02
(1,1223)	1:42:A:ARG:HA	1:45:A:LEU:HA	2	1.02
(1,1006)	1:109:B:LEU:HD12	1:86:B:LEU:H	9	1.02
(1,973)	1:7:A:GLN:HG2	1:44:B:ASP:HB2	4	1.02
(1,744)	1:87:B:THR:HG21	1:92:B:GLU:HG2	7	1.02
(1,743)	1:87:A:THR:HG21	1:92:A:GLU:HG2	7	1.02
(1,694)	1:74:B:LEU:HG	1:78:B:GLU:HG3	1	1.02
(1,590)	1:85:B:ARG:HG3	1:78:B:GLU:HG2	3	1.02
(1,589)	1:85:A:ARG:HG3	1:78:A:GLU:HG2	3	1.02
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	3	1.02
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	3	1.02
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	3	1.02
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	3	1.02
(1,335)	1:41:A:VAL:HG11	1:48:A:PHE:H	8	1.02
(1,288)	1:64:B:GLU:HB2	1:71:B:ASP:HA	10	1.02
(1,287)	1:64:A:GLU:HB2	1:71:A:ASP:HA	10	1.02
(1,230)	1:12:B:ILE:HG22	1:80:B:ILE:HD13	5	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:12:A:ILE:HG22	1:80:A:ILE:HD13	5	1.02
(3,546)	1:33:B:ASN:HA	1:31:B:THR:HG21	9	1.01
(3,83)	1:87:A:THR:HG21	1:92:A:GLU:HG2	9	1.01
(1,1826)	1:21:B:GLN:H	1:17:B:ASN:HB3	2	1.01
(1,1826)	1:94:B:MET:H	1:93:B:LYS:HE3	5	1.01
(1,1825)	1:21:A:GLN:H	1:17:A:ASN:HB3	2	1.01
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG13	9	1.01
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG13	9	1.01
(1,1643)	1:65:A:ASP:H	1:63:A:MET:HG2	7	1.01
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD23	1	1.01
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD23	1	1.01
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD13	3	1.01
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD13	3	1.01
(1,1224)	1:50:B:LYS:HA	1:45:B:LEU:HA	9	1.01
(1,1223)	1:50:A:LYS:HA	1:45:A:LEU:HA	9	1.01
(1,1005)	1:109:A:LEU:HD12	1:86:A:LEU:H	9	1.01
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	4	1.01
(1,743)	1:87:A:THR:HG21	1:92:A:GLU:HG2	9	1.01
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD21	10	1.01
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD21	10	1.01
(1,37)	1:58:A:VAL:HG12	1:61:A:HIS:HA	9	1.01
(3,639)	1:8:A:LEU:HD13	1:83:B:MET:HG3	2	1.0
(3,84)	1:87:B:THR:HG21	1:92:B:GLU:HG2	9	1.0
(1,1825)	1:94:A:MET:H	1:93:A:LYS:HE3	5	1.0
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG13	6	1.0
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG13	6	1.0
(1,1644)	1:65:B:ASP:H	1:63:B:MET:HG2	7	1.0
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD23	1	1.0
(1,1560)	1:46:B:GLN:H	1:45:B:LEU:HD22	7	1.0
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD23	1	1.0
(1,1559)	1:46:A:GLN:H	1:45:A:LEU:HD22	7	1.0
(1,1510)	1:39:B:GLU:H	1:38:B:LYS:HD2	6	1.0
(1,1509)	1:39:A:GLU:H	1:38:A:LYS:HD2	6	1.0
(1,1498)	1:44:B:ASP:H	1:49:B:LEU:HD12	7	1.0
(1,1497)	1:44:A:ASP:H	1:49:A:LEU:HD12	7	1.0
(1,1422)	1:22:B:TYR:H	1:36:B:GLU:HG2	8	1.0
(1,1421)	1:22:A:TYR:H	1:36:A:GLU:HG2	8	1.0
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD23	7	1.0
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD12	9	1.0
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD12	9	1.0
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG23	2	1.0
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG23	2	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1098)	1:59:B:ILE:HG23	1:42:B:ARG:HD2	5	1.0
(1,862)	1:25:B:LYS:HD2	1:33:B:ASN:HB3	9	1.0
(1,861)	1:25:A:LYS:HD2	1:33:A:ASN:HB3	9	1.0
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	4	1.0
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG2	5	1.0
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG2	5	1.0
(1,810)	1:74:B:LEU:HG	1:38:B:LYS:H	10	1.0
(1,809)	1:74:A:LEU:HG	1:38:A:LYS:H	10	1.0
(1,744)	1:87:B:THR:HG21	1:92:B:GLU:HG2	9	1.0
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG21	8	1.0
(1,566)	1:42:B:ARG:HA	1:49:B:LEU:H	2	1.0
(1,566)	1:42:B:ARG:HA	1:49:B:LEU:H	6	1.0
(1,565)	1:42:A:ARG:HA	1:49:A:LEU:H	2	1.0
(1,565)	1:42:A:ARG:HA	1:49:A:LEU:H	6	1.0
(1,440)	1:10:B:ARG:HG2	1:11:B:ASN:HB2	6	1.0
(1,50)	1:64:B:GLU:HG2	1:71:B:ASP:HA	4	1.0
(1,38)	1:58:B:VAL:HG12	1:61:B:HIS:HA	9	1.0
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	8	1.0
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	8	1.0
(3,1508)	1:113:B:THR:H	1:107:B:PRO:HD3	4	0.99
(3,1507)	1:113:A:THR:H	1:107:A:PRO:HD3	4	0.99
(3,668)	1:63:B:MET:HE3	1:32:B:LEU:HB2	3	0.99
(3,668)	1:63:B:MET:HE3	1:32:B:LEU:HB2	7	0.99
(3,667)	1:63:A:MET:HE3	1:32:A:LEU:HB2	7	0.99
(3,545)	1:33:A:ASN:HA	1:31:A:THR:HG21	9	0.99
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	8	0.99
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	8	0.99
(1,1820)	1:21:B:GLN:H	1:40:B:LEU:HG	8	0.99
(1,1819)	1:21:A:GLN:H	1:40:A:LEU:HG	8	0.99
(1,1797)	1:16:A:ILE:H	1:17:A:ASN:HB2	3	0.99
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	7	0.99
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	7	0.99
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD22	6	0.99
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD22	6	0.99
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD22	2	0.99
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD23	7	0.99
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD22	2	0.99
(1,1097)	1:59:A:ILE:HG23	1:42:A:ARG:HD2	5	0.99
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	7	0.99
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	10	0.99
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	10	0.99
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG21	8	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG2	2	0.99
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG2	2	0.99
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	2	0.99
(1,442)	1:10:B:ARG:HG2	1:4:B:LYS:HG3	6	0.99
(1,441)	1:10:A:ARG:HG2	1:4:A:LYS:HG3	6	0.99
(1,439)	1:10:A:ARG:HG2	1:11:A:ASN:HB2	6	0.99
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD21	7	0.99
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD21	7	0.99
(1,372)	1:7:B:GLN:HG2	1:17:A:ASN:HB2	4	0.99
(1,142)	1:80:B:ILE:HD11	1:83:A:MET:HE3	8	0.99
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	7	0.99
(1,49)	1:64:A:GLU:HG2	1:71:A:ASP:HA	4	0.99
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG23	3	0.98
(3,752)	1:59:B:ILE:HG21	1:61:B:HIS:HB3	8	0.98
(3,667)	1:63:A:MET:HE3	1:32:A:LEU:HB2	3	0.98
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	2	0.98
(3,228)	1:24:B:VAL:HB	1:32:B:LEU:HD22	6	0.98
(3,227)	1:24:A:VAL:HB	1:32:A:LEU:HD22	6	0.98
(3,90)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	8	0.98
(3,89)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	8	0.98
(1,1826)	1:16:B:ILE:H	1:17:B:ASN:HB2	3	0.98
(1,1825)	1:16:A:ILE:H	1:17:A:ASN:HB2	3	0.98
(1,1798)	1:16:B:ILE:H	1:17:B:ASN:HB2	3	0.98
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	10	0.98
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	5	0.98
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	10	0.98
(1,1522)	1:41:B:VAL:H	1:42:B:ARG:HG3	1	0.98
(1,1521)	1:41:A:VAL:H	1:42:A:ARG:HG3	1	0.98
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	2	0.98
(1,1444)	1:24:B:VAL:H	1:32:B:LEU:HD23	3	0.98
(1,1443)	1:24:A:VAL:H	1:32:A:LEU:HD23	3	0.98
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD21	5	0.98
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD21	5	0.98
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD12	4	0.98
(1,1216)	1:49:B:LEU:HB3	1:62:B:ILE:HB	6	0.98
(1,1215)	1:49:A:LEU:HB3	1:62:A:ILE:HB	6	0.98
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG21	5	0.98
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	7	0.98
(1,974)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	8	0.98
(1,973)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	8	0.98
(1,948)	1:86:B:LEU:HA	1:83:B:MET:HB3	4	0.98
(1,948)	1:86:B:LEU:HA	1:83:B:MET:HB3	7	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:86:A:LEU:HA	1:83:A:MET:HB3	4	0.98
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	9	0.98
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG2	9	0.98
(1,769)	1:59:A:ILE:HD12	1:42:A:ARG:HD2	2	0.98
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	5	0.98
(1,372)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	8	0.98
(1,371)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	8	0.98
(1,141)	1:80:A:ILE:HD11	1:83:B:MET:HE3	8	0.98
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	7	0.98
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	3	0.98
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	3	0.98
(3,751)	1:59:A:ILE:HG21	1:61:A:HIS:HB3	8	0.97
(3,720)	1:31:B:THR:HG22	1:74:B:LEU:HB2	2	0.97
(3,719)	1:31:A:THR:HG22	1:74:A:LEU:HB2	2	0.97
(3,667)	1:63:A:MET:HE3	1:32:A:LEU:HB2	1	0.97
(3,640)	1:8:B:LEU:HD13	1:83:A:MET:HG3	2	0.97
(3,516)	1:21:B:GLN:HG3	1:25:B:LYS:HE3	1	0.97
(3,515)	1:21:A:GLN:HG3	1:25:A:LYS:HE3	1	0.97
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	2	0.97
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	5	0.97
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	2	0.97
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD22	4	0.97
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD13	2	0.97
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD13	2	0.97
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD12	4	0.97
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG21	5	0.97
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	4	0.97
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	5	0.97
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	4	0.97
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD13	1	0.97
(1,947)	1:86:A:LEU:HA	1:83:A:MET:HB3	7	0.97
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	6	0.97
(1,770)	1:59:B:ILE:HD12	1:42:B:ARG:HD2	2	0.97
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	5	0.97
(1,555)	1:47:A:ASN:HA	1:5:B:MET:H	2	0.97
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	2	0.97
(1,472)	1:79:B:PHE:HB3	1:76:B:PHE:HB3	10	0.97
(1,471)	1:79:A:PHE:HB3	1:76:A:PHE:HB3	10	0.97
(1,371)	1:7:A:GLN:HG2	1:17:B:ASN:HB2	4	0.97
(1,336)	1:41:B:VAL:HG12	1:48:B:PHE:H	9	0.97
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	4	0.97
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	5	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	4	0.97
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD11	6	0.96
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD13	3	0.96
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD11	6	0.96
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG23	3	0.96
(3,970)	1:7:B:GLN:H	1:14:A:THR:HG22	10	0.96
(3,816)	1:51:B:LYS:HG2	1:109:B:LEU:HD21	6	0.96
(3,815)	1:51:A:LYS:HG2	1:109:A:LEU:HD21	6	0.96
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	9	0.96
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	9	0.96
(3,668)	1:63:B:MET:HE3	1:32:B:LEU:HB2	1	0.96
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD22	8	0.96
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD22	8	0.96
(1,1590)	1:10:B:ARG:H	1:12:B:ILE:HA	7	0.96
(1,1589)	1:10:A:ARG:H	1:12:A:ILE:HA	7	0.96
(1,1574)	1:48:B:PHE:H	1:41:B:VAL:HA	5	0.96
(1,1573)	1:48:A:PHE:H	1:41:A:VAL:HA	5	0.96
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	6	0.96
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	6	0.96
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD22	4	0.96
(1,1224)	1:50:B:LYS:HA	1:45:B:LEU:HA	1	0.96
(1,1223)	1:50:A:LYS:HA	1:45:A:LEU:HA	1	0.96
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD13	6	0.96
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD13	6	0.96
(1,994)	1:109:B:LEU:HD13	1:47:B:ASN:HB3	7	0.96
(1,993)	1:109:A:LEU:HD13	1:47:A:ASN:HB3	7	0.96
(1,991)	1:8:A:LEU:HD23	1:48:B:PHE:HB2	10	0.96
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	5	0.96
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	6	0.96
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	9	0.96
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	9	0.96
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD21	6	0.96
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD21	6	0.96
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	2	0.96
(1,394)	1:33:B:ASN:HB2	1:63:B:MET:HG3	10	0.96
(1,393)	1:33:A:ASN:HB2	1:63:A:MET:HG3	10	0.96
(1,335)	1:41:A:VAL:HG12	1:48:A:PHE:H	9	0.96
(1,70)	1:33:B:ASN:HB2	1:63:B:MET:HG3	10	0.96
(1,69)	1:33:A:ASN:HB2	1:63:A:MET:HG3	10	0.96
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	5	0.96
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	10	0.96
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	10	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1508)	1:113:B:THR:H	1:107:B:PRO:HD2	10	0.95
(3,1507)	1:113:A:THR:H	1:107:A:PRO:HD2	10	0.95
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD13	3	0.95
(3,969)	1:7:A:GLN:H	1:14:B:THR:HG22	10	0.95
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	2	0.95
(3,600)	1:53:B:ASN:HB2	1:46:B:GLN:HG3	7	0.95
(3,599)	1:53:A:ASN:HB2	1:46:A:GLN:HG3	7	0.95
(1,1573)	1:48:A:PHE:H	1:41:A:VAL:HA	10	0.95
(1,1548)	1:43:B:LYS:H	1:40:B:LEU:HG	2	0.95
(1,1547)	1:43:A:LYS:H	1:40:A:LEU:HG	2	0.95
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD23	10	0.95
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD23	10	0.95
(1,1389)	1:5:A:MET:H	1:110:B:GLY:H	10	0.95
(1,1218)	1:87:B:THR:HG22	1:83:B:MET:HB3	9	0.95
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD22	6	0.95
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD22	6	0.95
(1,992)	1:8:B:LEU:HD23	1:48:A:PHE:HB2	10	0.95
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	8	0.95
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	8	0.95
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG2	9	0.95
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	2	0.95
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	10	0.95
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	10	0.95
(1,230)	1:62:B:ILE:HG21	1:41:B:VAL:HG21	8	0.95
(1,229)	1:62:A:ILE:HG21	1:41:A:VAL:HG21	8	0.95
(1,190)	1:77:B:GLU:HA	1:87:A:THR:HG22	3	0.95
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG12	10	0.94
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG12	10	0.94
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	2	0.94
(3,515)	1:21:A:GLN:HG3	1:25:A:LYS:HE3	2	0.94
(1,1574)	1:48:B:PHE:H	1:41:B:VAL:HA	10	0.94
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	1	0.94
(1,1510)	1:39:B:GLU:H	1:38:B:LYS:HD3	7	0.94
(1,1509)	1:39:A:GLU:H	1:38:A:LYS:HD3	7	0.94
(1,1390)	1:5:B:MET:H	1:110:A:GLY:H	10	0.94
(1,1224)	1:42:B:ARG:HA	1:45:B:LEU:HA	5	0.94
(1,1223)	1:42:A:ARG:HA	1:45:A:LEU:HA	5	0.94
(1,1218)	1:87:B:THR:HG21	1:83:B:MET:HB3	8	0.94
(1,1217)	1:87:A:THR:HG21	1:83:A:MET:HB3	8	0.94
(1,1217)	1:87:A:THR:HG22	1:83:A:MET:HB3	9	0.94
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG2	9	0.94
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	2	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG2	10	0.94
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG2	10	0.94
(1,561)	1:16:A:ILE:HB	1:93:B:LYS:HB3	6	0.94
(1,534)	1:86:B:LEU:HD22	1:89:B:ALA:HA	4	0.94
(1,533)	1:86:A:LEU:HD22	1:89:A:ALA:HA	4	0.94
(1,480)	1:63:B:MET:HB2	1:82:B:LEU:HD23	9	0.94
(1,479)	1:63:A:MET:HB2	1:82:A:LEU:HD23	9	0.94
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD23	6	0.94
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD23	6	0.94
(1,189)	1:77:A:GLU:HA	1:87:B:THR:HG22	3	0.94
(1,38)	1:58:B:VAL:HG12	1:61:B:HIS:HA	8	0.94
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB3	5	0.93
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB3	5	0.93
(3,752)	1:59:B:ILE:HG21	1:61:B:HIS:HB3	10	0.93
(3,751)	1:59:A:ILE:HG21	1:61:A:HIS:HB3	10	0.93
(3,516)	1:21:B:GLN:HG3	1:25:B:LYS:HE3	2	0.93
(3,90)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	3	0.93
(3,89)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	3	0.93
(1,1826)	1:16:B:ILE:H	1:17:B:ASN:HB2	8	0.93
(1,1825)	1:16:A:ILE:H	1:17:A:ASN:HB2	8	0.93
(1,1804)	1:109:B:LEU:H	1:113:B:THR:H	10	0.93
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	2	0.93
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	1	0.93
(1,1546)	1:43:B:LYS:H	1:59:B:ILE:HD11	1	0.93
(1,1545)	1:43:A:LYS:H	1:59:A:ILE:HD11	1	0.93
(1,1544)	1:43:B:LYS:H	1:42:B:ARG:HG3	10	0.93
(1,1510)	1:67:B:ASP:H	1:66:B:LEU:HG	3	0.93
(1,1509)	1:67:A:ASP:H	1:66:A:LEU:HG	3	0.93
(1,1509)	1:67:A:ASP:H	1:66:A:LEU:HG	4	0.93
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD21	2	0.93
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD21	2	0.93
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	7	0.93
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	7	0.93
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG22	10	0.93
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG22	10	0.93
(1,994)	1:109:B:LEU:HD22	1:47:B:ASN:HB3	8	0.93
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD13	1	0.93
(1,974)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	3	0.93
(1,973)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	3	0.93
(1,757)	1:111:A:GLU:HG2	1:107:A:PRO:HD2	1	0.93
(1,598)	1:85:B:ARG:HG3	1:66:B:LEU:HD23	9	0.93
(1,597)	1:85:A:ARG:HG3	1:66:A:LEU:HD23	9	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:16:B:ILE:HB	1:93:A:LYS:HB3	6	0.93
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	1	0.93
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	3	0.93
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	7	0.93
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	7	0.93
(1,37)	1:58:A:VAL:HG12	1:61:A:HIS:HA	8	0.93
(1,17)	1:93:A:LYS:HA	1:109:A:LEU:HD12	10	0.93
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD12	4	0.92
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD13	5	0.92
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD12	4	0.92
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD13	5	0.92
(3,960)	1:75:B:SER:H	1:63:B:MET:HE1	4	0.92
(3,959)	1:75:A:SER:H	1:63:A:MET:HE1	4	0.92
(3,50)	1:78:B:GLU:HG2	1:77:B:GLU:H	3	0.92
(3,49)	1:78:A:GLU:HG2	1:77:A:GLU:H	3	0.92
(1,1803)	1:109:A:LEU:H	1:113:A:THR:H	10	0.92
(1,1581)	1:50:A:LYS:H	1:45:A:LEU:HD22	8	0.92
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	2	0.92
(1,1544)	1:43:B:LYS:H	1:42:B:ARG:HG3	2	0.92
(1,1543)	1:43:A:LYS:H	1:42:A:ARG:HG3	2	0.92
(1,1543)	1:43:A:LYS:H	1:42:A:ARG:HG3	10	0.92
(1,1510)	1:67:B:ASP:H	1:66:B:LEU:HG	4	0.92
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD21	10	0.92
(1,1224)	1:50:B:LYS:HA	1:45:B:LEU:HA	4	0.92
(1,1223)	1:50:A:LYS:HA	1:45:A:LEU:HA	4	0.92
(1,1138)	1:14:B:THR:HG22	1:12:B:ILE:HA	8	0.92
(1,1137)	1:14:A:THR:HG22	1:12:A:ILE:HA	8	0.92
(1,994)	1:109:B:LEU:HD21	1:47:B:ASN:HB2	4	0.92
(1,993)	1:109:A:LEU:HD21	1:47:A:ASN:HB2	4	0.92
(1,993)	1:109:A:LEU:HD22	1:47:A:ASN:HB3	8	0.92
(1,877)	1:34:A:GLN:HB2	1:72:A:LYS:HD2	9	0.92
(1,758)	1:111:B:GLU:HG2	1:107:B:PRO:HD2	1	0.92
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG11	10	0.92
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG11	10	0.92
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	1	0.92
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	3	0.92
(1,230)	1:12:B:ILE:HG21	1:80:B:ILE:HD12	6	0.92
(1,229)	1:12:A:ILE:HG21	1:80:A:ILE:HD12	6	0.92
(1,18)	1:93:B:LYS:HA	1:109:B:LEU:HD12	10	0.92
(3,642)	1:8:B:LEU:HD11	1:15:A:ILE:HD11	5	0.91
(3,641)	1:8:A:LEU:HD11	1:15:B:ILE:HD11	5	0.91
(3,384)	1:51:B:LYS:HD3	1:109:B:LEU:HD23	4	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,383)	1:51:A:LYS:HD3	1:109:A:LEU:HD23	4	0.91
(3,276)	1:53:B:ASN:HB2	1:52:B:GLU:HG3	7	0.91
(3,275)	1:53:A:ASN:HB2	1:52:A:GLU:HG3	7	0.91
(1,1708)	1:79:B:PHE:H	1:87:A:THR:HG21	5	0.91
(1,1707)	1:79:A:PHE:H	1:87:B:THR:HG21	5	0.91
(1,1632)	1:60:B:GLU:H	1:41:B:VAL:HG21	8	0.91
(1,1631)	1:60:A:GLU:H	1:41:A:VAL:HG21	8	0.91
(1,1582)	1:50:B:LYS:H	1:45:B:LEU:HD22	8	0.91
(1,1510)	1:39:B:GLU:H	1:38:B:LYS:HD3	8	0.91
(1,1509)	1:39:A:GLU:H	1:38:A:LYS:HD3	8	0.91
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD21	7	0.91
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD21	7	0.91
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD21	10	0.91
(1,1204)	1:60:B:GLU:HB2	1:62:B:ILE:HG13	1	0.91
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	2	0.91
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD23	8	0.91
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	2	0.91
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	2	0.91
(1,878)	1:34:B:GLN:HB2	1:72:B:LYS:HD2	9	0.91
(1,810)	1:68:B:THR:H	1:74:B:LEU:HG	7	0.91
(1,809)	1:68:A:THR:H	1:74:A:LEU:HG	7	0.91
(1,599)	1:18:A:THR:HG21	1:11:B:ASN:HB2	4	0.91
(1,280)	1:19:B:PHE:HB2	1:32:B:LEU:HB2	8	0.91
(1,279)	1:19:A:PHE:HB2	1:32:A:LEU:HB2	8	0.91
(1,230)	1:62:B:ILE:HG22	1:41:B:VAL:HG22	2	0.91
(1,229)	1:62:A:ILE:HG22	1:41:A:VAL:HG22	2	0.91
(1,130)	1:16:B:ILE:HD12	1:17:B:ASN:HA	4	0.91
(1,129)	1:16:A:ILE:HD12	1:17:A:ASN:HA	4	0.91
(1,105)	1:7:A:GLN:HG3	1:15:B:ILE:HD11	2	0.91
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	7	0.91
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD12	1	0.9
(3,794)	1:107:B:PRO:HG2	1:93:B:LYS:HG3	4	0.9
(3,793)	1:107:A:PRO:HG2	1:93:A:LYS:HG3	4	0.9
(1,1709)	1:79:A:PHE:H	1:66:A:LEU:HD22	8	0.9
(1,1509)	1:67:A:ASP:H	1:66:A:LEU:HG	9	0.9
(1,1498)	1:44:B:ASP:H	1:49:B:LEU:HD11	6	0.9
(1,1497)	1:44:A:ASP:H	1:49:A:LEU:HD11	6	0.9
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD21	3	0.9
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD21	3	0.9
(1,1203)	1:60:A:GLU:HB2	1:62:A:ILE:HG13	1	0.9
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	2	0.9
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG22	3	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG23	4	0.9
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG22	3	0.9
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD23	8	0.9
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	6	0.9
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	4	0.9
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	4	0.9
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	4	0.9
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	4	0.9
(1,698)	1:107:B:PRO:HG2	1:93:B:LYS:HG3	4	0.9
(1,697)	1:107:A:PRO:HG2	1:93:A:LYS:HG3	4	0.9
(1,680)	1:37:B:PHE:HB2	1:62:B:ILE:HG22	7	0.9
(1,679)	1:37:A:PHE:HB2	1:62:A:ILE:HG22	7	0.9
(1,662)	1:49:B:LEU:HG	1:52:B:GLU:HG3	7	0.9
(1,661)	1:49:A:LEU:HG	1:52:A:GLU:HG3	7	0.9
(1,600)	1:18:B:THR:HG21	1:11:A:ASN:HB2	4	0.9
(1,582)	1:42:B:ARG:HB3	1:53:B:ASN:HB2	3	0.9
(1,581)	1:42:A:ARG:HB3	1:53:A:ASN:HB2	3	0.9
(1,492)	1:37:B:PHE:HB2	1:62:B:ILE:HG22	7	0.9
(1,491)	1:37:A:PHE:HB2	1:62:A:ILE:HG22	7	0.9
(1,406)	1:42:B:ARG:HB3	1:53:B:ASN:HB2	3	0.9
(1,405)	1:42:A:ARG:HB3	1:53:A:ASN:HB2	3	0.9
(1,38)	1:58:B:VAL:HG23	1:53:B:ASN:HA	1	0.9
(1,37)	1:58:A:VAL:HG23	1:53:A:ASN:HA	1	0.9
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	7	0.9
(4,258)	1:108:B:GLY:H	1:111:B:GLU:HA	6	0.89
(4,257)	1:108:A:GLY:H	1:111:A:GLU:HA	6	0.89
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD23	8	0.89
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD12	1	0.89
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD23	8	0.89
(1,1710)	1:79:B:PHE:H	1:66:B:LEU:HD22	8	0.89
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	5	0.89
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	5	0.89
(1,1574)	1:48:B:PHE:H	1:41:B:VAL:HA	2	0.89
(1,1573)	1:48:A:PHE:H	1:41:A:VAL:HA	2	0.89
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	3	0.89
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	8	0.89
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	9	0.89
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	3	0.89
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	8	0.89
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	9	0.89
(1,1510)	1:67:B:ASP:H	1:66:B:LEU:HG	9	0.89
(1,1510)	1:67:B:ASP:H	1:66:B:LEU:HG	10	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:67:A:ASP:H	1:66:A:LEU:HG	10	0.89
(1,1270)	1:48:B:PHE:H	1:4:A:LYS:HE3	2	0.89
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD13	7	0.89
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD13	7	0.89
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG21	8	0.89
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG23	4	0.89
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG21	8	0.89
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	6	0.89
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB1	6	0.89
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB1	6	0.89
(1,862)	1:25:B:LYS:HD2	1:33:B:ASN:HB2	8	0.89
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD22	3	0.89
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD21	4	0.89
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD21	4	0.89
(1,395)	1:33:A:ASN:HB3	1:34:A:GLN:HG2	9	0.89
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	1	0.89
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	1	0.89
(1,262)	1:8:B:LEU:HG	1:40:A:LEU:HG	9	0.89
(1,261)	1:8:A:LEU:HG	1:40:B:LEU:HG	9	0.89
(1,230)	1:12:B:ILE:HG21	1:80:B:ILE:HD11	3	0.89
(1,229)	1:12:A:ILE:HG21	1:80:A:ILE:HD11	3	0.89
(1,118)	1:66:B:LEU:HG	1:62:B:ILE:HD11	1	0.89
(1,117)	1:66:A:LEU:HG	1:62:A:ILE:HD11	1	0.89
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD23	2	0.88
(1,1522)	1:41:B:VAL:H	1:49:B:LEU:HB2	4	0.88
(1,1521)	1:41:A:VAL:H	1:49:A:LEU:HB2	4	0.88
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	1	0.88
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	1	0.88
(1,1498)	1:38:B:LYS:H	1:59:B:ILE:HD11	3	0.88
(1,1497)	1:38:A:LYS:H	1:59:A:ILE:HD11	3	0.88
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD22	10	0.88
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD22	10	0.88
(1,1224)	1:50:B:LYS:HA	1:45:B:LEU:HA	8	0.88
(1,1224)	1:50:B:LYS:HA	1:45:B:LEU:HA	10	0.88
(1,1223)	1:50:A:LYS:HA	1:45:A:LEU:HA	8	0.88
(1,1223)	1:50:A:LYS:HA	1:45:A:LEU:HA	10	0.88
(1,1175)	1:107:A:PRO:HG2	1:109:A:LEU:H	1	0.88
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE1	7	0.88
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE1	7	0.88
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG21	9	0.88
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG21	9	0.88
(1,861)	1:25:A:LYS:HD2	1:33:A:ASN:HB2	8	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:107:A:PRO:HG2	1:109:A:LEU:H	1	0.88
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD22	3	0.88
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	10	0.88
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	2	0.88
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	2	0.88
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD12	3	0.88
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD12	3	0.88
(1,268)	1:66:B:LEU:HG	1:85:B:ARG:HB2	1	0.88
(1,267)	1:66:A:LEU:HG	1:85:A:ARG:HB2	1	0.88
(1,106)	1:7:B:GLN:HG3	1:15:A:ILE:HD11	2	0.88
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	1	0.88
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB3	2	0.87
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB3	2	0.87
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG12	5	0.87
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG12	5	0.87
(3,480)	1:111:B:GLU:HG2	1:109:B:LEU:HB3	7	0.87
(3,479)	1:111:A:GLU:HG2	1:109:A:LEU:HB3	7	0.87
(3,15)	1:101:A:PRO:HG3	1:102:A:GLY:HA2	8	0.87
(1,1797)	1:16:A:ILE:H	1:17:A:ASN:HB2	10	0.87
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD12	9	0.87
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD23	2	0.87
(1,1572)	1:47:B:ASN:H	1:45:B:LEU:HB3	4	0.87
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD22	4	0.87
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD12	3	0.87
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD12	3	0.87
(1,1176)	1:107:B:PRO:HG2	1:109:B:LEU:H	1	0.87
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG3	6	0.87
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG3	6	0.87
(1,746)	1:111:B:GLU:HG2	1:109:B:LEU:HB3	7	0.87
(1,745)	1:111:A:GLU:HG2	1:109:A:LEU:HB3	7	0.87
(1,688)	1:107:B:PRO:HG2	1:109:B:LEU:H	1	0.87
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD23	1	0.87
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD23	1	0.87
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG2	4	0.87
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG2	4	0.87
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	4	0.87
(1,478)	1:63:B:MET:HB2	1:37:B:PHE:HB3	9	0.87
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	10	0.87
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	4	0.87
(1,477)	1:63:A:MET:HB2	1:37:A:PHE:HB3	9	0.87
(1,396)	1:33:B:ASN:HB3	1:34:B:GLN:HG2	9	0.87
(1,262)	1:8:B:LEU:HG	1:40:A:LEU:HG	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:16:B:ILE:HD12	1:17:B:ASN:HA	3	0.87
(1,129)	1:16:A:ILE:HD12	1:17:A:ASN:HA	3	0.87
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	1	0.87
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	1	0.87
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD13	10	0.86
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD13	10	0.86
(3,960)	1:75:B:SER:H	1:63:B:MET:HE2	10	0.86
(3,959)	1:75:A:SER:H	1:63:A:MET:HE2	10	0.86
(3,50)	1:78:B:GLU:HG2	1:77:B:GLU:H	8	0.86
(3,49)	1:78:A:GLU:HG2	1:77:A:GLU:H	8	0.86
(3,16)	1:101:B:PRO:HG3	1:102:B:GLY:HA2	8	0.86
(1,1826)	1:16:B:ILE:H	1:17:B:ASN:HB2	10	0.86
(1,1825)	1:16:A:ILE:H	1:17:A:ASN:HB2	10	0.86
(1,1798)	1:16:B:ILE:H	1:17:B:ASN:HB2	10	0.86
(1,1782)	1:89:B:ALA:H	1:93:B:LYS:HB2	6	0.86
(1,1781)	1:89:A:ALA:H	1:93:A:LYS:HB2	6	0.86
(1,1781)	1:89:A:ALA:H	1:93:A:LYS:HB2	10	0.86
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD12	9	0.86
(1,1571)	1:47:A:ASN:H	1:45:A:LEU:HB3	4	0.86
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG3	9	0.86
(1,1269)	1:48:A:PHE:H	1:4:B:LYS:HE3	2	0.86
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD12	5	0.86
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD12	5	0.86
(1,1054)	1:31:B:THR:HG21	1:71:B:ASP:HB3	7	0.86
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB2	9	0.86
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	6	0.86
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	6	0.86
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	6	0.86
(1,612)	1:53:B:ASN:H	1:50:B:LYS:HD3	3	0.86
(1,611)	1:53:A:ASN:H	1:50:A:LYS:HD3	3	0.86
(1,354)	1:58:B:VAL:HG22	1:54:B:LYS:HA	2	0.86
(1,353)	1:58:A:VAL:HG22	1:54:A:LYS:HA	2	0.86
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	5	0.86
(1,261)	1:8:A:LEU:HG	1:40:B:LEU:HG	4	0.86
(1,234)	1:46:B:GLN:HA	1:44:B:ASP:HB2	7	0.86
(1,233)	1:46:A:GLN:HA	1:44:A:ASP:HB2	7	0.86
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG3	6	0.85
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG3	6	0.85
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD21	7	0.85
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD21	7	0.85
(3,794)	1:107:B:PRO:HG3	1:93:B:LYS:HG2	1	0.85
(3,793)	1:107:A:PRO:HG3	1:93:A:LYS:HG2	1	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	8	0.85
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	8	0.85
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD13	2	0.85
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD13	2	0.85
(1,1782)	1:89:B:ALA:H	1:93:B:LYS:HB2	10	0.85
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG3	6	0.85
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG3	6	0.85
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG3	9	0.85
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD22	4	0.85
(1,1053)	1:31:A:THR:HG21	1:71:A:ASP:HB3	7	0.85
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD21	8	0.85
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB2	9	0.85
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG2	6	0.85
(1,698)	1:107:B:PRO:HG3	1:93:B:LYS:HG2	1	0.85
(1,697)	1:107:A:PRO:HG3	1:93:A:LYS:HG2	1	0.85
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	2	0.85
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	2	0.85
(1,590)	1:85:B:ARG:HG3	1:83:B:MET:HG2	5	0.85
(1,589)	1:85:A:ARG:HG3	1:83:A:MET:HG2	5	0.85
(1,534)	1:86:B:LEU:HD23	1:89:B:ALA:HA	6	0.85
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	5	0.85
(1,130)	1:16:B:ILE:HD12	1:17:B:ASN:HA	5	0.85
(1,129)	1:16:A:ILE:HD12	1:17:A:ASN:HA	5	0.85
(3,720)	1:31:B:THR:HG23	1:74:B:LEU:HB2	4	0.84
(3,719)	1:31:A:THR:HG23	1:74:A:LEU:HB2	4	0.84
(1,1544)	1:43:B:LYS:H	1:42:B:ARG:HG3	3	0.84
(1,1543)	1:43:A:LYS:H	1:42:A:ARG:HG3	3	0.84
(1,1510)	1:67:B:ASP:H	1:66:B:LEU:HG	2	0.84
(1,1509)	1:67:A:ASP:H	1:66:A:LEU:HG	2	0.84
(1,1498)	1:38:B:LYS:H	1:59:B:ILE:HD12	2	0.84
(1,1497)	1:38:A:LYS:H	1:59:A:ILE:HD12	2	0.84
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG21	7	0.84
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG21	7	0.84
(1,1422)	1:22:B:TYR:H	1:36:B:GLU:HG2	1	0.84
(1,1421)	1:22:A:TYR:H	1:36:A:GLU:HG2	1	0.84
(1,1396)	1:19:B:PHE:H	1:15:B:ILE:HD12	1	0.84
(1,1395)	1:19:A:PHE:H	1:15:A:ILE:HD12	1	0.84
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD3	9	0.84
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD3	9	0.84
(1,1104)	1:58:B:VAL:H	1:59:B:ILE:HG21	1	0.84
(1,1103)	1:58:A:VAL:H	1:59:A:ILE:HG21	1	0.84
(1,996)	1:109:B:LEU:HD12	1:93:B:LYS:HD3	8	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:109:B:LEU:HD12	1:93:B:LYS:HB3	10	0.84
(1,995)	1:109:A:LEU:HD12	1:93:A:LYS:HD3	8	0.84
(1,995)	1:109:A:LEU:HD12	1:93:A:LYS:HB3	10	0.84
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD21	8	0.84
(1,600)	1:18:B:THR:HG21	1:43:B:LYS:HE2	7	0.84
(1,533)	1:86:A:LEU:HD23	1:89:A:ALA:HA	6	0.84
(1,66)	1:74:B:LEU:HG	1:62:B:ILE:HG22	7	0.84
(1,65)	1:74:A:LEU:HG	1:62:A:ILE:HG22	7	0.84
(4,258)	1:108:B:GLY:H	1:111:B:GLU:HA	9	0.83
(4,257)	1:108:A:GLY:H	1:111:A:GLU:HA	9	0.83
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB3	4	0.83
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG11	9	0.83
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG13	9	0.83
(3,16)	1:101:B:PRO:HG3	1:102:B:GLY:HA2	2	0.83
(3,15)	1:101:A:PRO:HG3	1:102:A:GLY:HA2	2	0.83
(1,1798)	1:5:B:MET:H	1:4:B:LYS:HE3	9	0.83
(1,1308)	1:10:B:ARG:H	1:11:B:ASN:HB2	1	0.83
(1,1307)	1:10:A:ARG:H	1:11:A:ASN:HB2	1	0.83
(1,1302)	1:9:B:GLU:H	1:40:A:LEU:HD11	7	0.83
(1,1204)	1:60:B:GLU:HB2	1:62:B:ILE:HG12	9	0.83
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	6	0.83
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	6	0.83
(1,754)	1:111:B:GLU:HG3	1:51:B:LYS:HE2	5	0.83
(1,753)	1:111:A:GLU:HG3	1:51:A:LYS:HE2	5	0.83
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	6	0.83
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	6	0.83
(1,710)	1:21:B:GLN:HG3	1:23:B:SER:HA	3	0.83
(1,709)	1:21:A:GLN:HG3	1:23:A:SER:HA	3	0.83
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	9	0.83
(1,623)	1:21:A:GLN:HA	1:25:A:LYS:HE3	3	0.83
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD22	9	0.83
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD22	9	0.83
(1,600)	1:18:B:THR:HG21	1:11:A:ASN:HB3	9	0.83
(1,599)	1:18:A:THR:HG21	1:43:A:LYS:HE2	7	0.83
(1,599)	1:18:A:THR:HG21	1:11:B:ASN:HB3	9	0.83
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	8	0.83
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	8	0.83
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	3	0.83
(1,456)	1:7:B:GLN:HB3	1:9:B:GLU:HG3	9	0.83
(1,455)	1:7:A:GLN:HB3	1:9:A:GLU:HG3	9	0.83
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	7	0.83
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	1	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG2	10	0.82
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG2	10	0.82
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB3	4	0.82
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG12	3	0.82
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG12	3	0.82
(3,780)	1:21:B:GLN:HG2	1:40:B:LEU:HB2	7	0.82
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE3	7	0.82
(3,526)	1:76:B:PHE:HB2	1:16:B:ILE:HA	2	0.82
(3,525)	1:76:A:PHE:HB2	1:16:A:ILE:HA	2	0.82
(1,1820)	1:21:B:GLN:H	1:40:B:LEU:HG	4	0.82
(1,1819)	1:21:A:GLN:H	1:40:A:LEU:HG	4	0.82
(1,1798)	1:5:B:MET:H	1:4:B:LYS:HE3	2	0.82
(1,1797)	1:5:A:MET:H	1:4:A:LYS:HE3	2	0.82
(1,1797)	1:5:A:MET:H	1:4:A:LYS:HE3	9	0.82
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG2	10	0.82
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG2	10	0.82
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD12	4	0.82
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB3	6	0.82
(1,1308)	1:10:B:ARG:H	1:11:B:ASN:HB2	10	0.82
(1,1307)	1:10:A:ARG:H	1:11:A:ASN:HB2	10	0.82
(1,1301)	1:9:A:GLU:H	1:40:B:LEU:HD11	7	0.82
(1,1203)	1:60:A:GLU:HB2	1:62:A:ILE:HG12	9	0.82
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB2	10	0.82
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB2	10	0.82
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD12	5	0.82
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD12	5	0.82
(1,812)	1:21:B:GLN:HG3	1:39:B:GLU:HG2	7	0.82
(1,811)	1:21:A:GLN:HG3	1:39:A:GLU:HG2	7	0.82
(1,714)	1:21:B:GLN:HG2	1:40:B:LEU:HB2	7	0.82
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	7	0.82
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	9	0.82
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	7	0.82
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	1	0.82
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	4	0.82
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	1	0.82
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	4	0.82
(1,555)	1:47:A:ASN:HA	1:5:B:MET:H	3	0.82
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	7	0.82
(1,23)	1:96:A:GLU:HA	1:107:A:PRO:HD2	10	0.82
(3,916)	1:47:B:ASN:H	1:5:A:MET:HG3	1	0.81
(3,779)	1:21:A:GLN:HG2	1:40:A:LEU:HB2	7	0.81
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE3	7	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD13	7	0.81
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD13	7	0.81
(3,276)	1:53:B:ASN:HB2	1:52:B:GLU:HG2	3	0.81
(3,275)	1:53:A:ASN:HB2	1:52:A:GLU:HG2	3	0.81
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG3	3	0.81
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG3	3	0.81
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD12	4	0.81
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB3	6	0.81
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD23	3	0.81
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD23	3	0.81
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD22	5	0.81
(1,988)	1:48:B:PHE:HB3	1:109:B:LEU:H	6	0.81
(1,987)	1:48:A:PHE:HB3	1:109:A:LEU:H	6	0.81
(1,713)	1:21:A:GLN:HG2	1:40:A:LEU:HB2	7	0.81
(1,624)	1:21:B:GLN:HA	1:25:B:LYS:HE3	3	0.81
(1,616)	1:42:B:ARG:HA	1:45:B:LEU:HD11	5	0.81
(1,615)	1:42:A:ARG:HA	1:45:A:LEU:HD11	5	0.81
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	3	0.81
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	3	0.81
(1,480)	1:63:B:MET:HB2	1:59:B:ILE:HD12	2	0.81
(1,479)	1:63:A:MET:HB2	1:59:A:ILE:HD12	2	0.81
(1,280)	1:19:B:PHE:HB3	1:32:B:LEU:HB2	1	0.81
(1,279)	1:19:A:PHE:HB3	1:32:A:LEU:HB2	1	0.81
(1,24)	1:96:B:GLU:HA	1:107:B:PRO:HD2	10	0.81
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	4	0.81
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	4	0.81
(3,494)	1:59:B:ILE:HD12	1:38:B:LYS:HE2	2	0.8
(3,493)	1:59:A:ILE:HD12	1:38:A:LYS:HE2	2	0.8
(1,1852)	1:5:B:MET:H	1:5:B:MET:HG3	2	0.8
(1,1825)	1:16:A:ILE:H	1:17:A:ASN:HB2	4	0.8
(1,1798)	1:16:B:ILE:H	1:17:B:ASN:HB2	4	0.8
(1,1797)	1:16:A:ILE:H	1:17:A:ASN:HB2	4	0.8
(1,1522)	1:41:B:VAL:H	1:49:B:LEU:HB2	9	0.8
(1,1521)	1:41:A:VAL:H	1:49:A:LEU:HB2	9	0.8
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	2	0.8
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	10	0.8
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD22	2	0.8
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD22	2	0.8
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD22	5	0.8
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD21	4	0.8
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD21	4	0.8
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD21	4	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	5	0.8
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	5	0.8
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	6	0.8
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	6	0.8
(1,442)	1:10:B:ARG:HG3	1:4:B:LYS:HG2	2	0.8
(1,441)	1:10:A:ARG:HG3	1:4:A:LYS:HG2	2	0.8
(1,130)	1:16:B:ILE:HD13	1:17:B:ASN:HA	8	0.8
(1,130)	1:16:B:ILE:HD13	1:17:B:ASN:HA	9	0.8
(1,129)	1:16:A:ILE:HD13	1:17:A:ASN:HA	8	0.8
(1,129)	1:16:A:ILE:HD13	1:17:A:ASN:HA	9	0.8
(1,27)	1:58:A:VAL:HG13	1:53:A:ASN:HA	3	0.8
(3,354)	1:47:B:ASN:HA	1:109:B:LEU:HD12	3	0.79
(3,353)	1:47:A:ASN:HA	1:109:A:LEU:HD12	3	0.79
(3,186)	1:19:B:PHE:HB2	1:83:B:MET:HG2	5	0.79
(3,185)	1:19:A:PHE:HB2	1:83:A:MET:HG2	5	0.79
(3,16)	1:101:B:PRO:HG3	1:102:B:GLY:HA2	5	0.79
(3,15)	1:101:A:PRO:HG3	1:102:A:GLY:HA2	5	0.79
(1,1851)	1:5:A:MET:H	1:5:A:MET:HG3	2	0.79
(1,1826)	1:16:B:ILE:H	1:17:B:ASN:HB2	4	0.79
(1,1510)	1:67:B:ASP:H	1:66:B:LEU:HG	5	0.79
(1,1509)	1:67:A:ASP:H	1:66:A:LEU:HG	5	0.79
(1,1498)	1:38:B:LYS:H	1:59:B:ILE:HD13	5	0.79
(1,1497)	1:38:A:LYS:H	1:59:A:ILE:HD13	5	0.79
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	2	0.79
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	10	0.79
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD21	4	0.79
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD21	4	0.79
(1,912)	1:66:B:LEU:HD12	1:64:B:GLU:HA	9	0.79
(1,911)	1:66:A:LEU:HD12	1:64:A:GLU:HA	9	0.79
(1,862)	1:25:B:LYS:HD2	1:33:B:ASN:HB2	4	0.79
(1,861)	1:25:A:LYS:HD2	1:33:A:ASN:HB2	4	0.79
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD21	4	0.79
(1,800)	1:111:B:GLU:HA	1:50:B:LYS:HE2	3	0.79
(1,799)	1:111:A:GLU:HA	1:50:A:LYS:HE2	3	0.79
(1,758)	1:111:B:GLU:HG2	1:107:B:PRO:HD3	8	0.79
(1,757)	1:111:A:GLU:HG2	1:107:A:PRO:HD3	8	0.79
(1,614)	1:50:B:LYS:HD2	1:50:B:LYS:HA	7	0.79
(1,613)	1:50:A:LYS:HD2	1:50:A:LYS:HA	7	0.79
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE3	8	0.79
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE3	8	0.79
(1,451)	1:7:A:GLN:HB3	1:15:B:ILE:HG12	2	0.79
(1,400)	1:63:B:MET:HB3	1:72:B:LYS:HE2	4	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:63:A:MET:HB3	1:72:A:LYS:HE2	4	0.79
(1,130)	1:16:B:ILE:HD11	1:17:B:ASN:HA	2	0.79
(1,129)	1:16:A:ILE:HD11	1:17:A:ASN:HA	2	0.79
(1,28)	1:58:B:VAL:HG13	1:53:B:ASN:HA	3	0.79
(3,815)	1:51:A:LYS:HG2	1:109:A:LEU:HD13	2	0.78
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB2	9	0.78
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB2	9	0.78
(3,280)	1:72:B:LYS:HG2	1:73:B:GLN:HB2	2	0.78
(3,279)	1:72:A:LYS:HG2	1:73:A:GLN:HB2	2	0.78
(3,240)	1:77:B:GLU:HB2	1:78:B:GLU:HG2	8	0.78
(3,239)	1:77:A:GLU:HB2	1:78:A:GLU:HG2	8	0.78
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG2	2	0.78
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG2	2	0.78
(1,1816)	1:110:B:GLY:H	1:48:B:PHE:HA	7	0.78
(1,1815)	1:110:A:GLY:H	1:48:A:PHE:HA	7	0.78
(1,1803)	1:109:A:LEU:H	1:113:A:THR:H	5	0.78
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD22	9	0.78
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD22	9	0.78
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	4	0.78
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	4	0.78
(1,1522)	1:41:B:VAL:H	1:49:B:LEU:HB2	7	0.78
(1,1521)	1:41:A:VAL:H	1:49:A:LEU:HB2	7	0.78
(1,1219)	1:51:A:LYS:HG2	1:109:A:LEU:HD13	2	0.78
(1,912)	1:66:B:LEU:HD11	1:64:B:GLU:HA	5	0.78
(1,911)	1:66:A:LEU:HD11	1:64:A:GLU:HA	5	0.78
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG23	1	0.78
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG23	1	0.78
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	2	0.78
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB2	9	0.78
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB2	9	0.78
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD11	3	0.78
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD11	9	0.78
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD11	9	0.78
(1,751)	1:111:A:GLU:HG2	1:5:B:MET:HG2	6	0.78
(1,616)	1:21:B:GLN:HA	1:32:B:LEU:HD22	7	0.78
(1,615)	1:21:A:GLN:HA	1:32:A:LEU:HD22	7	0.78
(1,613)	1:36:A:GLU:HA	1:25:A:LYS:HD2	3	0.78
(1,600)	1:18:B:THR:HG23	1:43:B:LYS:HE3	3	0.78
(1,599)	1:18:A:THR:HG23	1:43:A:LYS:HE3	3	0.78
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	7	0.78
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	7	0.78
(1,535)	1:51:A:LYS:HG2	1:109:A:LEU:HD13	2	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:49:B:LEU:HB2	1:86:B:LEU:HG	5	0.78
(1,521)	1:49:A:LEU:HB2	1:86:A:LEU:HG	5	0.78
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD12	9	0.78
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD12	9	0.78
(1,288)	1:64:B:GLU:HB2	1:71:B:ASP:HA	7	0.78
(1,223)	1:12:A:ILE:HG21	1:83:B:MET:HE1	8	0.78
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB3	10	0.77
(3,1088)	1:23:B:SER:H	1:40:B:LEU:HD23	2	0.77
(3,1087)	1:23:A:SER:H	1:40:A:LEU:HD23	2	0.77
(3,915)	1:47:A:ASN:H	1:5:B:MET:HG3	1	0.77
(3,816)	1:51:B:LYS:HG2	1:109:B:LEU:HD13	2	0.77
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB3	3	0.77
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB2	4	0.77
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB3	3	0.77
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB2	4	0.77
(1,1804)	1:109:B:LEU:H	1:113:B:THR:H	5	0.77
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD23	4	0.77
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD12	9	0.77
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD23	4	0.77
(1,1220)	1:51:B:LYS:HG2	1:109:B:LEU:HD13	2	0.77
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE1	5	0.77
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE1	5	0.77
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD13	4	0.77
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD13	4	0.77
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB2	1	0.77
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB3	3	0.77
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB2	4	0.77
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB3	3	0.77
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB2	4	0.77
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD11	3	0.77
(1,810)	1:68:B:THR:H	1:74:B:LEU:HG	1	0.77
(1,809)	1:68:A:THR:H	1:74:A:LEU:HG	1	0.77
(1,758)	1:96:B:GLU:HG2	1:107:B:PRO:HD2	3	0.77
(1,752)	1:111:B:GLU:HG2	1:5:A:MET:HG2	6	0.77
(1,694)	1:74:B:LEU:HG	1:78:B:GLU:HG2	6	0.77
(1,693)	1:74:A:LEU:HG	1:78:A:GLU:HG2	6	0.77
(1,614)	1:51:B:LYS:HA	1:51:B:LYS:HD3	2	0.77
(1,614)	1:36:B:GLU:HA	1:25:B:LYS:HD2	3	0.77
(1,613)	1:51:A:LYS:HA	1:51:A:LYS:HD3	2	0.77
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	9	0.77
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	9	0.77
(1,568)	1:42:B:ARG:HA	1:50:B:LYS:HE3	7	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:42:A:ARG:HA	1:50:A:LYS:HE3	7	0.77
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	8	0.77
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	8	0.77
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	10	0.77
(1,555)	1:47:A:ASN:HA	1:53:A:ASN:H	10	0.77
(1,536)	1:51:B:LYS:HG2	1:109:B:LEU:HD13	2	0.77
(1,452)	1:7:B:GLN:HB3	1:15:A:ILE:HG12	2	0.77
(1,348)	1:5:B:MET:HG2	1:4:B:LYS:HE3	7	0.77
(1,347)	1:5:A:MET:HG2	1:4:A:LYS:HE3	7	0.77
(1,287)	1:64:A:GLU:HB2	1:71:A:ASP:HA	7	0.77
(1,272)	1:12:B:ILE:H	1:8:B:LEU:HG	6	0.77
(1,271)	1:12:A:ILE:H	1:8:A:LEU:HG	6	0.77
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE3	2	0.77
(1,224)	1:12:B:ILE:HG21	1:83:A:MET:HE1	8	0.77
(1,130)	1:16:B:ILE:HD13	1:17:B:ASN:HA	7	0.77
(1,130)	1:16:B:ILE:HD12	1:17:B:ASN:HA	10	0.77
(1,129)	1:16:A:ILE:HD13	1:17:A:ASN:HA	7	0.77
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG2	2	0.76
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD12	5	0.76
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD12	5	0.76
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB3	10	0.76
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD11	5	0.76
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD11	5	0.76
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE3	1	0.76
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE1	3	0.76
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE3	1	0.76
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE1	3	0.76
(3,720)	1:31:B:THR:HG22	1:74:B:LEU:HB2	5	0.76
(3,719)	1:31:A:THR:HG22	1:74:A:LEU:HB2	5	0.76
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB3	6	0.76
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	4	0.76
(3,90)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	1	0.76
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG2	2	0.76
(1,1674)	1:66:B:LEU:H	1:63:B:MET:HE1	2	0.76
(1,1673)	1:66:A:LEU:H	1:63:A:MET:HE1	2	0.76
(1,1548)	1:43:B:LYS:H	1:40:B:LEU:HG	8	0.76
(1,1547)	1:43:A:LYS:H	1:40:A:LEU:HG	8	0.76
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	7	0.76
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD12	9	0.76
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	3	0.76
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	3	0.76
(1,1184)	1:81:B:MET:HB3	1:85:B:ARG:HG3	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:81:A:MET:HB3	1:85:A:ARG:HG3	6	0.76
(1,990)	1:48:B:PHE:HB2	1:13:A:GLU:H	3	0.76
(1,974)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	1	0.76
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB2	1	0.76
(1,925)	1:72:A:LYS:HA	1:70:A:ALA:HB1	7	0.76
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	2	0.76
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB3	6	0.76
(1,757)	1:96:A:GLU:HG2	1:107:A:PRO:HD2	3	0.76
(1,614)	1:50:B:LYS:HD3	1:50:B:LYS:HA	10	0.76
(1,600)	1:18:B:THR:HG22	1:11:A:ASN:HB2	1	0.76
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	4	0.76
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	4	0.76
(1,372)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	1	0.76
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG3	4	0.76
(1,129)	1:16:A:ILE:HD12	1:17:A:ASN:HA	10	0.76
(1,68)	1:48:B:PHE:HB2	1:13:A:GLU:H	3	0.76
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB2	3	0.75
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB2	3	0.75
(3,643)	1:8:A:LEU:HD13	1:40:B:LEU:HD21	6	0.75
(3,491)	1:59:A:ILE:HD11	1:52:A:GLU:HG2	6	0.75
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB3	2	0.75
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB3	6	0.75
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB3	2	0.75
(3,245)	1:7:A:GLN:HG3	1:18:B:THR:HB	2	0.75
(3,220)	1:66:B:LEU:HD11	1:74:B:LEU:HA	2	0.75
(3,219)	1:66:A:LEU:HD11	1:74:A:LEU:HA	2	0.75
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	4	0.75
(3,89)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	1	0.75
(3,89)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	2	0.75
(1,1738)	1:36:B:GLU:H	1:33:B:ASN:HB3	1	0.75
(1,1737)	1:36:A:GLU:H	1:33:A:ASN:HB3	1	0.75
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	3	0.75
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	3	0.75
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD11	6	0.75
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD11	6	0.75
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	3	0.75
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	8	0.75
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	3	0.75
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	8	0.75
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	7	0.75
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	5	0.75
(1,973)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,926)	1:72:B:LYS:HA	1:70:B:ALA:HB1	7	0.75
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	3	0.75
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HB3	8	0.75
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG2	3	0.75
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB3	2	0.75
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB3	6	0.75
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB3	2	0.75
(1,646)	1:86:B:LEU:HA	1:49:B:LEU:HA	9	0.75
(1,616)	1:42:B:ARG:HA	1:45:B:LEU:HD11	8	0.75
(1,615)	1:42:A:ARG:HA	1:45:A:LEU:HD11	8	0.75
(1,613)	1:50:A:LYS:HD3	1:50:A:LYS:HA	10	0.75
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	6	0.75
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	6	0.75
(1,534)	1:86:B:LEU:HD21	1:89:B:ALA:HA	8	0.75
(1,533)	1:86:A:LEU:HD21	1:89:A:ALA:HA	8	0.75
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG3	7	0.75
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG3	7	0.75
(1,371)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	1	0.75
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG3	4	0.75
(1,301)	1:44:A:ASP:HA	1:7:B:GLN:HA	9	0.75
(1,189)	1:77:A:GLU:HA	1:87:B:THR:HG22	9	0.75
(1,144)	1:75:B:SER:HB3	1:68:B:THR:HB	9	0.75
(1,143)	1:75:A:SER:HB3	1:68:A:THR:HB	9	0.75
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG3	7	0.75
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG3	7	0.75
(1,24)	1:96:B:GLU:HA	1:107:B:PRO:HD2	4	0.75
(1,23)	1:96:A:GLU:HA	1:107:A:PRO:HD2	4	0.75
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	2	0.75
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB3	7	0.74
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB3	7	0.74
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD23	2	0.74
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD21	9	0.74
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD23	2	0.74
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD21	9	0.74
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD22	6	0.74
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD22	6	0.74
(3,720)	1:31:B:THR:HG22	1:74:B:LEU:HB2	7	0.74
(3,719)	1:31:A:THR:HG22	1:74:A:LEU:HB2	7	0.74
(3,644)	1:8:B:LEU:HD13	1:40:A:LEU:HD21	6	0.74
(3,525)	1:76:A:PHE:HB3	1:16:A:ILE:HA	10	0.74
(3,516)	1:21:B:GLN:HG3	1:25:B:LYS:HE3	5	0.74
(3,515)	1:21:A:GLN:HG3	1:25:A:LYS:HE3	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,492)	1:59:B:ILE:HD11	1:52:B:GLU:HG2	6	0.74
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD13	3	0.74
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD13	3	0.74
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	6	0.74
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	6	0.74
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	5	0.74
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	4	0.74
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD11	4	0.74
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD11	4	0.74
(1,989)	1:48:A:PHE:HB2	1:13:B:GLU:H	3	0.74
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HB3	8	0.74
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG23	6	0.74
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG23	6	0.74
(1,646)	1:53:B:ASN:HA	1:49:B:LEU:HA	3	0.74
(1,645)	1:53:A:ASN:HA	1:49:A:LEU:HA	3	0.74
(1,645)	1:86:A:LEU:HA	1:49:A:LEU:HA	9	0.74
(1,614)	1:51:B:LYS:HA	1:51:B:LYS:HD3	8	0.74
(1,613)	1:51:A:LYS:HA	1:51:A:LYS:HD3	8	0.74
(1,599)	1:18:A:THR:HG22	1:11:B:ASN:HB2	1	0.74
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD22	3	0.74
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD22	3	0.74
(1,556)	1:47:B:ASN:HA	1:53:B:ASN:H	7	0.74
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	5	0.74
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD11	8	0.74
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD11	8	0.74
(1,302)	1:44:B:ASP:HA	1:7:A:GLN:HA	9	0.74
(1,280)	1:19:B:PHE:HB2	1:32:B:LEU:HB2	5	0.74
(1,279)	1:19:A:PHE:HB2	1:32:A:LEU:HB2	5	0.74
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE3	2	0.74
(1,67)	1:48:A:PHE:HB2	1:13:B:GLU:H	3	0.74
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	2	0.74
(4,11)	1:98:A:ASP:HA	1:96:A:GLU:HA	8	0.73
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG2	2	0.73
(3,746)	1:24:B:VAL:HG12	1:25:B:LYS:HG3	8	0.73
(3,526)	1:76:B:PHE:HB3	1:16:B:ILE:HA	10	0.73
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB3	5	0.73
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB3	5	0.73
(3,276)	1:53:B:ASN:HB2	1:52:B:GLU:HG2	5	0.73
(3,275)	1:53:A:ASN:HB2	1:52:A:GLU:HG2	5	0.73
(3,220)	1:66:B:LEU:HD23	1:74:B:LEU:HA	1	0.73
(3,90)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	2	0.73
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG2	2	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	4	0.73
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	8	0.73
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	2	0.73
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	8	0.73
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE1	2	0.73
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE1	2	0.73
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD22	10	0.73
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD22	10	0.73
(1,872)	1:34:B:GLN:HB2	1:64:B:GLU:HG3	1	0.73
(1,871)	1:34:A:GLN:HB2	1:64:A:GLU:HG3	1	0.73
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB3	5	0.73
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB3	5	0.73
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD22	6	0.73
(1,796)	1:111:B:GLU:HA	1:50:B:LYS:HB3	4	0.73
(1,795)	1:111:A:GLU:HA	1:50:A:LYS:HB3	4	0.73
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	10	0.73
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	10	0.73
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	10	0.73
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	10	0.73
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD23	6	0.73
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD23	6	0.73
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	9	0.73
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	9	0.73
(1,555)	1:47:A:ASN:HA	1:5:B:MET:H	4	0.73
(1,555)	1:47:A:ASN:HA	1:53:A:ASN:H	7	0.73
(1,458)	1:111:B:GLU:HA	1:50:B:LYS:HB3	4	0.73
(1,457)	1:111:A:GLU:HA	1:50:A:LYS:HB3	4	0.73
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	5	0.73
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG3	4	0.73
(1,272)	1:12:B:ILE:H	1:8:B:LEU:HG	1	0.73
(1,271)	1:12:A:ILE:H	1:8:A:LEU:HG	1	0.73
(1,190)	1:77:B:GLU:HA	1:87:A:THR:HG22	9	0.73
(1,95)	1:7:A:GLN:HG3	1:6:A:SER:HA	2	0.73
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG3	4	0.73
(1,38)	1:58:B:VAL:HG22	1:53:B:ASN:HA	10	0.73
(1,37)	1:58:A:VAL:HG22	1:53:A:ASN:HA	10	0.73
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	8	0.72
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB3	9	0.72
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB3	9	0.72
(3,745)	1:24:A:VAL:HG12	1:25:A:LYS:HG3	8	0.72
(3,642)	1:8:B:LEU:HD12	1:15:A:ILE:HD11	8	0.72
(3,641)	1:8:A:LEU:HD12	1:15:B:ILE:HD11	8	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,584)	1:66:B:LEU:HD22	1:67:B:ASP:HA	3	0.72
(3,583)	1:66:A:LEU:HD23	1:67:A:ASP:HA	3	0.72
(3,516)	1:21:B:GLN:HG3	1:25:B:LYS:HE2	6	0.72
(3,515)	1:21:A:GLN:HG3	1:25:A:LYS:HE2	6	0.72
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB2	1	0.72
(3,334)	1:86:B:LEU:HD23	1:48:B:PHE:HB3	4	0.72
(3,246)	1:7:B:GLN:HG3	1:18:A:THR:HB	2	0.72
(3,219)	1:66:A:LEU:HD23	1:74:A:LEU:HA	1	0.72
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	1	0.72
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	4	0.72
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	10	0.72
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	1	0.72
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	4	0.72
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	10	0.72
(1,1590)	1:10:B:ARG:H	1:12:B:ILE:HA	10	0.72
(1,1589)	1:10:A:ARG:H	1:12:A:ILE:HA	10	0.72
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	1	0.72
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG22	10	0.72
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG22	10	0.72
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	8	0.72
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	8	0.72
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD22	2	0.72
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD12	6	0.72
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD12	6	0.72
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	2	0.72
(1,1138)	1:14:B:THR:HG23	1:12:B:ILE:HA	9	0.72
(1,1137)	1:14:A:THR:HG23	1:12:A:ILE:HA	9	0.72
(1,1136)	1:5:B:MET:HG3	1:4:B:LYS:HE3	6	0.72
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD23	6	0.72
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD23	6	0.72
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	2	0.72
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	9	0.72
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	9	0.72
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB2	1	0.72
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD22	6	0.72
(1,680)	1:37:B:PHE:HB3	1:62:B:ILE:HG21	5	0.72
(1,679)	1:37:A:PHE:HB3	1:62:A:ILE:HG21	5	0.72
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	4	0.72
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG3	4	0.72
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD21	9	0.72
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD21	9	0.72
(1,348)	1:5:B:MET:HG3	1:4:B:LYS:HE3	6	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:66:B:LEU:HD22	1:67:B:ASP:HA	3	0.72
(1,327)	1:66:A:LEU:HD23	1:67:A:ASP:HA	3	0.72
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD21	9	0.72
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD21	9	0.72
(1,96)	1:7:B:GLN:HG3	1:18:A:THR:HB	2	0.72
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG3	4	0.72
(1,38)	1:58:B:VAL:HG13	1:61:B:HIS:HA	5	0.72
(1,37)	1:58:A:VAL:HG13	1:61:A:HIS:HA	5	0.72
(3,1507)	1:113:A:THR:H	1:107:A:PRO:HD3	8	0.71
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG2	3	0.71
(3,1198)	1:40:B:LEU:H	1:40:B:LEU:HD22	7	0.71
(3,1197)	1:40:A:LEU:H	1:40:A:LEU:HD22	7	0.71
(3,926)	1:77:B:GLU:H	1:87:A:THR:HG22	3	0.71
(3,925)	1:77:A:GLU:H	1:87:B:THR:HG22	3	0.71
(3,642)	1:8:B:LEU:HD21	1:15:A:ILE:HD12	1	0.71
(3,641)	1:8:A:LEU:HD13	1:15:B:ILE:HD12	2	0.71
(3,365)	1:85:A:ARG:HG2	1:77:B:GLU:HA	7	0.71
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB2	1	0.71
(3,333)	1:86:A:LEU:HD23	1:48:A:PHE:HB3	4	0.71
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG2	9	0.71
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG2	9	0.71
(3,89)	1:7:A:GLN:HG3	1:44:B:ASP:HB3	7	0.71
(1,1782)	1:89:B:ALA:H	1:85:B:ARG:HG2	2	0.71
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG2	3	0.71
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	5	0.71
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	5	0.71
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	1	0.71
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD22	2	0.71
(1,1270)	1:48:B:PHE:H	1:51:B:LYS:HE2	10	0.71
(1,1269)	1:48:A:PHE:H	1:51:A:LYS:HE2	10	0.71
(1,1248)	1:6:B:SER:H	1:12:B:ILE:HD13	4	0.71
(1,1247)	1:6:A:SER:H	1:12:A:ILE:HD13	4	0.71
(1,1154)	1:32:B:LEU:HG	1:36:B:GLU:HG2	1	0.71
(1,1153)	1:32:A:LEU:HG	1:36:A:GLU:HG2	1	0.71
(1,1135)	1:5:A:MET:HG2	1:4:A:LYS:HE3	6	0.71
(1,940)	1:5:B:MET:HB3	1:9:B:GLU:HA	2	0.71
(1,939)	1:5:A:MET:HB3	1:9:A:GLU:HA	2	0.71
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	3	0.71
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB2	1	0.71
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	5	0.71
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	5	0.71
(1,534)	1:86:B:LEU:HD21	1:89:B:ALA:HA	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD12	6	0.71
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD12	6	0.71
(1,347)	1:5:A:MET:HG2	1:4:A:LYS:HE3	6	0.71
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD23	6	0.71
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD23	6	0.71
(1,316)	1:109:B:LEU:HB3	1:111:B:GLU:HB2	5	0.71
(1,315)	1:109:A:LEU:HB3	1:111:A:GLU:HB2	5	0.71
(1,268)	1:66:B:LEU:HG	1:85:B:ARG:HB2	6	0.71
(1,267)	1:66:A:LEU:HG	1:85:A:ARG:HB2	6	0.71
(3,1508)	1:113:B:THR:H	1:107:B:PRO:HD3	8	0.7
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG2	3	0.7
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD12	9	0.7
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD12	9	0.7
(3,960)	1:75:B:SER:H	1:63:B:MET:HE3	6	0.7
(3,959)	1:75:A:SER:H	1:63:A:MET:HE3	6	0.7
(3,641)	1:8:A:LEU:HD21	1:15:B:ILE:HD12	1	0.7
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD23	6	0.7
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD23	6	0.7
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB3	8	0.7
(3,90)	1:7:B:GLN:HG3	1:44:A:ASP:HB3	7	0.7
(1,1781)	1:89:A:ALA:H	1:85:A:ARG:HG2	2	0.7
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG2	3	0.7
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD12	5	0.7
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	4	0.7
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	4	0.7
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	2	0.7
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	6	0.7
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	2	0.7
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	6	0.7
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD23	6	0.7
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD23	6	0.7
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG13	1	0.7
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG13	1	0.7
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD21	8	0.7
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	7	0.7
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	7	0.7
(1,1218)	1:87:B:THR:HG22	1:83:B:MET:HB3	1	0.7
(1,1217)	1:87:A:THR:HG22	1:83:A:MET:HB3	1	0.7
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE3	4	0.7
(1,1045)	1:53:A:ASN:HA	1:38:A:LYS:HA	7	0.7
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	1	0.7
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	3	0.7
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB3	8	0.7
(1,796)	1:111:B:GLU:HA	1:10:A:ARG:HG2	3	0.7
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	5	0.7
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	5	0.7
(1,720)	1:77:B:GLU:HB2	1:68:B:THR:HG23	10	0.7
(1,690)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	3	0.7
(1,604)	1:18:B:THR:HG21	1:21:B:GLN:HG2	8	0.7
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	5	0.7
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	5	0.7
(1,533)	1:86:A:LEU:HD21	1:89:A:ALA:HA	7	0.7
(1,458)	1:111:B:GLU:HA	1:10:A:ARG:HG2	3	0.7
(1,378)	1:34:B:GLN:HG3	1:63:B:MET:H	4	0.7
(1,377)	1:34:A:GLN:HG3	1:63:A:MET:H	4	0.7
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD21	9	0.7
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD21	9	0.7
(1,330)	1:66:B:LEU:HD12	1:84:B:ALA:H	3	0.7
(1,329)	1:66:A:LEU:HD12	1:84:A:ALA:H	3	0.7
(1,250)	1:36:B:GLU:HB3	1:25:B:LYS:HE2	7	0.7
(1,223)	1:62:A:ILE:HG22	1:66:A:LEU:HG	1	0.7
(1,218)	1:12:B:ILE:HG23	1:48:A:PHE:HB3	7	0.7
(1,94)	1:34:B:GLN:HG3	1:63:B:MET:H	4	0.7
(1,93)	1:34:A:GLN:HG3	1:63:A:MET:H	4	0.7
(1,27)	1:87:A:THR:HG21	1:85:A:ARG:HA	9	0.7
(1,20)	1:93:B:LYS:HA	1:109:B:LEU:HG	6	0.7
(1,19)	1:93:A:LYS:HA	1:109:A:LEU:HG	6	0.7
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG21	8	0.69
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG22	8	0.69
(3,642)	1:8:B:LEU:HD13	1:15:A:ILE:HD12	2	0.69
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD21	9	0.69
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD21	9	0.69
(3,572)	1:78:B:GLU:HB2	1:66:B:LEU:HB3	3	0.69
(3,366)	1:85:B:ARG:HG2	1:77:A:GLU:HA	7	0.69
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB3	8	0.69
(1,1826)	1:94:B:MET:H	1:95:B:HIS:HB3	9	0.69
(1,1825)	1:94:A:MET:H	1:95:A:HIS:HB3	9	0.69
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD12	4	0.69
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD12	4	0.69
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	2	0.69
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	2	0.69
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD12	5	0.69
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG22	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG22	6	0.69
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG22	1	0.69
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG22	6	0.69
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG22	10	0.69
(1,1643)	1:61:A:HIS:H	1:63:A:MET:HG3	3	0.69
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	1	0.69
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	1	0.69
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	3	0.69
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	5	0.69
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	3	0.69
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	9	0.69
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	1	0.69
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	4	0.69
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	1	0.69
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	4	0.69
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD21	8	0.69
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD13	6	0.69
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD13	6	0.69
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	1	0.69
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	4	0.69
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	1	0.69
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	4	0.69
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE3	4	0.69
(1,1046)	1:53:B:ASN:HA	1:38:B:LYS:HA	7	0.69
(1,995)	1:109:A:LEU:HD22	1:93:A:LYS:HB2	1	0.69
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	1	0.69
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG2	1	0.69
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB3	8	0.69
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG3	2	0.69
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG3	2	0.69
(1,810)	1:68:B:THR:H	1:74:B:LEU:HG	2	0.69
(1,809)	1:68:A:THR:H	1:74:A:LEU:HG	2	0.69
(1,795)	1:111:A:GLU:HA	1:10:B:ARG:HG2	3	0.69
(1,719)	1:77:A:GLU:HB2	1:68:A:THR:HG23	10	0.69
(1,689)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	3	0.69
(1,688)	1:107:B:PRO:HG2	1:109:B:LEU:H	9	0.69
(1,687)	1:107:A:PRO:HG2	1:109:A:LEU:H	9	0.69
(1,603)	1:18:A:THR:HG21	1:21:A:GLN:HG2	8	0.69
(1,600)	1:18:B:THR:HG22	1:11:A:ASN:HB2	6	0.69
(1,599)	1:18:A:THR:HG22	1:11:B:ASN:HB2	6	0.69
(1,599)	1:18:A:THR:HG23	1:11:B:ASN:HB3	8	0.69
(1,534)	1:86:B:LEU:HD22	1:89:B:ALA:HA	5	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:111:A:GLU:HA	1:10:B:ARG:HG2	3	0.69
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD21	2	0.69
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD21	2	0.69
(1,316)	1:109:B:LEU:HB3	1:111:B:GLU:HB2	7	0.69
(1,315)	1:109:A:LEU:HB3	1:111:A:GLU:HB2	7	0.69
(1,249)	1:36:A:GLU:HB3	1:25:A:LYS:HE2	7	0.69
(1,224)	1:62:B:ILE:HG22	1:66:B:LEU:HG	1	0.69
(1,217)	1:12:A:ILE:HG23	1:48:B:PHE:HB3	7	0.69
(1,144)	1:75:B:SER:HB3	1:68:B:THR:HB	2	0.69
(1,140)	1:16:B:ILE:HD13	1:13:B:GLU:HG2	6	0.69
(1,139)	1:16:A:ILE:HD13	1:13:A:GLU:HG2	6	0.69
(1,130)	1:16:B:ILE:HD11	1:17:B:ASN:HA	1	0.69
(1,129)	1:16:A:ILE:HD11	1:17:A:ASN:HA	1	0.69
(1,28)	1:87:B:THR:HG21	1:85:B:ARG:HA	9	0.69
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG23	8	0.68
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG23	8	0.68
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG3	10	0.68
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG3	10	0.68
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG22	4	0.68
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG23	5	0.68
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG21	6	0.68
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG21	10	0.68
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG23	4	0.68
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG23	5	0.68
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG21	6	0.68
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG22	8	0.68
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG22	8	0.68
(3,866)	1:52:B:GLU:H	1:51:B:LYS:HG3	2	0.68
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD21	2	0.68
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD21	2	0.68
(3,571)	1:78:A:GLU:HB2	1:66:A:LEU:HB3	3	0.68
(3,491)	1:59:A:ILE:HD12	1:52:A:GLU:HG2	7	0.68
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	5	0.68
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	5	0.68
(3,239)	1:77:A:GLU:HB2	1:78:A:GLU:HG2	3	0.68
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD13	6	0.68
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	6	0.68
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	6	0.68
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG21	2	0.68
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG21	7	0.68
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG23	8	0.68
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG21	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG21	7	0.68
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG23	8	0.68
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG23	7	0.68
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG23	7	0.68
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG22	10	0.68
(1,1644)	1:61:B:HIS:H	1:63:B:MET:HG3	3	0.68
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	9	0.68
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	5	0.68
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	5	0.68
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	5	0.68
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	6	0.68
(1,1184)	1:96:B:GLU:HB2	1:93:B:LYS:HD3	3	0.68
(1,1183)	1:96:A:GLU:HB2	1:93:A:LYS:HD3	3	0.68
(1,1135)	1:5:A:MET:HG3	1:4:A:LYS:HE3	4	0.68
(1,996)	1:109:B:LEU:HD22	1:93:B:LYS:HB2	1	0.68
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD22	10	0.68
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD22	10	0.68
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	1	0.68
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG21	4	0.68
(1,836)	1:76:B:PHE:HB3	1:29:B:PRO:HB2	4	0.68
(1,835)	1:76:A:PHE:HB3	1:29:A:PRO:HB2	4	0.68
(1,758)	1:111:B:GLU:HG2	1:107:B:PRO:HD2	9	0.68
(1,690)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	8	0.68
(1,689)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	8	0.68
(1,680)	1:37:B:PHE:HB2	1:62:B:ILE:HG23	9	0.68
(1,679)	1:37:A:PHE:HB2	1:62:A:ILE:HG23	9	0.68
(1,600)	1:18:B:THR:HG23	1:11:A:ASN:HB3	8	0.68
(1,566)	1:39:B:GLU:H	1:42:B:ARG:HA	9	0.68
(1,565)	1:39:A:GLU:H	1:42:A:ARG:HA	9	0.68
(1,533)	1:86:A:LEU:HD22	1:89:A:ALA:HA	5	0.68
(1,528)	1:49:B:LEU:HB3	1:51:B:LYS:HG3	5	0.68
(1,527)	1:49:A:LEU:HB3	1:51:A:LYS:HG3	5	0.68
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	7	0.68
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	5	0.68
(1,478)	1:37:B:PHE:HB2	1:74:B:LEU:HG	8	0.68
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	5	0.68
(1,477)	1:37:A:PHE:HB2	1:74:A:LEU:HG	8	0.68
(1,347)	1:5:A:MET:HG3	1:4:A:LYS:HE3	4	0.68
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD21	5	0.68
(1,50)	1:64:B:GLU:HG3	1:71:B:ASP:HA	2	0.68
(4,258)	1:108:B:GLY:H	1:111:B:GLU:HA	1	0.67
(4,257)	1:108:A:GLY:H	1:111:A:GLU:HA	1	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB2	9	0.67
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB2	9	0.67
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG23	1	0.67
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG23	1	0.67
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG23	1	0.67
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG23	1	0.67
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG21	10	0.67
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG22	2	0.67
(3,865)	1:52:A:GLU:H	1:51:A:LYS:HG3	2	0.67
(3,584)	1:66:B:LEU:HD22	1:67:B:ASP:HA	8	0.67
(3,583)	1:66:A:LEU:HD22	1:67:A:ASP:HA	8	0.67
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD21	5	0.67
(3,516)	1:21:B:GLN:HG3	1:25:B:LYS:HE3	7	0.67
(3,515)	1:21:A:GLN:HG3	1:25:A:LYS:HE3	7	0.67
(3,492)	1:59:B:ILE:HD12	1:52:B:GLU:HG2	7	0.67
(3,456)	1:21:B:GLN:HG2	1:20:B:HIS:HB2	4	0.67
(3,455)	1:21:A:GLN:HG2	1:20:A:HIS:HB2	4	0.67
(3,450)	1:107:B:PRO:HG3	1:111:B:GLU:HB3	7	0.67
(3,449)	1:107:A:PRO:HG3	1:111:A:GLU:HB3	7	0.67
(3,240)	1:77:B:GLU:HB2	1:78:B:GLU:HG2	3	0.67
(3,92)	1:7:B:GLN:HG3	1:6:B:SER:HB3	2	0.67
(3,92)	1:7:B:GLN:HG3	1:6:B:SER:HB3	3	0.67
(3,91)	1:7:A:GLN:HG3	1:6:A:SER:HB3	2	0.67
(3,91)	1:7:A:GLN:HG3	1:6:A:SER:HB3	3	0.67
(3,90)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	10	0.67
(3,89)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	10	0.67
(3,35)	1:58:A:VAL:HG23	1:57:A:LYS:HE3	8	0.67
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD13	6	0.67
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	5	0.67
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	9	0.67
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	5	0.67
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	9	0.67
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG21	4	0.67
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG23	9	0.67
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG21	4	0.67
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG23	9	0.67
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG22	5	0.67
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG22	5	0.67
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	10	0.67
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	10	0.67
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB2	10	0.67
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD13	2	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD13	2	0.67
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD12	4	0.67
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	6	0.67
(1,1196)	1:98:B:ASP:HA	1:104:B:HIS:HB3	1	0.67
(1,1196)	1:98:B:ASP:HA	1:104:B:HIS:HB3	8	0.67
(1,1195)	1:98:A:ASP:HA	1:104:A:HIS:HB3	1	0.67
(1,1195)	1:98:A:ASP:HA	1:104:A:HIS:HB3	8	0.67
(1,1136)	1:5:B:MET:HG3	1:4:B:LYS:HE3	4	0.67
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG21	4	0.67
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD21	2	0.67
(1,770)	1:59:B:ILE:HD11	1:42:B:ARG:HD2	9	0.67
(1,769)	1:59:A:ILE:HD11	1:42:A:ARG:HD2	9	0.67
(1,757)	1:111:A:GLU:HG2	1:107:A:PRO:HD2	9	0.67
(1,690)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	2	0.67
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	4	0.67
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	4	0.67
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	7	0.67
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	3	0.67
(1,348)	1:5:B:MET:HG3	1:4:B:LYS:HE3	4	0.67
(1,336)	1:41:B:VAL:HG13	1:48:B:PHE:H	10	0.67
(1,335)	1:41:A:VAL:HG13	1:48:A:PHE:H	10	0.67
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD21	5	0.67
(1,328)	1:66:B:LEU:HD22	1:67:B:ASP:HA	8	0.67
(1,327)	1:66:A:LEU:HD22	1:67:A:ASP:HA	8	0.67
(1,268)	1:8:B:LEU:HG	1:15:A:ILE:HB	4	0.67
(1,267)	1:8:A:LEU:HG	1:15:B:ILE:HB	4	0.67
(1,143)	1:75:A:SER:HB3	1:68:A:THR:HB	2	0.67
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD11	8	0.67
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD11	8	0.67
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	9	0.67
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	9	0.67
(1,49)	1:64:A:GLU:HG3	1:71:A:ASP:HA	2	0.67
(1,20)	1:93:B:LYS:HA	1:109:B:LEU:HG	9	0.67
(1,19)	1:93:A:LYS:HA	1:109:A:LEU:HG	9	0.67
(3,1466)	1:110:B:GLY:H	1:108:B:GLY:HA3	9	0.66
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG2	1	0.66
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG2	5	0.66
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG2	5	0.66
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG22	2	0.66
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG23	7	0.66
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG21	10	0.66
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG23	7	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG21	10	0.66
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG22	2	0.66
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG23	3	0.66
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG22	2	0.66
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG23	3	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG22	2	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG22	3	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG22	4	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG22	5	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG21	7	0.66
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG23	9	0.66
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG22	3	0.66
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG22	4	0.66
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG22	5	0.66
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG21	7	0.66
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG23	9	0.66
(3,600)	1:53:B:ASN:HB3	1:46:B:GLN:HG3	6	0.66
(3,599)	1:53:A:ASN:HB3	1:46:A:GLN:HG3	6	0.66
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD21	5	0.66
(3,252)	1:33:B:ASN:HB2	1:72:B:LYS:HA	9	0.66
(3,251)	1:33:A:ASN:HB2	1:72:A:LYS:HA	9	0.66
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	2	0.66
(3,106)	1:38:B:LYS:HG3	1:34:B:GLN:HA	3	0.66
(3,36)	1:58:B:VAL:HG23	1:57:B:LYS:HE3	8	0.66
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG2	1	0.66
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG2	5	0.66
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG2	5	0.66
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD23	7	0.66
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD23	7	0.66
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG23	4	0.66
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG23	4	0.66
(1,1673)	1:66:A:LEU:H	1:62:A:ILE:HG12	8	0.66
(1,1498)	1:38:B:LYS:H	1:59:B:ILE:HD13	4	0.66
(1,1497)	1:38:A:LYS:H	1:59:A:ILE:HD13	4	0.66
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	4	0.66
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	4	0.66
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG12	8	0.66
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB2	10	0.66
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD12	4	0.66
(1,1228)	1:76:B:PHE:H	1:32:B:LEU:HB2	7	0.66
(1,1227)	1:76:A:PHE:H	1:32:A:LEU:HB2	7	0.66
(1,1078)	1:31:B:THR:HG21	1:68:B:THR:HG23	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,940)	1:5:B:MET:HB3	1:9:B:GLU:HA	10	0.66
(1,939)	1:5:A:MET:HB3	1:9:A:GLU:HA	10	0.66
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD21	5	0.66
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	10	0.66
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	10	0.66
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD21	2	0.66
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	1	0.66
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	1	0.66
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	1	0.66
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	1	0.66
(1,689)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	2	0.66
(1,642)	1:86:B:LEU:HA	1:85:B:ARG:HD2	3	0.66
(1,641)	1:86:A:LEU:HA	1:85:A:ARG:HD2	3	0.66
(1,534)	1:86:B:LEU:HD22	1:89:B:ALA:HA	2	0.66
(1,533)	1:86:A:LEU:HD22	1:89:A:ALA:HA	2	0.66
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	1	0.66
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	1	0.66
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	4	0.66
(1,507)	1:11:A:ASN:HB2	1:15:B:ILE:HG13	7	0.66
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	3	0.66
(1,318)	1:82:B:LEU:HB3	1:80:B:ILE:HD13	3	0.66
(1,317)	1:82:A:LEU:HB3	1:80:A:ILE:HD13	3	0.66
(1,214)	1:62:B:ILE:HG22	1:63:B:MET:HA	10	0.66
(1,213)	1:62:A:ILE:HG22	1:63:A:MET:HA	10	0.66
(3,1465)	1:110:A:GLY:H	1:108:A:GLY:HA3	9	0.65
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG22	2	0.65
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG2	1	0.65
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG2	5	0.65
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG2	5	0.65
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG21	1	0.65
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG21	1	0.65
(3,720)	1:31:B:THR:HG21	1:74:B:LEU:HB2	10	0.65
(3,719)	1:31:A:THR:HG21	1:74:A:LEU:HB2	10	0.65
(3,105)	1:38:A:LYS:HG3	1:34:A:GLN:HA	3	0.65
(3,42)	1:58:B:VAL:HG13	1:57:B:LYS:HB2	2	0.65
(3,41)	1:58:A:VAL:HG13	1:57:A:LYS:HB2	2	0.65
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	8	0.65
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	8	0.65
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD13	1	0.65
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG21	3	0.65
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG21	3	0.65
(1,1674)	1:66:B:LEU:H	1:62:B:ILE:HG12	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	3	0.65
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG13	9	0.65
(1,1527)	1:42:A:ARG:H	1:42:A:ARG:HG3	1	0.65
(1,1521)	1:41:A:VAL:H	1:43:A:LYS:HD2	5	0.65
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	6	0.65
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	6	0.65
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG12	8	0.65
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	6	0.65
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	6	0.65
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	7	0.65
(1,1292)	1:7:B:GLN:H	1:7:B:GLN:HG3	2	0.65
(1,1291)	1:7:A:GLN:H	1:7:A:GLN:HG3	2	0.65
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE2	3	0.65
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE2	3	0.65
(1,1077)	1:31:A:THR:HG21	1:68:A:THR:HG23	8	0.65
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD21	5	0.65
(1,810)	1:68:B:THR:H	1:74:B:LEU:HG	9	0.65
(1,809)	1:68:A:THR:H	1:74:A:LEU:HG	9	0.65
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	8	0.65
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	8	0.65
(1,604)	1:18:B:THR:HG22	1:21:B:GLN:HG2	2	0.65
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	2	0.65
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	2	0.65
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE2	5	0.65
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE2	5	0.65
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	4	0.65
(1,508)	1:11:B:ASN:HB2	1:15:A:ILE:HG13	7	0.65
(1,456)	1:7:B:GLN:HB3	1:9:B:GLU:HG3	2	0.65
(1,455)	1:7:A:GLN:HB3	1:9:A:GLU:HG3	2	0.65
(1,335)	1:41:A:VAL:HG13	1:48:A:PHE:H	7	0.65
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG2	1	0.64
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD13	3	0.64
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD13	3	0.64
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG21	3	0.64
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG23	6	0.64
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG21	3	0.64
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG23	6	0.64
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG3	2	0.64
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG2	1	0.64
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG3	2	0.64
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG22	9	0.64
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG22	9	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG23	6	0.64
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG23	6	0.64
(3,1015)	1:14:A:THR:H	1:14:A:THR:HG21	10	0.64
(3,642)	1:8:B:LEU:HD13	1:15:A:ILE:HD11	9	0.64
(3,641)	1:8:A:LEU:HD13	1:15:B:ILE:HD11	9	0.64
(3,584)	1:66:B:LEU:HD23	1:67:B:ASP:HA	1	0.64
(3,583)	1:66:A:LEU:HD23	1:67:A:ASP:HA	1	0.64
(3,492)	1:59:B:ILE:HD13	1:52:B:GLU:HG2	3	0.64
(3,491)	1:59:A:ILE:HD13	1:52:A:GLU:HG2	3	0.64
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	9	0.64
(3,408)	1:69:B:ASN:HB2	1:68:B:THR:HG21	1	0.64
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG2	3	0.64
(3,116)	1:75:B:SER:HB2	1:67:B:ASP:HA	5	0.64
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	2	0.64
(3,115)	1:75:A:SER:HB2	1:67:A:ASP:HA	5	0.64
(3,92)	1:7:B:GLN:HG3	1:6:B:SER:HB3	8	0.64
(3,91)	1:7:A:GLN:HG3	1:6:A:SER:HB3	8	0.64
(3,16)	1:101:B:PRO:HG2	1:102:B:GLY:HA2	10	0.64
(3,15)	1:101:A:PRO:HG2	1:102:A:GLY:HA2	10	0.64
(1,1782)	1:89:B:ALA:H	1:93:B:LYS:HB2	5	0.64
(1,1781)	1:89:A:ALA:H	1:93:A:LYS:HB2	5	0.64
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG2	1	0.64
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	10	0.64
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	10	0.64
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD21	3	0.64
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD21	3	0.64
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG23	9	0.64
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG23	9	0.64
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	3	0.64
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG13	9	0.64
(1,1580)	1:50:B:LYS:H	1:50:B:LYS:HG3	6	0.64
(1,1579)	1:50:A:LYS:H	1:50:A:LYS:HG3	6	0.64
(1,1528)	1:42:B:ARG:H	1:42:B:ARG:HG3	1	0.64
(1,1522)	1:41:B:VAL:H	1:43:B:LYS:HD2	5	0.64
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	2	0.64
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	8	0.64
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	8	0.64
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG11	2	0.64
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG12	4	0.64
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG12	7	0.64
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG12	4	0.64
(1,1401)	1:20:A:HIS:H	1:24:A:VAL:HG12	8	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	7	0.64
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD21	10	0.64
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD21	10	0.64
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD22	9	0.64
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD21	10	0.64
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	10	0.64
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	10	0.64
(1,884)	1:78:B:GLU:HB3	1:62:B:ILE:HG22	10	0.64
(1,883)	1:78:A:GLU:HB3	1:62:A:ILE:HG22	10	0.64
(1,796)	1:111:B:GLU:HA	1:50:B:LYS:HB2	6	0.64
(1,795)	1:111:A:GLU:HA	1:50:A:LYS:HB2	6	0.64
(1,690)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	10	0.64
(1,689)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	10	0.64
(1,680)	1:37:B:PHE:HB3	1:62:B:ILE:HG21	3	0.64
(1,679)	1:37:A:PHE:HB3	1:62:A:ILE:HG21	3	0.64
(1,660)	1:7:B:GLN:HG2	1:8:B:LEU:HG	6	0.64
(1,603)	1:18:A:THR:HG22	1:21:A:GLN:HG2	2	0.64
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	8	0.64
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	8	0.64
(1,458)	1:111:B:GLU:HA	1:50:B:LYS:HB2	6	0.64
(1,457)	1:111:A:GLU:HA	1:50:A:LYS:HB2	6	0.64
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG2	8	0.64
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG2	8	0.64
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD13	5	0.64
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD13	5	0.64
(1,336)	1:41:B:VAL:HG13	1:48:B:PHE:H	7	0.64
(1,328)	1:66:B:LEU:HD23	1:67:B:ASP:HA	1	0.64
(1,327)	1:66:A:LEU:HD23	1:67:A:ASP:HA	1	0.64
(1,232)	1:12:B:ILE:HG22	1:80:B:ILE:HG23	8	0.64
(1,231)	1:12:A:ILE:HG22	1:80:A:ILE:HG23	8	0.64
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG2	8	0.64
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG2	8	0.64
(1,24)	1:93:B:LYS:HA	1:107:B:PRO:HD3	7	0.64
(1,23)	1:93:A:LYS:HA	1:107:A:PRO:HD3	7	0.64
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD13	1	0.63
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD13	8	0.63
(3,1038)	1:18:B:THR:H	1:18:B:THR:HG21	7	0.63
(3,1037)	1:18:A:THR:H	1:18:A:THR:HG21	7	0.63
(3,1016)	1:14:B:THR:H	1:14:B:THR:HG21	10	0.63
(3,642)	1:8:B:LEU:HD13	1:15:A:ILE:HD12	3	0.63
(3,407)	1:69:A:ASN:HB2	1:68:A:THR:HG21	1	0.63
(3,286)	1:7:B:GLN:HB3	1:8:B:LEU:HD13	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,252)	1:33:B:ASN:HB2	1:72:B:LYS:HA	3	0.63
(3,251)	1:33:A:ASN:HB2	1:72:A:LYS:HA	3	0.63
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG2	3	0.63
(3,90)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	9	0.63
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD13	1	0.63
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	1	0.63
(1,1728)	1:81:B:MET:H	1:80:B:ILE:HG13	4	0.63
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	1	0.63
(1,1727)	1:81:A:MET:H	1:80:A:ILE:HG13	4	0.63
(1,1694)	1:62:B:ILE:H	1:62:B:ILE:HG21	10	0.63
(1,1693)	1:62:A:ILE:H	1:62:A:ILE:HG21	10	0.63
(1,1580)	1:50:B:LYS:H	1:51:B:LYS:HG3	5	0.63
(1,1579)	1:50:A:LYS:H	1:51:A:LYS:HG3	5	0.63
(1,1547)	1:43:A:LYS:H	1:8:B:LEU:HD13	1	0.63
(1,1528)	1:42:B:ARG:H	1:42:B:ARG:HG3	4	0.63
(1,1528)	1:42:B:ARG:H	1:42:B:ARG:HG3	5	0.63
(1,1527)	1:42:A:ARG:H	1:42:A:ARG:HG3	4	0.63
(1,1527)	1:42:A:ARG:H	1:42:A:ARG:HG3	5	0.63
(1,1492)	1:37:B:PHE:H	1:35:B:GLY:HA2	7	0.63
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	2	0.63
(1,1491)	1:37:A:PHE:H	1:35:A:GLY:HA2	7	0.63
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG11	10	0.63
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG11	2	0.63
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG12	7	0.63
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG11	10	0.63
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	7	0.63
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	7	0.63
(1,1402)	1:20:B:HIS:H	1:24:B:VAL:HG12	8	0.63
(1,1278)	1:48:B:PHE:H	1:45:B:LEU:HD21	8	0.63
(1,1277)	1:48:A:PHE:H	1:45:A:LEU:HD21	8	0.63
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	10	0.63
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	7	0.63
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	7	0.63
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD22	9	0.63
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD21	10	0.63
(1,1045)	1:85:A:ARG:HA	1:77:B:GLU:HA	2	0.63
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD21	1	0.63
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD23	3	0.63
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD21	1	0.63
(1,996)	1:109:B:LEU:HD11	1:93:B:LYS:HB2	6	0.63
(1,974)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	9	0.63
(1,872)	1:34:B:GLN:HB2	1:64:B:GLU:HG3	9	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,871)	1:34:A:GLN:HB2	1:64:A:GLU:HG3	9	0.63
(1,659)	1:7:A:GLN:HG2	1:8:A:LEU:HG	6	0.63
(1,646)	1:53:B:ASN:HA	1:49:B:LEU:HA	7	0.63
(1,645)	1:53:A:ASN:HA	1:49:A:LEU:HA	7	0.63
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE2	3	0.63
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE2	3	0.63
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	1	0.63
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	1	0.63
(1,372)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	9	0.63
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG2	10	0.63
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG2	10	0.63
(1,214)	1:62:B:ILE:HG23	1:63:B:MET:HA	1	0.63
(1,213)	1:62:A:ILE:HG23	1:63:A:MET:HA	1	0.63
(1,20)	1:93:B:LYS:HA	1:109:B:LEU:HG	2	0.63
(1,19)	1:93:A:LYS:HA	1:109:A:LEU:HG	2	0.63
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG23	9	0.62
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG21	5	0.62
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG23	9	0.62
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD13	1	0.62
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD13	8	0.62
(3,641)	1:8:A:LEU:HD13	1:15:B:ILE:HD12	3	0.62
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	9	0.62
(3,285)	1:7:A:GLN:HB3	1:8:A:LEU:HD13	4	0.62
(3,256)	1:33:B:ASN:HB2	1:31:B:THR:HG23	3	0.62
(3,255)	1:33:A:ASN:HB2	1:31:A:THR:HG23	3	0.62
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG2	1	0.62
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG2	1	0.62
(3,92)	1:7:B:GLN:HG2	1:6:B:SER:HB3	1	0.62
(3,91)	1:7:A:GLN:HG2	1:6:A:SER:HB3	1	0.62
(3,89)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	9	0.62
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	2	0.62
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	2	0.62
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD11	3	0.62
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD11	3	0.62
(1,1580)	1:50:B:LYS:H	1:50:B:LYS:HG3	10	0.62
(1,1579)	1:50:A:LYS:H	1:50:A:LYS:HG3	10	0.62
(1,1574)	1:75:B:SER:H	1:68:B:THR:HA	8	0.62
(1,1573)	1:75:A:SER:H	1:68:A:THR:HA	8	0.62
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	3	0.62
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	3	0.62
(1,1527)	1:42:A:ARG:H	1:42:A:ARG:HG3	9	0.62
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	10	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG11	9	0.62
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG11	9	0.62
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	3	0.62
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	9	0.62
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	3	0.62
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	9	0.62
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD21	7	0.62
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD13	10	0.62
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD13	10	0.62
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	10	0.62
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD12	8	0.62
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD12	8	0.62
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	3	0.62
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	9	0.62
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	3	0.62
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	9	0.62
(1,1133)	1:72:A:LYS:HE2	1:63:A:MET:HG3	7	0.62
(1,1131)	1:72:A:LYS:HE2	1:63:A:MET:HG3	7	0.62
(1,1056)	1:33:B:ASN:HB2	1:31:B:THR:HG23	3	0.62
(1,1055)	1:33:A:ASN:HB2	1:31:A:THR:HG23	3	0.62
(1,1046)	1:85:B:ARG:HA	1:77:A:GLU:HA	2	0.62
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD23	3	0.62
(1,995)	1:109:A:LEU:HD11	1:93:A:LYS:HB2	6	0.62
(1,983)	1:48:A:PHE:HB3	1:16:B:ILE:HD12	9	0.62
(1,973)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	9	0.62
(1,876)	1:78:B:GLU:HB2	1:66:B:LEU:HG	3	0.62
(1,875)	1:78:A:GLU:HB2	1:66:A:LEU:HG	3	0.62
(1,757)	1:111:A:GLU:HG2	1:107:A:PRO:HD2	7	0.62
(1,754)	1:111:B:GLU:HG3	1:4:A:LYS:HE2	9	0.62
(1,753)	1:111:A:GLU:HG3	1:4:B:LYS:HE2	9	0.62
(1,688)	1:107:B:PRO:HG2	1:109:B:LEU:H	6	0.62
(1,687)	1:107:A:PRO:HG2	1:109:A:LEU:H	6	0.62
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	1	0.62
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	1	0.62
(1,600)	1:18:B:THR:HG21	1:43:B:LYS:HE3	10	0.62
(1,599)	1:18:A:THR:HG21	1:43:A:LYS:HE3	10	0.62
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD12	8	0.62
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	10	0.62
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	10	0.62
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	2	0.62
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	2	0.62
(1,371)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	9	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:41:A:VAL:HG11	1:48:A:PHE:H	4	0.62
(1,214)	1:62:B:ILE:HG21	1:63:B:MET:HA	4	0.62
(1,213)	1:62:A:ILE:HG21	1:63:A:MET:HA	4	0.62
(1,140)	1:16:B:ILE:HD13	1:13:B:GLU:HG2	3	0.62
(1,139)	1:16:A:ILE:HD13	1:13:A:GLU:HG2	3	0.62
(1,28)	1:87:B:THR:HG21	1:85:B:ARG:HA	4	0.62
(1,27)	1:87:A:THR:HG21	1:85:A:ARG:HA	4	0.62
(1,18)	1:93:B:LYS:HA	1:109:B:LEU:HD12	8	0.62
(1,17)	1:93:A:LYS:HA	1:109:A:LEU:HD12	8	0.62
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG23	4	0.61
(3,1300)	1:59:B:ILE:H	1:59:B:ILE:HG21	5	0.61
(3,1299)	1:59:A:ILE:H	1:59:A:ILE:HG23	4	0.61
(3,797)	1:107:A:PRO:HG3	1:108:A:GLY:HA3	1	0.61
(3,530)	1:67:B:ASP:HB2	1:64:B:GLU:HG2	3	0.61
(3,529)	1:67:A:ASP:HB2	1:64:A:GLU:HG2	3	0.61
(3,245)	1:7:A:GLN:HG3	1:18:B:THR:HB	8	0.61
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG2	4	0.61
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG2	4	0.61
(3,90)	1:7:B:GLN:HG2	1:44:A:ASP:HB2	6	0.61
(1,1858)	1:110:B:GLY:H	1:111:B:GLU:HA	3	0.61
(1,1857)	1:110:A:GLY:H	1:111:A:GLU:HA	3	0.61
(1,1781)	1:89:A:ALA:H	1:16:B:ILE:HG12	7	0.61
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD22	1	0.61
(1,1643)	1:61:A:HIS:H	1:63:A:MET:HG3	1	0.61
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD13	5	0.61
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD13	5	0.61
(1,1528)	1:42:B:ARG:H	1:42:B:ARG:HG3	9	0.61
(1,1518)	1:40:B:LEU:H	1:25:B:LYS:HD2	4	0.61
(1,1517)	1:40:A:LEU:H	1:43:A:LYS:HD3	4	0.61
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	10	0.61
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD13	6	0.61
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD13	6	0.61
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD22	5	0.61
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD21	7	0.61
(1,1230)	1:76:B:PHE:H	1:32:B:LEU:HD11	7	0.61
(1,1229)	1:76:A:PHE:H	1:32:A:LEU:HD11	7	0.61
(1,1227)	1:76:A:PHE:H	1:32:A:LEU:HB2	8	0.61
(1,1134)	1:72:B:LYS:HE2	1:63:B:MET:HG3	7	0.61
(1,1132)	1:72:B:LYS:HE2	1:63:B:MET:HG3	7	0.61
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE3	8	0.61
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE3	8	0.61
(1,984)	1:48:B:PHE:HB3	1:16:A:ILE:HD12	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	10	0.61
(1,758)	1:111:B:GLU:HG2	1:107:B:PRO:HD2	7	0.61
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG23	9	0.61
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG22	6	0.61
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG22	6	0.61
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD12	8	0.61
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	10	0.61
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	10	0.61
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG11	7	0.61
(1,456)	1:7:B:GLN:HB3	1:9:B:GLU:HG3	3	0.61
(1,455)	1:7:A:GLN:HB3	1:9:A:GLU:HG3	3	0.61
(1,394)	1:33:B:ASN:HB3	1:63:B:MET:HG2	2	0.61
(1,356)	1:54:B:LYS:HA	1:50:B:LYS:HD3	5	0.61
(1,355)	1:54:A:LYS:HA	1:50:A:LYS:HD3	5	0.61
(1,336)	1:41:B:VAL:HG11	1:48:B:PHE:H	4	0.61
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD21	10	0.61
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD21	10	0.61
(1,248)	1:63:B:MET:HB2	1:61:B:HIS:HB3	7	0.61
(1,247)	1:63:A:MET:HB2	1:61:A:HIS:HB3	7	0.61
(1,130)	1:16:B:ILE:HD12	1:17:B:ASN:HA	6	0.61
(1,129)	1:16:A:ILE:HD12	1:17:A:ASN:HA	6	0.61
(1,95)	1:7:A:GLN:HG3	1:18:B:THR:HB	8	0.61
(1,70)	1:33:B:ASN:HB3	1:63:B:MET:HG2	2	0.61
(1,42)	1:78:B:GLU:HG3	1:76:B:PHE:HA	9	0.61
(3,1466)	1:110:B:GLY:H	1:108:B:GLY:HA2	7	0.6
(3,973)	1:5:A:MET:H	1:4:A:LYS:HB2	5	0.6
(3,973)	1:5:A:MET:H	1:4:A:LYS:HB3	7	0.6
(3,798)	1:107:B:PRO:HG3	1:108:B:GLY:HA3	1	0.6
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	4	0.6
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	4	0.6
(3,772)	1:14:B:THR:HG21	1:17:B:ASN:HB3	1	0.6
(3,771)	1:14:A:THR:HG21	1:17:A:ASN:HB3	1	0.6
(3,746)	1:24:B:VAL:HG11	1:25:B:LYS:HG3	9	0.6
(3,745)	1:24:A:VAL:HG11	1:25:A:LYS:HG3	9	0.6
(3,584)	1:66:B:LEU:HD21	1:67:B:ASP:HA	6	0.6
(3,583)	1:66:A:LEU:HD21	1:67:A:ASP:HA	6	0.6
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD21	10	0.6
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD21	10	0.6
(3,334)	1:86:B:LEU:HD22	1:48:B:PHE:HB3	7	0.6
(3,333)	1:86:A:LEU:HD22	1:48:A:PHE:HB3	7	0.6
(3,246)	1:7:B:GLN:HG3	1:18:A:THR:HB	8	0.6
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	8	0.6
(3,92)	1:7:B:GLN:HG2	1:6:B:SER:HB3	4	0.6
(3,91)	1:7:A:GLN:HG2	1:6:A:SER:HB3	4	0.6
(1,1782)	1:89:B:ALA:H	1:16:A:ILE:HG12	7	0.6
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD12	3	0.6
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD22	1	0.6
(1,1644)	1:61:B:HIS:H	1:63:B:MET:HG3	1	0.6
(1,1598)	1:53:B:ASN:H	1:58:B:VAL:HB	2	0.6
(1,1597)	1:53:A:ASN:H	1:58:A:VAL:HB	2	0.6
(1,1548)	1:43:B:LYS:H	1:8:A:LEU:HD13	1	0.6
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG21	8	0.6
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG21	8	0.6
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG13	6	0.6
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD22	5	0.6
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	5	0.6
(1,1228)	1:76:B:PHE:H	1:32:B:LEU:HB2	8	0.6
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD22	3	0.6
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD21	4	0.6
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD21	4	0.6
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	5	0.6
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG2	10	0.6
(1,796)	1:111:B:GLU:HA	1:50:B:LYS:HB3	8	0.6
(1,795)	1:111:A:GLU:HA	1:50:A:LYS:HB3	8	0.6
(1,785)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	2	0.6
(1,723)	1:77:A:GLU:HB3	1:80:A:ILE:HG12	2	0.6
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	4	0.6
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	4	0.6
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG23	9	0.6
(1,646)	1:53:B:ASN:HA	1:49:B:LEU:HA	6	0.6
(1,614)	1:51:B:LYS:HA	1:51:B:LYS:HD3	9	0.6
(1,613)	1:51:A:LYS:HA	1:51:A:LYS:HD3	9	0.6
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	9	0.6
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	9	0.6
(1,458)	1:111:B:GLU:HA	1:50:B:LYS:HB3	8	0.6
(1,457)	1:111:A:GLU:HA	1:50:A:LYS:HB3	8	0.6
(1,393)	1:33:A:ASN:HB3	1:63:A:MET:HG2	2	0.6
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD23	2	0.6
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD23	2	0.6
(1,328)	1:66:B:LEU:HD21	1:67:B:ASP:HA	6	0.6
(1,327)	1:66:A:LEU:HD21	1:67:A:ASP:HA	6	0.6
(1,272)	1:49:B:LEU:HG	1:51:B:LYS:H	2	0.6
(1,271)	1:49:A:LEU:HG	1:51:A:LYS:H	2	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD23	2	0.6
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD23	2	0.6
(1,96)	1:7:B:GLN:HG3	1:18:A:THR:HB	8	0.6
(1,69)	1:33:A:ASN:HB3	1:63:A:MET:HG2	2	0.6
(1,41)	1:78:A:GLU:HG3	1:76:A:PHE:HA	9	0.6
(1,38)	1:58:B:VAL:HG12	1:61:B:HIS:HA	4	0.6
(1,37)	1:58:A:VAL:HG12	1:61:A:HIS:HA	4	0.6
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB3	7	0.59
(3,1465)	1:110:A:GLY:H	1:108:A:GLY:HA2	7	0.59
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE3	3	0.59
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	7	0.59
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	7	0.59
(3,974)	1:5:B:MET:H	1:4:B:LYS:HB2	5	0.59
(3,974)	1:5:B:MET:H	1:4:B:LYS:HB3	7	0.59
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG3	6	0.59
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG3	6	0.59
(3,788)	1:67:B:ASP:HB2	1:78:B:GLU:HB3	6	0.59
(3,787)	1:67:A:ASP:HB2	1:78:A:GLU:HB3	6	0.59
(3,745)	1:24:A:VAL:HG12	1:25:A:LYS:HG3	7	0.59
(3,89)	1:7:A:GLN:HG2	1:44:B:ASP:HB2	6	0.59
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD12	10	0.59
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD12	3	0.59
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD12	10	0.59
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	5	0.59
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	5	0.59
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD12	3	0.59
(1,1590)	1:51:B:LYS:H	1:46:B:GLN:HA	9	0.59
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG13	6	0.59
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	10	0.59
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	10	0.59
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	5	0.59
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	10	0.59
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	10	0.59
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD22	10	0.59
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD22	10	0.59
(1,994)	1:109:B:LEU:HD22	1:47:B:ASN:HB2	10	0.59
(1,988)	1:48:B:PHE:HB3	1:109:B:LEU:H	1	0.59
(1,940)	1:5:B:MET:HB3	1:9:B:GLU:HA	1	0.59
(1,939)	1:5:A:MET:HB3	1:9:A:GLU:HA	1	0.59
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG2	4	0.59
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG2	5	0.59
(1,786)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:111:A:GLU:HG2	1:108:A:GLY:HA2	3	0.59
(1,724)	1:77:B:GLU:HB3	1:80:B:ILE:HG12	2	0.59
(1,646)	1:53:B:ASN:HA	1:49:B:LEU:HA	4	0.59
(1,645)	1:53:A:ASN:HA	1:49:A:LEU:HA	4	0.59
(1,645)	1:53:A:ASN:HA	1:49:A:LEU:HA	6	0.59
(1,624)	1:21:B:GLN:HA	1:25:B:LYS:HE3	8	0.59
(1,623)	1:21:A:GLN:HA	1:25:A:LYS:HE3	8	0.59
(1,613)	1:36:A:GLU:HA	1:25:A:LYS:HD3	6	0.59
(1,603)	1:18:A:THR:HG22	1:21:A:GLN:HG2	4	0.59
(1,603)	1:18:A:THR:HG22	1:21:A:GLN:HG2	9	0.59
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	4	0.59
(1,582)	1:42:B:ARG:HB3	1:53:B:ASN:HB2	8	0.59
(1,581)	1:42:A:ARG:HB3	1:53:A:ASN:HB2	8	0.59
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE2	4	0.59
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE2	4	0.59
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	10	0.59
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG11	7	0.59
(1,406)	1:42:B:ARG:HB3	1:53:B:ASN:HB2	8	0.59
(1,405)	1:42:A:ARG:HB3	1:53:A:ASN:HB2	8	0.59
(1,214)	1:62:B:ILE:HG22	1:63:B:MET:HA	7	0.59
(1,37)	1:58:A:VAL:HG13	1:53:A:ASN:HA	7	0.59
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB3	7	0.58
(3,1458)	1:89:B:ALA:H	1:16:A:ILE:HD12	3	0.58
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG2	4	0.58
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE3	3	0.58
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD22	10	0.58
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD22	10	0.58
(3,794)	1:107:B:PRO:HG2	1:93:B:LYS:HG2	8	0.58
(3,793)	1:107:A:PRO:HG2	1:93:A:LYS:HG2	8	0.58
(3,746)	1:24:B:VAL:HG12	1:25:B:LYS:HG3	7	0.58
(3,600)	1:53:B:ASN:HB2	1:46:B:GLN:HG3	4	0.58
(3,584)	1:66:B:LEU:HD22	1:67:B:ASP:HA	2	0.58
(3,246)	1:7:B:GLN:HG3	1:18:A:THR:HB	7	0.58
(3,245)	1:7:A:GLN:HG3	1:18:B:THR:HB	3	0.58
(3,245)	1:7:A:GLN:HG3	1:18:B:THR:HB	7	0.58
(1,1858)	1:110:B:GLY:H	1:111:B:GLU:HA	2	0.58
(1,1857)	1:110:A:GLY:H	1:111:A:GLU:HA	2	0.58
(1,1792)	1:16:B:ILE:H	1:12:B:ILE:HG23	8	0.58
(1,1791)	1:16:A:ILE:H	1:12:A:ILE:HG23	8	0.58
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG2	4	0.58
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD12	3	0.58
(1,1589)	1:51:A:LYS:H	1:46:A:GLN:HA	9	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG21	9	0.58
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG21	9	0.58
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG12	3	0.58
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG23	8	0.58
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD13	2	0.58
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD13	2	0.58
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD22	3	0.58
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	1	0.58
(1,1007)	1:8:A:LEU:HD22	1:40:B:LEU:HA	2	0.58
(1,993)	1:109:A:LEU:HD22	1:47:A:ASN:HB2	10	0.58
(1,987)	1:48:A:PHE:HB3	1:109:A:LEU:H	1	0.58
(1,974)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	7	0.58
(1,973)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	7	0.58
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	5	0.58
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	8	0.58
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	5	0.58
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	8	0.58
(1,756)	1:111:B:GLU:HG2	1:108:B:GLY:HA2	3	0.58
(1,698)	1:107:B:PRO:HG2	1:93:B:LYS:HG2	8	0.58
(1,697)	1:107:A:PRO:HG2	1:93:A:LYS:HG2	8	0.58
(1,614)	1:36:B:GLU:HA	1:25:B:LYS:HD3	6	0.58
(1,604)	1:18:B:THR:HG22	1:21:B:GLN:HG2	4	0.58
(1,604)	1:18:B:THR:HG22	1:21:B:GLN:HG2	9	0.58
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	4	0.58
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	1	0.58
(1,534)	1:86:B:LEU:HD12	1:89:B:ALA:HA	3	0.58
(1,533)	1:86:A:LEU:HD22	1:13:B:GLU:HA	3	0.58
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	10	0.58
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG21	7	0.58
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG21	7	0.58
(1,372)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	7	0.58
(1,371)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	7	0.58
(1,328)	1:66:B:LEU:HD22	1:67:B:ASP:HA	2	0.58
(1,324)	1:41:B:VAL:HG12	1:52:B:GLU:HG2	7	0.58
(1,213)	1:62:A:ILE:HG22	1:63:A:MET:HA	7	0.58
(1,96)	1:7:B:GLN:HG3	1:18:A:THR:HB	7	0.58
(1,95)	1:7:A:GLN:HG3	1:18:B:THR:HB	3	0.58
(1,95)	1:7:A:GLN:HG3	1:18:B:THR:HB	7	0.58
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	2	0.58
(1,38)	1:58:B:VAL:HG12	1:61:B:HIS:HA	3	0.58
(1,38)	1:58:B:VAL:HG13	1:53:B:ASN:HA	7	0.58
(1,28)	1:87:B:THR:HG21	1:85:B:ARG:HA	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:87:A:THR:HG21	1:85:A:ARG:HA	1	0.58
(3,1268)	1:55:B:ASN:H	1:41:B:VAL:HG13	8	0.57
(3,1267)	1:55:A:ASN:H	1:41:A:VAL:HG13	8	0.57
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD12	4	0.57
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD12	4	0.57
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	10	0.57
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD11	9	0.57
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	4	0.57
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	4	0.57
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	6	0.57
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	10	0.57
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	6	0.57
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	10	0.57
(3,599)	1:53:A:ASN:HB2	1:46:A:GLN:HG3	4	0.57
(3,584)	1:66:B:LEU:HD21	1:67:B:ASP:HA	4	0.57
(3,583)	1:66:A:LEU:HD22	1:67:A:ASP:HA	2	0.57
(3,583)	1:66:A:LEU:HD21	1:67:A:ASP:HA	4	0.57
(3,22)	1:101:B:PRO:HG3	1:104:B:HIS:HA	3	0.57
(3,21)	1:101:A:PRO:HG3	1:104:A:HIS:HA	3	0.57
(1,1826)	1:94:B:MET:H	1:93:B:LYS:HE2	6	0.57
(1,1825)	1:94:A:MET:H	1:93:A:LYS:HE2	6	0.57
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG23	8	0.57
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG23	8	0.57
(1,1804)	1:109:B:LEU:H	1:113:B:THR:H	4	0.57
(1,1798)	1:94:B:MET:H	1:93:B:LYS:HE2	6	0.57
(1,1797)	1:94:A:MET:H	1:93:A:LYS:HE2	6	0.57
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD13	2	0.57
(1,1738)	1:36:B:GLU:H	1:33:B:ASN:HB2	10	0.57
(1,1737)	1:36:A:GLU:H	1:33:A:ASN:HB2	10	0.57
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD11	7	0.57
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD11	7	0.57
(1,1528)	1:42:B:ARG:H	1:42:B:ARG:HG2	7	0.57
(1,1527)	1:42:A:ARG:H	1:42:A:ARG:HG2	7	0.57
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	1	0.57
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG12	3	0.57
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG23	8	0.57
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	8	0.57
(1,1328)	1:12:B:ILE:H	1:45:A:LEU:HD23	4	0.57
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD23	9	0.57
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD13	1	0.57
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD13	1	0.57
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	9	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	9	0.57
(1,1129)	1:4:A:LYS:HE3	1:6:A:SER:HB3	5	0.57
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE2	6	0.57
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE2	6	0.57
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	2	0.57
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	6	0.57
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	1	0.57
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	2	0.57
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	6	0.57
(1,1008)	1:8:B:LEU:HD22	1:40:A:LEU:HA	2	0.57
(1,1006)	1:109:B:LEU:HD13	1:86:B:LEU:H	8	0.57
(1,1005)	1:109:A:LEU:HD13	1:86:A:LEU:H	8	0.57
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	4	0.57
(1,800)	1:111:B:GLU:HA	1:93:B:LYS:HE3	7	0.57
(1,799)	1:111:A:GLU:HA	1:93:A:LYS:HE3	7	0.57
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	6	0.57
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	10	0.57
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	6	0.57
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	10	0.57
(1,672)	1:49:B:LEU:HG	1:53:B:ASN:H	6	0.57
(1,671)	1:49:A:LEU:HG	1:53:A:ASN:H	6	0.57
(1,524)	1:49:B:LEU:HB3	1:58:B:VAL:HB	6	0.57
(1,523)	1:49:A:LEU:HB3	1:58:A:VAL:HB	6	0.57
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD22	7	0.57
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD22	7	0.57
(1,359)	1:77:A:GLU:HB2	1:31:A:THR:HG23	9	0.57
(1,336)	1:41:B:VAL:HG11	1:48:B:PHE:H	5	0.57
(1,335)	1:41:A:VAL:HG11	1:48:A:PHE:H	5	0.57
(1,328)	1:66:B:LEU:HD21	1:67:B:ASP:HA	4	0.57
(1,327)	1:66:A:LEU:HD22	1:67:A:ASP:HA	2	0.57
(1,327)	1:66:A:LEU:HD21	1:67:A:ASP:HA	4	0.57
(1,323)	1:41:A:VAL:HG12	1:52:A:GLU:HG2	7	0.57
(1,267)	1:8:A:LEU:HG	1:15:B:ILE:HB	8	0.57
(1,248)	1:63:B:MET:HB3	1:61:B:HIS:HB3	5	0.57
(1,248)	1:63:B:MET:HB3	1:61:B:HIS:HB3	8	0.57
(1,247)	1:63:A:MET:HB3	1:61:A:HIS:HB3	5	0.57
(1,247)	1:63:A:MET:HB3	1:61:A:HIS:HB3	8	0.57
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD22	7	0.57
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD22	7	0.57
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	10	0.57
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	8	0.57
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:58:A:VAL:HG12	1:61:A:HIS:HA	3	0.57
(1,24)	1:93:B:LYS:HA	1:107:B:PRO:HD2	8	0.57
(1,23)	1:93:A:LYS:HA	1:107:A:PRO:HD2	8	0.57
(3,1457)	1:89:A:ALA:H	1:16:B:ILE:HD12	3	0.56
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG2	4	0.56
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	10	0.56
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD11	9	0.56
(3,974)	1:5:B:MET:H	1:4:B:LYS:HB3	3	0.56
(3,746)	1:24:B:VAL:HG13	1:25:B:LYS:HG3	6	0.56
(3,745)	1:24:A:VAL:HG13	1:25:A:LYS:HG3	6	0.56
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	5	0.56
(3,600)	1:53:B:ASN:HB3	1:46:B:GLN:HG3	2	0.56
(3,599)	1:53:A:ASN:HB3	1:46:A:GLN:HG3	2	0.56
(3,276)	1:53:B:ASN:HB3	1:52:B:GLU:HG2	6	0.56
(3,275)	1:53:A:ASN:HB3	1:52:A:GLU:HG2	6	0.56
(3,246)	1:7:B:GLN:HG3	1:18:A:THR:HB	3	0.56
(1,1826)	1:94:B:MET:H	1:93:B:LYS:HE2	7	0.56
(1,1803)	1:109:A:LEU:H	1:113:A:THR:H	4	0.56
(1,1798)	1:94:B:MET:H	1:93:B:LYS:HE2	7	0.56
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG2	4	0.56
(1,1543)	1:43:A:LYS:H	1:43:A:LYS:HD2	8	0.56
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	10	0.56
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	1	0.56
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	10	0.56
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	8	0.56
(1,1327)	1:12:A:ILE:H	1:45:B:LEU:HD23	4	0.56
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD21	1	0.56
(1,1297)	1:8:A:LEU:H	1:40:B:LEU:HD23	9	0.56
(1,1228)	1:76:B:PHE:H	1:80:B:ILE:HB	6	0.56
(1,1227)	1:76:A:PHE:H	1:80:A:ILE:HB	6	0.56
(1,1154)	1:32:B:LEU:HG	1:36:B:GLU:HG2	3	0.56
(1,1153)	1:32:A:LEU:HG	1:36:A:GLU:HG2	3	0.56
(1,1130)	1:4:B:LYS:HE3	1:6:B:SER:HB3	5	0.56
(1,1010)	1:8:B:LEU:HD13	1:41:A:VAL:HA	1	0.56
(1,850)	1:15:B:ILE:HA	1:7:A:GLN:HB3	1	0.56
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG3	3	0.56
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG3	3	0.56
(1,796)	1:111:B:GLU:HA	1:50:B:LYS:HB3	9	0.56
(1,604)	1:18:B:THR:HG21	1:21:B:GLN:HG2	10	0.56
(1,603)	1:18:A:THR:HG21	1:21:A:GLN:HG2	10	0.56
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	1	0.56
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	5	0.56
(1,555)	1:47:A:ASN:HA	1:5:B:MET:H	1	0.56
(1,458)	1:111:B:GLU:HA	1:50:B:LYS:HB3	9	0.56
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	10	0.56
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	10	0.56
(1,396)	1:33:B:ASN:HB2	1:34:B:GLN:HG2	1	0.56
(1,378)	1:34:B:GLN:HG3	1:63:B:MET:H	5	0.56
(1,360)	1:77:B:GLU:HB2	1:31:B:THR:HG23	9	0.56
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD22	3	0.56
(1,318)	1:82:B:LEU:HB3	1:80:B:ILE:HD12	7	0.56
(1,317)	1:82:A:LEU:HB3	1:80:A:ILE:HD12	7	0.56
(1,268)	1:8:B:LEU:HG	1:15:A:ILE:HB	8	0.56
(1,214)	1:62:B:ILE:HG23	1:63:B:MET:HA	6	0.56
(1,213)	1:62:A:ILE:HG23	1:63:A:MET:HA	6	0.56
(1,140)	1:16:B:ILE:HD11	1:13:B:GLU:HG2	9	0.56
(1,139)	1:16:A:ILE:HD11	1:13:A:GLU:HG2	9	0.56
(1,96)	1:7:B:GLN:HG3	1:18:A:THR:HB	3	0.56
(1,94)	1:34:B:GLN:HG3	1:63:B:MET:H	5	0.56
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	10	0.56
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	2	0.56
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	2	0.56
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	10	0.56
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	2	0.56
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	10	0.56
(1,72)	1:48:B:PHE:HB2	1:9:A:GLU:HB3	2	0.56
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE2	7	0.55
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG3	4	0.55
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG3	6	0.55
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG3	6	0.55
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	5	0.55
(3,973)	1:5:A:MET:H	1:4:A:LYS:HB3	3	0.55
(3,973)	1:5:A:MET:H	1:4:A:LYS:HB2	8	0.55
(3,960)	1:75:B:SER:H	1:63:B:MET:HE2	8	0.55
(3,959)	1:75:A:SER:H	1:63:A:MET:HE2	8	0.55
(3,798)	1:107:B:PRO:HG2	1:108:B:GLY:HA3	7	0.55
(3,797)	1:107:A:PRO:HG2	1:108:A:GLY:HA3	7	0.55
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	5	0.55
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD22	3	0.55
(1,1825)	1:94:A:MET:H	1:93:A:LYS:HE2	7	0.55
(1,1797)	1:94:A:MET:H	1:93:A:LYS:HE2	7	0.55
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD13	2	0.55
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:43:B:LYS:H	1:43:B:LYS:HD2	8	0.55
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	5	0.55
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	5	0.55
(1,1402)	1:20:B:HIS:H	1:24:B:VAL:HG11	10	0.55
(1,1401)	1:20:A:HIS:H	1:24:A:VAL:HG11	10	0.55
(1,1298)	1:8:B:LEU:H	1:40:A:LEU:HD21	1	0.55
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD11	5	0.55
(1,1228)	1:76:B:PHE:H	1:80:B:ILE:HB	3	0.55
(1,1227)	1:76:A:PHE:H	1:80:A:ILE:HB	3	0.55
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	5	0.55
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	5	0.55
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	9	0.55
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	9	0.55
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD22	1	0.55
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD22	1	0.55
(1,1082)	1:37:B:PHE:HA	1:35:B:GLY:HA2	7	0.55
(1,1081)	1:37:A:PHE:HA	1:35:A:GLY:HA2	7	0.55
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD21	9	0.55
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD21	9	0.55
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG2	10	0.55
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG2	10	0.55
(1,795)	1:111:A:GLU:HA	1:50:A:LYS:HB3	9	0.55
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	5	0.55
(1,660)	1:7:B:GLN:HG3	1:8:B:LEU:HG	8	0.55
(1,659)	1:7:A:GLN:HG3	1:8:A:LEU:HG	8	0.55
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	7	0.55
(1,555)	1:47:A:ASN:HA	1:5:B:MET:H	5	0.55
(1,471)	1:79:A:PHE:HB3	1:76:A:PHE:HB3	6	0.55
(1,457)	1:111:A:GLU:HA	1:50:A:LYS:HB3	9	0.55
(1,395)	1:33:A:ASN:HB2	1:34:A:GLN:HG2	1	0.55
(1,377)	1:34:A:GLN:HG3	1:63:A:MET:H	5	0.55
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD22	3	0.55
(1,93)	1:34:A:GLN:HG3	1:63:A:MET:H	5	0.55
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	3	0.55
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	3	0.55
(3,1508)	1:113:B:THR:H	1:107:B:PRO:HD2	2	0.54
(3,1466)	1:110:B:GLY:H	1:108:B:GLY:HA3	1	0.54
(3,1465)	1:110:A:GLY:H	1:108:A:GLY:HA3	1	0.54
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB3	1	0.54
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB3	1	0.54
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG21	1	0.54
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG21	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE3	1	0.54
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE2	7	0.54
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE3	1	0.54
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG3	4	0.54
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	5	0.54
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	6	0.54
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	3	0.54
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	6	0.54
(3,974)	1:5:B:MET:H	1:4:B:LYS:HB2	8	0.54
(3,960)	1:75:B:SER:H	1:63:B:MET:HE3	9	0.54
(3,959)	1:75:A:SER:H	1:63:A:MET:HE3	9	0.54
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG3	9	0.54
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	1	0.54
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	1	0.54
(3,746)	1:24:B:VAL:HG12	1:25:B:LYS:HG3	5	0.54
(3,745)	1:24:A:VAL:HG12	1:25:A:LYS:HG3	5	0.54
(3,668)	1:63:B:MET:HE1	1:32:B:LEU:HB2	4	0.54
(3,668)	1:63:B:MET:HE1	1:32:B:LEU:HB3	8	0.54
(3,667)	1:63:A:MET:HE1	1:32:A:LEU:HB2	4	0.54
(3,667)	1:63:A:MET:HE1	1:32:A:LEU:HB3	8	0.54
(3,628)	1:48:B:PHE:HB2	1:9:A:GLU:HG3	8	0.54
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD22	3	0.54
(3,504)	1:111:B:GLU:HA	1:107:B:PRO:HB2	3	0.54
(3,503)	1:111:A:GLU:HA	1:107:A:PRO:HB2	3	0.54
(3,226)	1:66:B:LEU:HD11	1:82:B:LEU:HA	3	0.54
(3,225)	1:66:A:LEU:HD11	1:82:A:LEU:HA	3	0.54
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	9	0.54
(1,1858)	1:110:B:GLY:H	1:111:B:GLU:HA	10	0.54
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	9	0.54
(1,1544)	1:43:B:LYS:H	1:43:B:LYS:HD2	6	0.54
(1,1543)	1:43:A:LYS:H	1:43:A:LYS:HD2	6	0.54
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD11	5	0.54
(1,1218)	1:87:B:THR:HG23	1:15:A:ILE:HB	7	0.54
(1,1204)	1:34:B:GLN:HB2	1:72:B:LYS:HD3	8	0.54
(1,1203)	1:34:A:GLN:HB2	1:72:A:LYS:HD3	8	0.54
(1,1176)	1:107:B:PRO:HG2	1:109:B:LEU:H	5	0.54
(1,1175)	1:107:A:PRO:HG2	1:109:A:LEU:H	5	0.54
(1,1162)	1:21:B:GLN:HG2	1:19:B:PHE:HB2	7	0.54
(1,1161)	1:21:A:GLN:HG2	1:19:A:PHE:HB2	7	0.54
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG2	8	0.54
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	4	0.54
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	4	0.54
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	5	0.54
(1,992)	1:8:B:LEU:HD21	1:48:A:PHE:HB2	5	0.54
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	7	0.54
(1,878)	1:34:B:GLN:HB2	1:72:B:LYS:HD3	8	0.54
(1,877)	1:34:A:GLN:HB2	1:72:A:LYS:HD3	8	0.54
(1,849)	1:15:A:ILE:HA	1:7:B:GLN:HB3	1	0.54
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD11	10	0.54
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	9	0.54
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	9	0.54
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	1	0.54
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	1	0.54
(1,688)	1:107:B:PRO:HG2	1:109:B:LEU:H	5	0.54
(1,687)	1:107:A:PRO:HG2	1:109:A:LEU:H	5	0.54
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG22	8	0.54
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG22	8	0.54
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	5	0.54
(1,604)	1:18:B:THR:HG23	1:21:B:GLN:HG2	5	0.54
(1,603)	1:18:A:THR:HG23	1:21:A:GLN:HG2	5	0.54
(1,600)	1:18:B:THR:HG23	1:43:B:LYS:HE3	2	0.54
(1,599)	1:18:A:THR:HG23	1:43:A:LYS:HE3	2	0.54
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	7	0.54
(1,555)	1:47:A:ASN:HA	1:5:B:MET:H	9	0.54
(1,511)	1:51:A:LYS:HE3	1:58:A:VAL:HG11	6	0.54
(1,472)	1:79:B:PHE:HB3	1:76:B:PHE:HB3	6	0.54
(1,446)	1:53:B:ASN:HB3	1:41:B:VAL:HB	7	0.54
(1,332)	1:66:B:LEU:H	1:66:B:LEU:HD23	4	0.54
(1,331)	1:66:A:LEU:H	1:66:A:LEU:HD23	4	0.54
(1,330)	1:78:B:GLU:H	1:66:B:LEU:HD22	9	0.54
(1,329)	1:78:A:GLU:H	1:66:A:LEU:HD22	9	0.54
(1,280)	1:19:B:PHE:HB3	1:32:B:LEU:HB2	4	0.54
(1,279)	1:19:A:PHE:HB3	1:32:A:LEU:HB2	4	0.54
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE2	10	0.54
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	4	0.54
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	4	0.54
(1,71)	1:48:A:PHE:HB2	1:9:B:GLU:HB3	2	0.54
(1,66)	1:74:B:LEU:HG	1:62:B:ILE:HG21	5	0.54
(1,65)	1:74:A:LEU:HG	1:62:A:ILE:HG21	5	0.54
(3,1507)	1:113:A:THR:H	1:107:A:PRO:HD2	2	0.53
(3,1374)	1:70:B:ALA:H	1:78:B:GLU:HB2	8	0.53
(3,1373)	1:70:A:ALA:H	1:78:A:GLU:HB2	8	0.53
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD23	6	0.53
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD23	6	0.53
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG3	9	0.53
(3,638)	1:109:B:LEU:HD21	1:48:B:PHE:HA	5	0.53
(3,637)	1:109:A:LEU:HD21	1:48:A:PHE:HA	5	0.53
(3,627)	1:48:A:PHE:HB2	1:9:B:GLU:HG3	8	0.53
(3,582)	1:66:B:LEU:H	1:66:B:LEU:HD23	4	0.53
(3,581)	1:66:A:LEU:H	1:66:A:LEU:HD23	4	0.53
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	9	0.53
(1,1857)	1:110:A:GLY:H	1:111:A:GLU:HA	10	0.53
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	2	0.53
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	2	0.53
(1,1674)	1:66:B:LEU:H	1:63:B:MET:HE1	9	0.53
(1,1466)	1:35:B:GLY:H	1:73:B:GLN:HG2	1	0.53
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB2	7	0.53
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	1	0.53
(1,1217)	1:87:A:THR:HG23	1:15:B:ILE:HB	7	0.53
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE3	10	0.53
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE3	10	0.53
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG3	7	0.53
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG2	8	0.53
(1,1009)	1:8:A:LEU:HD13	1:41:B:VAL:HA	1	0.53
(1,1004)	1:49:B:LEU:H	1:49:B:LEU:HD21	7	0.53
(1,1003)	1:49:A:LEU:H	1:49:A:LEU:HD21	7	0.53
(1,991)	1:8:A:LEU:HD21	1:48:B:PHE:HB2	5	0.53
(1,974)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	10	0.53
(1,973)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	10	0.53
(1,756)	1:111:B:GLU:HG3	1:108:B:GLY:HA3	6	0.53
(1,755)	1:111:A:GLU:HG3	1:108:A:GLY:HA3	6	0.53
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG23	10	0.53
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG23	10	0.53
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	10	0.53
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	10	0.53
(1,660)	1:8:B:LEU:HG	1:83:A:MET:HG3	3	0.53
(1,659)	1:8:A:LEU:HG	1:83:B:MET:HG3	3	0.53
(1,597)	1:85:A:ARG:HG3	1:66:A:LEU:HD23	10	0.53
(1,592)	1:85:B:ARG:HG3	1:66:B:LEU:HG	3	0.53
(1,591)	1:85:A:ARG:HG3	1:66:A:LEU:HG	3	0.53
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	7	0.53
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	7	0.53
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	9	0.53
(1,512)	1:51:B:LYS:HE3	1:58:B:VAL:HG11	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD11	10	0.53
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD11	10	0.53
(1,445)	1:53:A:ASN:HB3	1:41:A:VAL:HB	7	0.53
(1,372)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	10	0.53
(1,371)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	10	0.53
(1,368)	1:34:B:GLN:HG2	1:38:B:LYS:HA	5	0.53
(1,261)	1:8:A:LEU:HG	1:40:B:LEU:HG	7	0.53
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE2	10	0.53
(1,214)	1:62:B:ILE:HG21	1:63:B:MET:HA	5	0.53
(1,213)	1:62:A:ILE:HG21	1:63:A:MET:HA	5	0.53
(1,12)	1:90:B:SER:H	1:92:B:GLU:HA	9	0.53
(1,11)	1:90:A:SER:H	1:92:A:GLU:HA	9	0.53
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	2	0.52
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	4	0.52
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	4	0.52
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD12	8	0.52
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD12	8	0.52
(3,746)	1:24:B:VAL:HG11	1:25:B:LYS:HG3	10	0.52
(3,745)	1:24:A:VAL:HG11	1:25:A:LYS:HG3	10	0.52
(3,602)	1:46:B:GLN:HG3	1:4:A:LYS:HE2	7	0.52
(3,492)	1:59:B:ILE:HD13	1:52:B:GLU:HG2	9	0.52
(3,491)	1:59:A:ILE:HD13	1:52:A:GLU:HG2	9	0.52
(1,1858)	1:110:B:GLY:H	1:111:B:GLU:HA	5	0.52
(1,1857)	1:110:A:GLY:H	1:111:A:GLU:HA	5	0.52
(1,1798)	1:109:B:LEU:H	1:93:B:LYS:HE2	5	0.52
(1,1797)	1:109:A:LEU:H	1:93:A:LYS:HE2	5	0.52
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	5	0.52
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	5	0.52
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD12	9	0.52
(1,1673)	1:66:A:LEU:H	1:63:A:MET:HE1	9	0.52
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD11	8	0.52
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD11	8	0.52
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	8	0.52
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	8	0.52
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG22	5	0.52
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG22	5	0.52
(1,1465)	1:35:A:GLY:H	1:73:A:GLN:HG2	1	0.52
(1,1422)	1:22:B:TYR:H	1:36:B:GLU:HG3	6	0.52
(1,1421)	1:22:A:TYR:H	1:36:A:GLU:HG3	4	0.52
(1,1418)	1:21:B:GLN:H	1:24:B:VAL:HG12	5	0.52
(1,1417)	1:21:A:GLN:H	1:24:A:VAL:HG12	5	0.52
(1,1232)	1:33:B:ASN:H	1:34:B:GLN:HB3	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	1	0.52
(1,1231)	1:33:A:ASN:H	1:34:A:GLN:HB3	4	0.52
(1,1160)	1:21:B:GLN:HG3	1:25:B:LYS:HD2	4	0.52
(1,1159)	1:21:A:GLN:HG3	1:25:A:LYS:HD2	4	0.52
(1,1153)	1:32:A:LEU:HG	1:36:A:GLU:HG2	6	0.52
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG3	7	0.52
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	7	0.52
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD11	10	0.52
(1,810)	1:68:B:THR:H	1:74:B:LEU:HG	5	0.52
(1,809)	1:68:A:THR:H	1:74:A:LEU:HG	5	0.52
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	5	0.52
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	5	0.52
(1,598)	1:85:B:ARG:HG3	1:66:B:LEU:HD23	10	0.52
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE2	6	0.52
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE2	6	0.52
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	3	0.52
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	3	0.52
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG22	5	0.52
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG22	5	0.52
(1,394)	1:33:B:ASN:HB2	1:63:B:MET:HG2	1	0.52
(1,393)	1:33:A:ASN:HB2	1:63:A:MET:HG2	1	0.52
(1,367)	1:34:A:GLN:HG2	1:38:A:LYS:HA	5	0.52
(1,262)	1:8:B:LEU:HG	1:40:A:LEU:HG	7	0.52
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE3	5	0.52
(1,70)	1:33:B:ASN:HB2	1:63:B:MET:HG2	1	0.52
(1,69)	1:33:A:ASN:HB2	1:63:A:MET:HG2	1	0.52
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG11	8	0.51
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	2	0.51
(3,1088)	1:23:B:SER:H	1:40:B:LEU:HD22	7	0.51
(3,1087)	1:23:A:SER:H	1:40:A:LEU:HD22	7	0.51
(3,980)	1:9:B:GLU:H	1:5:B:MET:HG2	1	0.51
(3,979)	1:9:A:GLU:H	1:5:A:MET:HG2	1	0.51
(3,798)	1:107:B:PRO:HG3	1:108:B:GLY:HA3	9	0.51
(3,797)	1:107:A:PRO:HG3	1:108:A:GLY:HA3	9	0.51
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE1	8	0.51
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE1	8	0.51
(3,668)	1:63:B:MET:HE3	1:32:B:LEU:HB2	5	0.51
(3,667)	1:63:A:MET:HE3	1:32:A:LEU:HB2	5	0.51
(3,660)	1:72:B:LYS:HB3	1:64:B:GLU:HA	3	0.51
(3,659)	1:72:A:LYS:HB3	1:64:A:GLU:HA	3	0.51
(3,92)	1:7:B:GLN:HG3	1:6:B:SER:HB3	7	0.51
(3,36)	1:58:B:VAL:HG23	1:57:B:LYS:HE2	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,35)	1:58:A:VAL:HG23	1:57:A:LYS:HE2	7	0.51
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD12	9	0.51
(1,1694)	1:62:B:ILE:H	1:58:B:VAL:HG11	5	0.51
(1,1693)	1:62:A:ILE:H	1:58:A:VAL:HG11	5	0.51
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	7	0.51
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	8	0.51
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	8	0.51
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG23	2	0.51
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG23	2	0.51
(1,1422)	1:22:B:TYR:H	1:36:B:GLU:HG3	4	0.51
(1,1421)	1:22:A:TYR:H	1:36:A:GLU:HG3	6	0.51
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB2	7	0.51
(1,1377)	1:18:A:THR:H	1:20:A:HIS:H	4	0.51
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD12	7	0.51
(1,1327)	1:12:A:ILE:H	1:86:B:LEU:HD12	8	0.51
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD13	6	0.51
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD13	6	0.51
(1,1154)	1:32:B:LEU:HG	1:36:B:GLU:HG2	6	0.51
(1,1154)	1:32:B:LEU:HG	1:36:B:GLU:HG2	10	0.51
(1,1153)	1:32:A:LEU:HG	1:36:A:GLU:HG3	9	0.51
(1,1153)	1:32:A:LEU:HG	1:36:A:GLU:HG2	10	0.51
(1,1150)	1:32:B:LEU:HG	1:40:B:LEU:HB2	10	0.51
(1,1149)	1:32:A:LEU:HG	1:40:A:LEU:HB2	10	0.51
(1,1123)	1:84:A:ALA:HA	1:83:A:MET:HE1	9	0.51
(1,924)	1:87:B:THR:HA	1:86:B:LEU:HG	8	0.51
(1,923)	1:87:A:THR:HA	1:86:A:LEU:HG	8	0.51
(1,788)	1:32:B:LEU:HG	1:40:B:LEU:HB2	10	0.51
(1,787)	1:32:A:LEU:HG	1:40:A:LEU:HB2	10	0.51
(1,719)	1:77:A:GLU:HB3	1:68:A:THR:HG22	9	0.51
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	5	0.51
(1,680)	1:37:B:PHE:HB2	1:62:B:ILE:HG23	1	0.51
(1,679)	1:37:A:PHE:HB2	1:62:A:ILE:HG23	1	0.51
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG23	2	0.51
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG23	2	0.51
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE3	5	0.51
(1,42)	1:78:B:GLU:HG3	1:76:B:PHE:HA	4	0.51
(1,19)	1:93:A:LYS:HA	1:109:A:LEU:HG	8	0.51
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG3	7	0.5
(3,1280)	1:57:B:LYS:H	1:57:B:LYS:HD3	3	0.5
(3,1279)	1:57:A:LYS:H	1:57:A:LYS:HD3	3	0.5
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG11	8	0.5
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG13	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,960)	1:75:B:SER:H	1:63:B:MET:HE2	1	0.5
(3,959)	1:75:A:SER:H	1:63:A:MET:HE2	1	0.5
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD23	4	0.5
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD22	5	0.5
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD23	4	0.5
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD22	5	0.5
(3,667)	1:63:A:MET:HE3	1:32:A:LEU:HB2	9	0.5
(3,660)	1:72:B:LYS:HB3	1:64:B:GLU:HA	5	0.5
(3,659)	1:72:A:LYS:HB3	1:64:A:GLU:HA	5	0.5
(3,601)	1:46:A:GLN:HG3	1:4:B:LYS:HE2	7	0.5
(3,595)	1:72:A:LYS:HG2	1:72:A:LYS:HA	2	0.5
(3,584)	1:66:B:LEU:HD22	1:67:B:ASP:HA	9	0.5
(3,583)	1:66:A:LEU:HD22	1:67:A:ASP:HA	9	0.5
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	9	0.5
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	2	0.5
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	9	0.5
(3,149)	1:77:A:GLU:HA	1:81:B:MET:HE2	8	0.5
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	6	0.5
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	6	0.5
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG3	7	0.5
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD11	9	0.5
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	7	0.5
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	2	0.5
(1,1378)	1:18:B:THR:H	1:20:B:HIS:H	4	0.5
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD13	1	0.5
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD12	7	0.5
(1,1328)	1:12:B:ILE:H	1:86:A:LEU:HD12	8	0.5
(1,1318)	1:11:B:ASN:H	1:12:B:ILE:HG13	8	0.5
(1,1317)	1:11:A:ASN:H	1:12:A:ILE:HG13	8	0.5
(1,1196)	1:98:B:ASP:HA	1:104:B:HIS:HB2	5	0.5
(1,1195)	1:98:A:ASP:HA	1:104:A:HIS:HB2	5	0.5
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	2	0.5
(1,1154)	1:32:B:LEU:HG	1:36:B:GLU:HG3	9	0.5
(1,1150)	1:32:B:LEU:HG	1:40:B:LEU:HB2	7	0.5
(1,1149)	1:32:A:LEU:HG	1:40:A:LEU:HB2	7	0.5
(1,1124)	1:84:B:ALA:HA	1:83:B:MET:HE1	9	0.5
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	9	0.5
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	9	0.5
(1,788)	1:32:B:LEU:HG	1:40:B:LEU:HB2	7	0.5
(1,787)	1:32:A:LEU:HG	1:40:A:LEU:HB2	7	0.5
(1,720)	1:77:B:GLU:HB3	1:68:B:THR:HG22	9	0.5
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD23	2	0.5
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD12	9	0.5
(1,328)	1:66:B:LEU:HD22	1:67:B:ASP:HA	9	0.5
(1,327)	1:66:A:LEU:HD22	1:67:A:ASP:HA	9	0.5
(1,248)	1:63:B:MET:HB3	1:61:B:HIS:HB3	2	0.5
(1,247)	1:63:A:MET:HB3	1:61:A:HIS:HB3	2	0.5
(1,186)	1:60:B:GLU:HG2	1:61:B:HIS:HA	5	0.5
(1,185)	1:60:A:GLU:HG2	1:61:A:HIS:HA	5	0.5
(1,41)	1:78:A:GLU:HG3	1:76:A:PHE:HA	4	0.5
(1,20)	1:93:B:LYS:HA	1:109:B:LEU:HG	8	0.5
(3,1507)	1:113:A:THR:H	1:107:A:PRO:HD3	7	0.49
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB3	10	0.49
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB3	10	0.49
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG3	7	0.49
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG13	10	0.49
(3,740)	1:59:B:ILE:HG23	1:58:B:VAL:HG13	4	0.49
(3,739)	1:59:A:ILE:HG23	1:58:A:VAL:HG13	4	0.49
(3,704)	1:11:B:ASN:HB3	1:9:B:GLU:HA	7	0.49
(3,668)	1:63:B:MET:HE3	1:32:B:LEU:HB2	9	0.49
(3,596)	1:72:B:LYS:HG2	1:72:B:LYS:HA	2	0.49
(3,492)	1:59:B:ILE:HD12	1:52:B:GLU:HG2	10	0.49
(3,491)	1:59:A:ILE:HD12	1:52:A:GLU:HG2	10	0.49
(3,383)	1:51:A:LYS:HD3	1:109:A:LEU:HD21	6	0.49
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	2	0.49
(3,164)	1:13:B:GLU:HB3	1:14:B:THR:HG21	7	0.49
(3,163)	1:13:A:GLU:HB3	1:14:A:THR:HG21	7	0.49
(3,150)	1:77:B:GLU:HA	1:81:A:MET:HE2	8	0.49
(3,147)	1:60:A:GLU:HG2	1:56:A:GLU:H	5	0.49
(3,91)	1:7:A:GLN:HG3	1:6:A:SER:HB3	7	0.49
(1,1804)	1:93:B:LYS:H	1:88:B:TRP:H	3	0.49
(1,1803)	1:93:A:LYS:H	1:88:A:TRP:H	3	0.49
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	1	0.49
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	6	0.49
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	1	0.49
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	6	0.49
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG3	7	0.49
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	3	0.49
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	3	0.49
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD23	2	0.49
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD23	2	0.49
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD11	9	0.49
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	4	0.49
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	8	0.49
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	2	0.49
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	8	0.49
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD13	1	0.49
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	8	0.49
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	2	0.49
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	8	0.49
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	10	0.49
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	10	0.49
(1,1046)	1:53:B:ASN:HA	1:38:B:LYS:HA	5	0.49
(1,1045)	1:53:A:ASN:HA	1:38:A:LYS:HA	5	0.49
(1,836)	1:76:B:PHE:HB3	1:29:B:PRO:HB2	7	0.49
(1,835)	1:76:A:PHE:HB3	1:29:A:PRO:HB2	7	0.49
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG3	4	0.49
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG3	4	0.49
(1,769)	1:59:A:ILE:HD11	1:42:A:ARG:HD2	1	0.49
(1,646)	1:53:B:ASN:HA	1:49:B:LEU:HA	2	0.49
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	1	0.49
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	6	0.49
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	1	0.49
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	6	0.49
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD23	2	0.49
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	6	0.49
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	6	0.49
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD12	9	0.49
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	7	0.49
(3,1508)	1:113:B:THR:H	1:107:B:PRO:HD3	7	0.48
(3,1468)	1:110:B:GLY:H	1:48:B:PHE:HB3	1	0.48
(3,1467)	1:110:A:GLY:H	1:48:A:PHE:HB3	1	0.48
(3,1366)	1:69:B:ASN:H	1:73:B:GLN:HB2	9	0.48
(3,960)	1:75:B:SER:H	1:63:B:MET:HE1	5	0.48
(3,959)	1:75:A:SER:H	1:63:A:MET:HE1	5	0.48
(3,746)	1:24:B:VAL:HG12	1:25:B:LYS:HG3	4	0.48
(3,745)	1:24:A:VAL:HG12	1:25:A:LYS:HG3	4	0.48
(3,703)	1:11:A:ASN:HB3	1:9:A:GLU:HA	7	0.48
(3,668)	1:63:B:MET:HE1	1:32:B:LEU:HB2	10	0.48
(3,667)	1:63:A:MET:HE1	1:32:A:LEU:HB2	10	0.48
(3,660)	1:72:B:LYS:HB3	1:64:B:GLU:HA	8	0.48
(3,659)	1:72:A:LYS:HB3	1:64:A:GLU:HA	8	0.48
(3,485)	1:96:A:GLU:HG2	1:97:A:GLY:H	9	0.48
(3,384)	1:51:B:LYS:HD3	1:109:B:LEU:HD21	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	4	0.48
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	4	0.48
(3,148)	1:60:B:GLU:HG2	1:56:B:GLU:H	5	0.48
(3,132)	1:78:B:GLU:HB3	1:31:B:THR:HA	8	0.48
(3,131)	1:78:A:GLU:HB3	1:31:A:THR:HA	8	0.48
(3,15)	1:101:A:PRO:HG2	1:102:A:GLY:HA2	7	0.48
(1,1858)	1:110:B:GLY:H	1:111:B:GLU:HA	8	0.48
(1,1857)	1:110:A:GLY:H	1:111:A:GLU:HA	8	0.48
(1,1694)	1:62:B:ILE:H	1:58:B:VAL:HG13	3	0.48
(1,1693)	1:62:A:ILE:H	1:58:A:VAL:HG13	3	0.48
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	2	0.48
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	2	0.48
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG21	6	0.48
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG21	6	0.48
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	8	0.48
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	8	0.48
(1,1370)	1:17:B:ASN:H	1:15:B:ILE:HG13	6	0.48
(1,1369)	1:17:A:ASN:H	1:15:A:ILE:HG13	6	0.48
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB3	1	0.48
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB3	1	0.48
(1,1098)	1:59:B:ILE:HG23	1:42:B:ARG:HD2	3	0.48
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	6	0.48
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	6	0.48
(1,770)	1:59:B:ILE:HD11	1:42:B:ARG:HD2	1	0.48
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG22	4	0.48
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	3	0.48
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	3	0.48
(1,671)	1:49:A:LEU:HG	1:53:A:ASN:H	1	0.48
(1,652)	1:93:B:LYS:H	1:92:B:GLU:HB2	5	0.48
(1,652)	1:93:B:LYS:H	1:92:B:GLU:HB2	8	0.48
(1,651)	1:93:A:LYS:H	1:92:A:GLU:HB2	5	0.48
(1,651)	1:93:A:LYS:H	1:92:A:GLU:HB2	8	0.48
(1,646)	1:53:B:ASN:HA	1:49:B:LEU:HA	8	0.48
(1,645)	1:53:A:ASN:HA	1:49:A:LEU:HA	2	0.48
(1,645)	1:53:A:ASN:HA	1:49:A:LEU:HA	8	0.48
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB3	7	0.48
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB3	7	0.48
(1,248)	1:63:B:MET:HB3	1:61:B:HIS:HB3	10	0.48
(1,247)	1:63:A:MET:HB3	1:61:A:HIS:HB3	10	0.48
(1,118)	1:66:B:LEU:HG	1:62:B:ILE:HD11	3	0.48
(1,117)	1:66:A:LEU:HG	1:62:A:ILE:HD11	3	0.48
(1,103)	1:34:A:GLN:HG3	1:74:A:LEU:HD22	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:13:A:GLU:HG2	1:17:A:ASN:HA	3	0.48
(3,1365)	1:69:A:ASN:H	1:73:A:GLN:HB2	9	0.47
(3,1067)	1:21:A:GLN:H	1:20:A:HIS:HB2	4	0.47
(3,792)	1:47:B:ASN:HB3	1:6:A:SER:HB2	10	0.47
(3,668)	1:63:B:MET:HE3	1:32:B:LEU:HB2	2	0.47
(3,667)	1:63:A:MET:HE3	1:32:A:LEU:HB2	2	0.47
(3,660)	1:72:B:LYS:HB3	1:64:B:GLU:HA	10	0.47
(3,659)	1:72:A:LYS:HB3	1:64:A:GLU:HA	10	0.47
(3,486)	1:96:B:GLU:HG2	1:97:B:GLY:H	9	0.47
(3,462)	1:5:B:MET:HB2	1:4:B:LYS:HE3	6	0.47
(3,461)	1:5:A:MET:HB2	1:4:A:LYS:HE3	6	0.47
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG2	8	0.47
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG2	8	0.47
(3,16)	1:101:B:PRO:HG2	1:102:B:GLY:HA2	7	0.47
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	4	0.47
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	4	0.47
(1,1759)	1:24:A:VAL:H	1:25:A:LYS:HG3	6	0.47
(1,1754)	1:84:B:ALA:H	1:80:A:ILE:HD13	5	0.47
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD13	10	0.47
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD13	10	0.47
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD13	4	0.47
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD13	4	0.47
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	6	0.47
(1,1228)	1:76:B:PHE:H	1:80:B:ILE:HB	5	0.47
(1,1227)	1:76:A:PHE:H	1:80:A:ILE:HB	5	0.47
(1,1183)	1:56:A:GLU:HB3	1:57:A:LYS:HD2	7	0.47
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG22	3	0.47
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG22	3	0.47
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB3	6	0.47
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	7	0.47
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB3	6	0.47
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG2	10	0.47
(1,1097)	1:59:A:ILE:HG23	1:42:A:ARG:HD2	3	0.47
(1,974)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	6	0.47
(1,940)	1:5:B:MET:HB3	1:9:B:GLU:HA	7	0.47
(1,939)	1:5:A:MET:HB3	1:9:A:GLU:HA	7	0.47
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG22	4	0.47
(1,679)	1:37:A:PHE:HB2	1:62:A:ILE:HG22	10	0.47
(1,672)	1:49:B:LEU:HG	1:53:B:ASN:H	1	0.47
(1,672)	1:49:B:LEU:HG	1:53:B:ASN:H	9	0.47
(1,671)	1:49:A:LEU:HG	1:53:A:ASN:H	9	0.47
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	4	0.47
(1,582)	1:42:B:ARG:HB3	1:53:B:ASN:HB2	10	0.47
(1,581)	1:42:A:ARG:HB3	1:53:A:ASN:HB2	10	0.47
(1,527)	1:49:A:LEU:HB3	1:51:A:LYS:HG3	7	0.47
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG21	9	0.47
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG21	9	0.47
(1,406)	1:42:B:ARG:HB3	1:53:B:ASN:HB2	10	0.47
(1,405)	1:42:A:ARG:HB3	1:53:A:ASN:HB2	10	0.47
(1,372)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	6	0.47
(1,186)	1:60:B:GLU:HG2	1:61:B:HIS:HA	1	0.47
(1,186)	1:60:B:GLU:HG2	1:61:B:HIS:HA	3	0.47
(1,186)	1:60:B:GLU:HG3	1:61:B:HIS:HA	4	0.47
(1,185)	1:60:A:GLU:HG2	1:61:A:HIS:HA	1	0.47
(1,185)	1:60:A:GLU:HG2	1:61:A:HIS:HA	3	0.47
(1,185)	1:60:A:GLU:HG3	1:61:A:HIS:HA	4	0.47
(1,104)	1:34:B:GLN:HG3	1:74:B:LEU:HD22	3	0.47
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	7	0.47
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	9	0.47
(1,50)	1:13:B:GLU:HG2	1:17:B:ASN:HA	3	0.47
(1,49)	1:64:A:GLU:HG2	1:71:A:ASP:HA	8	0.47
(3,1068)	1:21:B:GLN:H	1:20:B:HIS:HB2	4	0.46
(3,788)	1:67:B:ASP:HB2	1:78:B:GLU:HB2	3	0.46
(3,787)	1:67:A:ASP:HB2	1:78:A:GLU:HB2	3	0.46
(3,726)	1:38:B:LYS:HA	1:42:B:ARG:HD2	9	0.46
(3,725)	1:38:A:LYS:HA	1:42:A:ARG:HD2	9	0.46
(3,628)	1:48:B:PHE:HB2	1:9:A:GLU:HG3	5	0.46
(3,566)	1:111:B:GLU:HB2	1:108:B:GLY:HA3	6	0.46
(3,565)	1:111:A:GLU:HB2	1:108:A:GLY:HA3	6	0.46
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	1	0.46
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	1	0.46
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	10	0.46
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG3	7	0.46
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG3	7	0.46
(3,15)	1:101:A:PRO:HG2	1:102:A:GLY:HA2	9	0.46
(1,1760)	1:24:B:VAL:H	1:25:B:LYS:HG3	6	0.46
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	6	0.46
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	6	0.46
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	6	0.46
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	6	0.46
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	6	0.46
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB2	8	0.46
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB2	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1370)	1:17:B:ASN:H	1:15:B:ILE:HG13	1	0.46
(1,1369)	1:17:A:ASN:H	1:15:A:ILE:HG13	1	0.46
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD13	7	0.46
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD13	7	0.46
(1,1184)	1:56:B:GLU:HB3	1:57:B:LYS:HD2	7	0.46
(1,1184)	1:56:B:GLU:HB3	1:57:B:LYS:HD2	8	0.46
(1,1184)	1:81:B:MET:HB3	1:85:B:ARG:HG3	10	0.46
(1,1183)	1:56:A:GLU:HB3	1:57:A:LYS:HD2	8	0.46
(1,1183)	1:81:A:MET:HB3	1:85:A:ARG:HG3	10	0.46
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	7	0.46
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG2	10	0.46
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD23	9	0.46
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD23	9	0.46
(1,1046)	1:53:B:ASN:HA	1:38:B:LYS:HA	8	0.46
(1,1045)	1:53:A:ASN:HA	1:38:A:LYS:HA	8	0.46
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD21	4	0.46
(1,862)	1:25:B:LYS:HD2	1:33:B:ASN:HB3	3	0.46
(1,861)	1:25:A:LYS:HD2	1:33:A:ASN:HB3	3	0.46
(1,696)	1:74:B:LEU:HG	1:31:B:THR:HG23	6	0.46
(1,695)	1:74:A:LEU:HG	1:31:A:THR:HG23	6	0.46
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG23	5	0.46
(1,680)	1:37:B:PHE:HB3	1:62:B:ILE:HG23	8	0.46
(1,680)	1:37:B:PHE:HB2	1:62:B:ILE:HG22	10	0.46
(1,679)	1:37:A:PHE:HB3	1:62:A:ILE:HG23	8	0.46
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	6	0.46
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	8	0.46
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	6	0.46
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	8	0.46
(1,672)	1:49:B:LEU:HG	1:53:B:ASN:H	3	0.46
(1,671)	1:49:A:LEU:HG	1:53:A:ASN:H	3	0.46
(1,671)	1:49:A:LEU:HG	1:53:A:ASN:H	4	0.46
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD21	5	0.46
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD21	5	0.46
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	5	0.46
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	5	0.46
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE3	2	0.46
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE3	2	0.46
(1,564)	1:16:B:ILE:HB	1:15:B:ILE:HG13	2	0.46
(1,563)	1:16:A:ILE:HB	1:15:A:ILE:HG13	2	0.46
(1,528)	1:49:B:LEU:HB3	1:51:B:LYS:HG3	7	0.46
(1,480)	1:36:B:GLU:HB2	1:31:B:THR:HG22	5	0.46
(1,479)	1:36:A:GLU:HB2	1:31:A:THR:HG22	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:41:B:VAL:HG11	1:48:B:PHE:H	6	0.46
(1,335)	1:41:A:VAL:HG11	1:48:A:PHE:H	6	0.46
(1,262)	1:49:B:LEU:HG	1:89:B:ALA:HB1	5	0.46
(1,261)	1:49:A:LEU:HG	1:89:A:ALA:HB1	5	0.46
(1,247)	1:63:A:MET:HB3	1:61:A:HIS:HB3	9	0.46
(1,190)	1:77:B:GLU:HA	1:87:A:THR:HG21	2	0.46
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	9	0.46
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	5	0.46
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	5	0.46
(1,55)	1:13:A:GLU:HG2	1:109:B:LEU:HD11	8	0.46
(1,50)	1:64:B:GLU:HG2	1:71:B:ASP:HA	8	0.46
(1,28)	1:87:B:THR:HG21	1:85:B:ARG:HA	7	0.46
(1,27)	1:87:A:THR:HG21	1:85:A:ARG:HA	7	0.46
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD23	2	0.45
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD23	2	0.45
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD12	4	0.45
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD12	4	0.45
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	3	0.45
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	7	0.45
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	7	0.45
(3,639)	1:8:A:LEU:HD12	1:83:B:MET:HG3	8	0.45
(3,627)	1:48:A:PHE:HB2	1:9:B:GLU:HG3	5	0.45
(3,618)	1:57:B:LYS:HA	1:57:B:LYS:HG2	8	0.45
(3,617)	1:57:A:LYS:HA	1:57:A:LYS:HG2	8	0.45
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	10	0.45
(3,220)	1:66:B:LEU:HD11	1:74:B:LEU:HA	9	0.45
(3,219)	1:66:A:LEU:HD11	1:74:A:LEU:HA	9	0.45
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	7	0.45
(3,54)	1:39:B:GLU:HG3	1:43:B:LYS:HD3	4	0.45
(3,53)	1:39:A:GLU:HG3	1:43:A:LYS:HD3	4	0.45
(3,42)	1:58:B:VAL:HG22	1:57:B:LYS:HB2	4	0.45
(3,41)	1:58:A:VAL:HG22	1:57:A:LYS:HB2	4	0.45
(3,16)	1:101:B:PRO:HG2	1:102:B:GLY:HA2	9	0.45
(3,6)	1:73:B:GLN:HG3	1:72:B:LYS:HG3	8	0.45
(3,5)	1:73:A:GLN:HG3	1:72:A:LYS:HG3	8	0.45
(1,1753)	1:84:A:ALA:H	1:80:B:ILE:HD13	5	0.45
(1,1580)	1:50:B:LYS:H	1:51:B:LYS:HG3	7	0.45
(1,1579)	1:50:A:LYS:H	1:51:A:LYS:HG3	7	0.45
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG22	3	0.45
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG22	3	0.45
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG21	4	0.45
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	5	0.45
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD12	4	0.45
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD12	4	0.45
(1,1318)	1:13:B:GLU:H	1:12:B:ILE:HG13	2	0.45
(1,1317)	1:13:A:GLU:H	1:12:A:ILE:HG13	2	0.45
(1,1160)	1:21:B:GLN:HG3	1:25:B:LYS:HD2	10	0.45
(1,1159)	1:21:A:GLN:HG3	1:25:A:LYS:HD2	10	0.45
(1,1150)	1:32:B:LEU:HG	1:40:B:LEU:HB2	5	0.45
(1,1149)	1:32:A:LEU:HG	1:40:A:LEU:HB2	5	0.45
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG22	2	0.45
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG22	2	0.45
(1,1048)	1:53:B:ASN:HA	1:59:B:ILE:HA	1	0.45
(1,1047)	1:53:A:ASN:HA	1:59:A:ILE:HA	1	0.45
(1,1046)	1:85:B:ARG:HA	1:77:A:GLU:HA	10	0.45
(1,1045)	1:85:A:ARG:HA	1:77:B:GLU:HA	10	0.45
(1,973)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	6	0.45
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD21	4	0.45
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD22	7	0.45
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD22	7	0.45
(1,924)	1:87:B:THR:HA	1:86:B:LEU:HG	5	0.45
(1,923)	1:87:A:THR:HA	1:86:A:LEU:HG	5	0.45
(1,918)	1:87:B:THR:HA	1:12:A:ILE:HB	3	0.45
(1,917)	1:87:A:THR:HA	1:12:B:ILE:HB	3	0.45
(1,904)	1:86:B:LEU:HB3	1:109:B:LEU:HG	8	0.45
(1,903)	1:86:A:LEU:HB3	1:109:A:LEU:HG	8	0.45
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG23	5	0.45
(1,680)	1:37:B:PHE:HB3	1:62:B:ILE:HG21	2	0.45
(1,679)	1:37:A:PHE:HB3	1:62:A:ILE:HG21	2	0.45
(1,672)	1:49:B:LEU:HG	1:53:B:ASN:H	4	0.45
(1,660)	1:7:B:GLN:HG2	1:8:B:LEU:HG	4	0.45
(1,659)	1:7:A:GLN:HG2	1:8:A:LEU:HG	4	0.45
(1,614)	1:36:B:GLU:HA	1:25:B:LYS:HD2	4	0.45
(1,613)	1:36:A:GLU:HA	1:25:A:LYS:HD2	4	0.45
(1,598)	1:85:B:ARG:HG3	1:82:B:LEU:HD21	1	0.45
(1,597)	1:85:A:ARG:HG3	1:82:A:LEU:HD21	1	0.45
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD13	4	0.45
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD13	4	0.45
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG22	10	0.45
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG22	10	0.45
(1,371)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	6	0.45
(1,268)	1:66:B:LEU:HG	1:85:B:ARG:HB2	2	0.45
(1,267)	1:66:A:LEU:HG	1:85:A:ARG:HB2	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:63:B:MET:HB3	1:61:B:HIS:HB3	9	0.45
(1,214)	1:62:B:ILE:HG23	1:63:B:MET:HA	8	0.45
(1,214)	1:62:B:ILE:HG23	1:63:B:MET:HA	9	0.45
(1,213)	1:62:A:ILE:HG23	1:63:A:MET:HA	8	0.45
(1,213)	1:62:A:ILE:HG23	1:63:A:MET:HA	9	0.45
(1,189)	1:77:A:GLU:HA	1:87:B:THR:HG21	2	0.45
(1,138)	1:80:B:ILE:HD11	1:85:A:ARG:HD2	8	0.45
(1,137)	1:80:A:ILE:HD11	1:85:B:ARG:HD2	8	0.45
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD11	9	0.45
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD11	9	0.45
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	1	0.45
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	1	0.45
(1,56)	1:13:B:GLU:HG2	1:109:A:LEU:HD11	8	0.45
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG2	9	0.44
(3,1152)	1:96:B:GLU:H	1:96:B:GLU:HG2	3	0.44
(3,1151)	1:96:A:GLU:H	1:96:A:GLU:HG2	3	0.44
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	1	0.44
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	8	0.44
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	1	0.44
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	8	0.44
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD23	3	0.44
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD23	3	0.44
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	3	0.44
(3,791)	1:47:A:ASN:HB3	1:6:B:SER:HB2	10	0.44
(3,640)	1:8:B:LEU:HD12	1:83:A:MET:HG3	8	0.44
(3,630)	1:48:B:PHE:HB3	1:45:B:LEU:HA	4	0.44
(3,629)	1:48:A:PHE:HB3	1:45:A:LEU:HA	4	0.44
(3,618)	1:57:B:LYS:HA	1:57:B:LYS:HG2	7	0.44
(3,617)	1:57:A:LYS:HA	1:57:A:LYS:HG2	7	0.44
(3,332)	1:86:B:LEU:HD12	1:9:A:GLU:HG2	5	0.44
(3,331)	1:86:A:LEU:HD12	1:9:B:GLU:HG2	5	0.44
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	6	0.44
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	6	0.44
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG23	5	0.44
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG23	5	0.44
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	7	0.44
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG2	9	0.44
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	1	0.44
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	10	0.44
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	1	0.44
(1,1518)	1:40:B:LEU:H	1:43:B:LYS:HD3	7	0.44
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG21	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	2	0.44
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	2	0.44
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD13	10	0.44
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD13	10	0.44
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG2	3	0.44
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG2	3	0.44
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD23	3	0.44
(1,904)	1:82:B:LEU:HB3	1:80:B:ILE:HB	7	0.44
(1,903)	1:82:A:LEU:HB3	1:80:A:ILE:HB	7	0.44
(1,550)	1:32:B:LEU:HA	1:32:B:LEU:HG	3	0.44
(1,550)	1:32:B:LEU:HA	1:36:B:GLU:HB2	5	0.44
(1,549)	1:32:A:LEU:HA	1:32:A:LEU:HG	3	0.44
(1,549)	1:32:A:LEU:HA	1:36:A:GLU:HB2	5	0.44
(1,368)	1:34:B:GLN:HG3	1:38:B:LYS:HA	6	0.44
(1,367)	1:34:A:GLN:HG3	1:38:A:LYS:HA	6	0.44
(1,336)	1:41:B:VAL:HG11	1:48:B:PHE:H	1	0.44
(1,335)	1:41:A:VAL:HG11	1:48:A:PHE:H	1	0.44
(1,262)	1:49:B:LEU:HG	1:89:B:ALA:HB3	1	0.44
(1,261)	1:49:A:LEU:HG	1:89:A:ALA:HB3	1	0.44
(1,232)	1:12:B:ILE:HG21	1:80:B:ILE:HG22	7	0.44
(1,231)	1:12:A:ILE:HG21	1:80:A:ILE:HG22	7	0.44
(1,186)	1:60:B:GLU:HG3	1:61:B:HIS:HA	6	0.44
(1,185)	1:60:A:GLU:HG3	1:61:A:HIS:HA	6	0.44
(1,138)	1:16:B:ILE:HD12	1:93:A:LYS:HE3	5	0.44
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD13	3	0.44
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD13	10	0.44
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD13	10	0.44
(1,72)	1:33:B:ASN:HB3	1:73:B:GLN:HG2	4	0.44
(1,62)	1:67:B:ASP:H	1:74:B:LEU:HG	3	0.44
(1,61)	1:67:A:ASP:H	1:74:A:LEU:HG	3	0.44
(1,28)	1:87:B:THR:HG23	1:85:B:ARG:HA	10	0.44
(3,1468)	1:110:B:GLY:H	1:48:B:PHE:HB2	7	0.43
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG2	9	0.43
(3,1355)	1:69:A:ASN:H	1:78:A:GLU:HB2	6	0.43
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG23	6	0.43
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG23	6	0.43
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG11	5	0.43
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG11	5	0.43
(3,1147)	1:35:A:GLY:H	1:32:A:LEU:HB3	9	0.43
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	6	0.43
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	6	0.43
(3,777)	1:21:A:GLN:HG2	1:32:A:LEU:HD23	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,692)	1:32:B:LEU:HA	1:36:B:GLU:HB2	10	0.43
(3,691)	1:32:A:LEU:HA	1:36:A:GLU:HB2	10	0.43
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	3	0.43
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG2	7	0.43
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	7	0.43
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	7	0.43
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	9	0.43
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	9	0.43
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG2	9	0.43
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	8	0.43
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	8	0.43
(1,1674)	1:66:B:LEU:H	1:62:B:ILE:HG12	5	0.43
(1,1636)	1:65:B:ASP:H	1:62:B:ILE:HG13	7	0.43
(1,1635)	1:65:A:ASP:H	1:62:A:ILE:HG13	7	0.43
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	10	0.43
(1,1517)	1:40:A:LEU:H	1:43:A:LYS:HD3	7	0.43
(1,1406)	1:20:B:HIS:H	1:32:B:LEU:HG	6	0.43
(1,1405)	1:20:A:HIS:H	1:32:A:LEU:HG	6	0.43
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	9	0.43
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	9	0.43
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB2	5	0.43
(1,1382)	1:18:B:THR:H	1:8:A:LEU:HB2	9	0.43
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB2	5	0.43
(1,1381)	1:18:A:THR:H	1:8:B:LEU:HB2	9	0.43
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	5	0.43
(1,1318)	1:13:B:GLU:H	1:12:B:ILE:HG13	7	0.43
(1,1317)	1:13:A:GLU:H	1:12:A:ILE:HG13	7	0.43
(1,1266)	1:77:B:GLU:H	1:84:A:ALA:HB1	8	0.43
(1,1265)	1:77:A:GLU:H	1:84:B:ALA:HB1	8	0.43
(1,1184)	1:56:B:GLU:HB3	1:57:B:LYS:HD3	4	0.43
(1,1183)	1:56:A:GLU:HB3	1:57:A:LYS:HD3	4	0.43
(1,1162)	1:21:B:GLN:HG2	1:19:B:PHE:HB2	1	0.43
(1,1161)	1:21:A:GLN:HG2	1:19:A:PHE:HB2	1	0.43
(1,1158)	1:20:B:HIS:H	1:32:B:LEU:HG	6	0.43
(1,1157)	1:20:A:HIS:H	1:32:A:LEU:HG	6	0.43
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	3	0.43
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG2	9	0.43
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG2	9	0.43
(1,1046)	1:53:B:ASN:HA	1:38:B:LYS:HA	4	0.43
(1,1045)	1:53:A:ASN:HA	1:38:A:LYS:HA	4	0.43
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	9	0.43
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD23	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,924)	1:87:B:THR:HA	1:86:B:LEU:HG	6	0.43
(1,923)	1:87:A:THR:HA	1:86:A:LEU:HG	6	0.43
(1,671)	1:49:A:LEU:HG	1:53:A:ASN:H	2	0.43
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	7	0.43
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	7	0.43
(1,604)	1:18:B:THR:HG23	1:21:B:GLN:HG2	3	0.43
(1,603)	1:18:A:THR:HG23	1:21:A:GLN:HG2	3	0.43
(1,542)	1:51:B:LYS:HG3	1:48:B:PHE:HA	7	0.43
(1,541)	1:51:A:LYS:HG3	1:48:A:PHE:HA	7	0.43
(1,396)	1:33:B:ASN:HB2	1:71:B:ASP:HB3	3	0.43
(1,395)	1:33:A:ASN:HB2	1:71:A:ASP:HB3	3	0.43
(1,364)	1:46:B:GLN:HB3	1:42:B:ARG:HG2	8	0.43
(1,363)	1:46:A:GLN:HB3	1:42:A:ARG:HG2	8	0.43
(1,214)	1:62:B:ILE:HG21	1:63:B:MET:HA	2	0.43
(1,213)	1:62:A:ILE:HG21	1:63:A:MET:HA	2	0.43
(1,137)	1:16:A:ILE:HD12	1:93:B:LYS:HE3	5	0.43
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD12	5	0.43
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD13	3	0.43
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD12	5	0.43
(1,71)	1:33:A:ASN:HB3	1:73:A:GLN:HG2	4	0.43
(1,60)	1:46:B:GLN:HB3	1:42:B:ARG:HG2	8	0.43
(1,59)	1:46:A:GLN:HB3	1:42:A:ARG:HG2	8	0.43
(1,27)	1:87:A:THR:HG23	1:85:A:ARG:HA	10	0.43
(3,1467)	1:110:A:GLY:H	1:48:A:PHE:HB2	7	0.42
(3,1356)	1:69:B:ASN:H	1:78:B:GLU:HB2	6	0.42
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG21	9	0.42
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG21	9	0.42
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD23	9	0.42
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD22	10	0.42
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD23	9	0.42
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD21	3	0.42
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD21	3	0.42
(3,778)	1:21:B:GLN:HG2	1:32:B:LEU:HD23	1	0.42
(3,712)	1:11:B:ASN:HB3	1:8:B:LEU:HA	7	0.42
(3,711)	1:11:A:ASN:HB3	1:8:A:LEU:HA	7	0.42
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	3	0.42
(3,584)	1:66:B:LEU:HD13	1:67:B:ASP:HA	5	0.42
(3,583)	1:66:A:LEU:HD13	1:67:A:ASP:HA	5	0.42
(3,438)	1:37:B:PHE:HB2	1:63:B:MET:HE3	9	0.42
(3,437)	1:37:A:PHE:HB2	1:63:A:MET:HE3	9	0.42
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG2	7	0.42
(3,252)	1:33:B:ASN:HB3	1:72:B:LYS:HA	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,251)	1:33:A:ASN:HB3	1:72:A:LYS:HA	8	0.42
(3,195)	1:46:A:GLN:HA	1:50:A:LYS:HG3	5	0.42
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	10	0.42
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	10	0.42
(1,1673)	1:66:A:LEU:H	1:62:A:ILE:HG12	5	0.42
(1,1606)	1:80:B:ILE:H	1:78:B:GLU:HG3	6	0.42
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD23	5	0.42
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD23	5	0.42
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	7	0.42
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	9	0.42
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	7	0.42
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	9	0.42
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	5	0.42
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD13	10	0.42
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD13	10	0.42
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	5	0.42
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	5	0.42
(1,1150)	1:32:B:LEU:HG	1:40:B:LEU:HB2	2	0.42
(1,1150)	1:32:B:LEU:HG	1:40:B:LEU:HB2	6	0.42
(1,1149)	1:32:A:LEU:HG	1:40:A:LEU:HB2	2	0.42
(1,1149)	1:32:A:LEU:HG	1:40:A:LEU:HB2	6	0.42
(1,1133)	1:51:A:LYS:HE3	1:53:A:ASN:HB2	3	0.42
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	3	0.42
(1,1008)	1:8:B:LEU:HD11	1:83:A:MET:HA	6	0.42
(1,1007)	1:8:A:LEU:HD11	1:83:B:MET:HA	6	0.42
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	9	0.42
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	1	0.42
(1,756)	1:111:B:GLU:HG3	1:108:B:GLY:HA2	10	0.42
(1,755)	1:111:A:GLU:HG3	1:108:A:GLY:HA2	10	0.42
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	9	0.42
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	9	0.42
(1,676)	1:37:B:PHE:HB2	1:22:B:TYR:HB3	10	0.42
(1,675)	1:37:A:PHE:HB2	1:22:A:TYR:HB3	10	0.42
(1,672)	1:49:B:LEU:HG	1:53:B:ASN:H	2	0.42
(1,661)	1:49:A:LEU:HG	1:52:A:GLU:HG2	1	0.42
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	10	0.42
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	10	0.42
(1,596)	1:85:B:ARG:HG3	1:62:B:ILE:HG22	8	0.42
(1,595)	1:85:A:ARG:HG3	1:62:A:ILE:HG22	8	0.42
(1,556)	1:47:B:ASN:HA	1:5:A:MET:H	8	0.42
(1,550)	1:32:B:LEU:HA	1:32:B:LEU:HG	6	0.42
(1,550)	1:32:B:LEU:HA	1:32:B:LEU:HG	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:32:A:LEU:HA	1:32:A:LEU:HG	6	0.42
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	8	0.42
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	8	0.42
(1,371)	1:7:A:GLN:HG2	1:17:B:ASN:HB3	3	0.42
(1,328)	1:66:B:LEU:HD13	1:67:B:ASP:HA	5	0.42
(1,327)	1:66:A:LEU:HD13	1:67:A:ASP:HA	5	0.42
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD12	2	0.42
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD13	8	0.42
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD12	2	0.42
(3,1480)	1:100:B:GLY:H	1:99:B:GLU:HB2	9	0.41
(3,1479)	1:100:A:GLY:H	1:99:A:GLU:HB2	9	0.41
(3,1474)	1:100:B:GLY:H	1:98:B:ASP:HA	9	0.41
(3,1468)	1:110:B:GLY:H	1:48:B:PHE:HB2	5	0.41
(3,1467)	1:110:A:GLY:H	1:48:A:PHE:HB2	5	0.41
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG23	4	0.41
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG23	4	0.41
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG11	4	0.41
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG12	9	0.41
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG11	4	0.41
(3,1148)	1:35:B:GLY:H	1:32:B:LEU:HB3	9	0.41
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD22	10	0.41
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD23	7	0.41
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD23	7	0.41
(3,668)	1:63:B:MET:HE2	1:32:B:LEU:HB2	6	0.41
(3,667)	1:63:A:MET:HE2	1:32:A:LEU:HB2	6	0.41
(3,630)	1:48:B:PHE:HB3	1:45:B:LEU:HA	7	0.41
(3,629)	1:48:A:PHE:HB3	1:45:A:LEU:HA	7	0.41
(3,526)	1:76:B:PHE:HB2	1:16:B:ILE:HA	3	0.41
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB3	10	0.41
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB3	10	0.41
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	5	0.41
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG2	8	0.41
(3,252)	1:33:B:ASN:HB3	1:72:B:LYS:HA	7	0.41
(3,251)	1:33:A:ASN:HB3	1:72:A:LYS:HA	7	0.41
(3,196)	1:46:B:GLN:HA	1:50:B:LYS:HG3	5	0.41
(3,149)	1:77:A:GLU:HA	1:81:B:MET:HE3	1	0.41
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG22	6	0.41
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG22	6	0.41
(3,132)	1:78:B:GLU:HB2	1:31:B:THR:HA	6	0.41
(3,131)	1:78:A:GLU:HB2	1:31:A:THR:HA	6	0.41
(3,42)	1:58:B:VAL:HG21	1:57:B:LYS:HB2	9	0.41
(3,41)	1:58:A:VAL:HG21	1:57:A:LYS:HB2	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:80:A:ILE:H	1:78:A:GLU:HG3	6	0.41
(1,1574)	1:75:B:SER:H	1:68:B:THR:HA	3	0.41
(1,1573)	1:75:A:SER:H	1:68:A:THR:HA	3	0.41
(1,1544)	1:43:B:LYS:H	1:42:B:ARG:HG2	1	0.41
(1,1543)	1:43:A:LYS:H	1:42:A:ARG:HG2	1	0.41
(1,1508)	1:67:B:ASP:H	1:64:B:GLU:HG2	6	0.41
(1,1507)	1:67:A:ASP:H	1:64:A:GLU:HG2	6	0.41
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	3	0.41
(1,1318)	1:13:B:GLU:H	1:12:B:ILE:HG13	9	0.41
(1,1317)	1:13:A:GLU:H	1:12:A:ILE:HG13	9	0.41
(1,1135)	1:5:A:MET:HG2	1:4:A:LYS:HE3	3	0.41
(1,1134)	1:51:B:LYS:HE3	1:53:B:ASN:HB2	3	0.41
(1,1082)	1:37:B:PHE:HA	1:39:B:GLU:HA	3	0.41
(1,1081)	1:37:A:PHE:HA	1:39:A:GLU:HA	3	0.41
(1,924)	1:87:B:THR:HA	1:86:B:LEU:HG	7	0.41
(1,923)	1:87:A:THR:HA	1:86:A:LEU:HG	7	0.41
(1,912)	1:66:B:LEU:HD12	1:64:B:GLU:HA	1	0.41
(1,911)	1:66:A:LEU:HD12	1:64:A:GLU:HA	1	0.41
(1,907)	1:86:A:LEU:HB3	1:13:B:GLU:HG2	4	0.41
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB3	10	0.41
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB3	10	0.41
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG2	8	0.41
(1,808)	1:74:B:LEU:HG	1:64:B:GLU:HA	3	0.41
(1,807)	1:74:A:LEU:HG	1:64:A:GLU:HA	3	0.41
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	1	0.41
(1,756)	1:96:B:GLU:HG3	1:97:B:GLY:HA3	4	0.41
(1,755)	1:96:A:GLU:HG3	1:97:A:GLY:HA3	4	0.41
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	7	0.41
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	7	0.41
(1,680)	1:37:B:PHE:HB3	1:62:B:ILE:HG23	6	0.41
(1,679)	1:37:A:PHE:HB3	1:62:A:ILE:HG23	6	0.41
(1,662)	1:49:B:LEU:HG	1:52:B:GLU:HG2	1	0.41
(1,604)	1:18:B:THR:HG23	1:21:B:GLN:HG2	6	0.41
(1,603)	1:18:A:THR:HG23	1:21:A:GLN:HG2	6	0.41
(1,596)	1:85:B:ARG:HG3	1:80:A:ILE:HG12	3	0.41
(1,549)	1:32:A:LEU:HA	1:32:A:LEU:HG	10	0.41
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD12	2	0.41
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD12	2	0.41
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	4	0.41
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	4	0.41
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG21	1	0.41
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG21	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:34:B:GLN:HG3	1:63:B:MET:H	10	0.41
(1,377)	1:34:A:GLN:HG3	1:63:A:MET:H	10	0.41
(1,347)	1:5:A:MET:HG2	1:4:A:LYS:HE3	3	0.41
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD13	8	0.41
(1,94)	1:34:B:GLN:HG3	1:63:B:MET:H	10	0.41
(1,93)	1:34:A:GLN:HG3	1:63:A:MET:H	10	0.41
(1,80)	1:59:B:ILE:HB	1:37:B:PHE:HB3	6	0.41
(1,79)	1:59:A:ILE:HB	1:37:A:PHE:HB3	6	0.41
(3,1473)	1:100:A:GLY:H	1:98:A:ASP:HA	9	0.4
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG12	9	0.4
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE2	10	0.4
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE2	10	0.4
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD23	7	0.4
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	10	0.4
(3,726)	1:38:B:LYS:HA	1:42:B:ARG:HD2	4	0.4
(3,725)	1:38:A:LYS:HA	1:42:A:ARG:HD2	4	0.4
(3,525)	1:76:A:PHE:HB2	1:16:A:ILE:HA	3	0.4
(3,504)	1:111:B:GLU:HA	1:107:B:PRO:HB2	5	0.4
(3,503)	1:111:A:GLU:HA	1:107:A:PRO:HB2	5	0.4
(3,486)	1:96:B:GLU:HG3	1:97:B:GLY:H	7	0.4
(3,485)	1:96:A:GLU:HG3	1:97:A:GLY:H	6	0.4
(3,390)	1:51:B:LYS:H	1:51:B:LYS:HD3	3	0.4
(3,389)	1:51:A:LYS:H	1:51:A:LYS:HD3	3	0.4
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	5	0.4
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG2	8	0.4
(3,207)	1:44:A:ASP:HA	1:9:B:GLU:HG3	7	0.4
(3,164)	1:13:B:GLU:HB3	1:14:B:THR:HG22	9	0.4
(3,163)	1:13:A:GLU:HB3	1:14:A:THR:HG22	9	0.4
(3,150)	1:77:B:GLU:HA	1:81:A:MET:HE3	1	0.4
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG22	7	0.4
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG22	7	0.4
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	3	0.4
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	6	0.4
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	3	0.4
(3,34)	1:87:B:THR:HG23	1:88:B:TRP:HA	5	0.4
(3,33)	1:87:A:THR:HG23	1:88:A:TRP:HA	5	0.4
(1,1636)	1:65:B:ASP:H	1:66:B:LEU:HG	8	0.4
(1,1635)	1:65:A:ASP:H	1:66:A:LEU:HG	8	0.4
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD11	1	0.4
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD11	1	0.4
(1,1562)	1:44:B:ASP:H	1:40:B:LEU:HD23	3	0.4
(1,1543)	1:43:A:LYS:H	1:43:A:LYS:HD2	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	3	0.4
(1,1450)	1:45:B:LEU:H	1:46:B:GLN:HB3	6	0.4
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	3	0.4
(1,1449)	1:45:A:LEU:H	1:46:A:GLN:HB3	6	0.4
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG23	8	0.4
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG23	8	0.4
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	3	0.4
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD13	2	0.4
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD13	2	0.4
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD13	3	0.4
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	4	0.4
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	4	0.4
(1,1327)	1:12:A:ILE:H	1:45:B:LEU:HD23	2	0.4
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD12	5	0.4
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD12	5	0.4
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD3	8	0.4
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD3	8	0.4
(1,1270)	1:48:B:PHE:H	1:51:B:LYS:HE2	7	0.4
(1,1228)	1:76:B:PHE:H	1:80:B:ILE:HB	10	0.4
(1,1227)	1:76:A:PHE:H	1:80:A:ILE:HB	10	0.4
(1,1136)	1:5:B:MET:HG2	1:4:B:LYS:HE3	3	0.4
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG2	2	0.4
(1,1046)	1:85:B:ARG:HA	1:77:A:GLU:HA	1	0.4
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	3	0.4
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	3	0.4
(1,912)	1:66:B:LEU:HD11	1:64:B:GLU:HA	7	0.4
(1,908)	1:86:B:LEU:HB3	1:13:A:GLU:HG2	4	0.4
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG2	8	0.4
(1,742)	1:81:B:MET:HA	1:84:B:ALA:HB3	8	0.4
(1,741)	1:81:A:MET:HA	1:84:A:ALA:HB3	8	0.4
(1,680)	1:37:B:PHE:HB2	1:62:B:ILE:HG21	4	0.4
(1,679)	1:37:A:PHE:HB2	1:62:A:ILE:HG21	4	0.4
(1,672)	1:49:B:LEU:HG	1:53:B:ASN:H	8	0.4
(1,671)	1:49:A:LEU:HG	1:53:A:ASN:H	8	0.4
(1,595)	1:85:A:ARG:HG3	1:80:B:ILE:HG12	3	0.4
(1,555)	1:47:A:ASN:HA	1:5:B:MET:H	8	0.4
(1,549)	1:32:A:LEU:HA	1:32:A:LEU:HG	2	0.4
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD13	3	0.4
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD13	3	0.4
(1,372)	1:7:B:GLN:HG2	1:17:A:ASN:HB3	3	0.4
(1,348)	1:5:B:MET:HG2	1:4:B:LYS:HE3	3	0.4
(1,190)	1:77:B:GLU:HA	1:87:A:THR:HG22	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD13	3	0.4
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD13	3	0.4
(1,72)	1:48:B:PHE:HB2	1:9:A:GLU:HB3	5	0.4
(1,65)	1:74:A:LEU:HG	1:62:A:ILE:HG21	2	0.4
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB3	8	0.39
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB3	8	0.39
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG22	3	0.39
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG22	3	0.39
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD23	3	0.39
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD23	7	0.39
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD23	3	0.39
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	10	0.39
(3,494)	1:59:B:ILE:HD13	1:38:B:LYS:HE2	4	0.39
(3,486)	1:96:B:GLU:HG2	1:97:B:GLY:H	6	0.39
(3,485)	1:96:A:GLU:HG3	1:97:A:GLY:H	7	0.39
(3,252)	1:33:B:ASN:HB2	1:72:B:LYS:HA	10	0.39
(3,251)	1:33:A:ASN:HB2	1:72:A:LYS:HA	10	0.39
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	6	0.39
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE2	9	0.39
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE2	9	0.39
(1,1770)	1:87:B:THR:H	1:82:B:LEU:HD12	7	0.39
(1,1769)	1:87:A:THR:H	1:82:A:LEU:HD12	7	0.39
(1,1606)	1:90:B:SER:H	1:13:A:GLU:HG2	5	0.39
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD13	1	0.39
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD13	1	0.39
(1,1561)	1:44:A:ASP:H	1:40:A:LEU:HD23	3	0.39
(1,1544)	1:43:B:LYS:H	1:43:B:LYS:HD2	5	0.39
(1,1500)	1:44:B:ASP:H	1:40:B:LEU:HD23	3	0.39
(1,1499)	1:44:A:ASP:H	1:40:A:LEU:HD23	3	0.39
(1,1482)	1:37:B:PHE:H	1:59:B:ILE:HG21	1	0.39
(1,1481)	1:37:A:PHE:H	1:59:A:ILE:HG21	1	0.39
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD13	3	0.39
(1,1328)	1:12:B:ILE:H	1:45:A:LEU:HD23	2	0.39
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD12	1	0.39
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD12	1	0.39
(1,1269)	1:48:A:PHE:H	1:51:A:LYS:HE2	7	0.39
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	8	0.39
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	8	0.39
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	4	0.39
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	4	0.39
(1,1122)	1:84:B:ALA:HA	1:81:B:MET:HG2	4	0.39
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG2	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1121)	1:84:A:ALA:HA	1:81:A:MET:HG2	4	0.39
(1,1033)	1:63:A:MET:HE3	1:32:A:LEU:HD13	1	0.39
(1,911)	1:66:A:LEU:HD11	1:64:A:GLU:HA	7	0.39
(1,810)	1:68:B:THR:H	1:74:B:LEU:HG	4	0.39
(1,809)	1:68:A:THR:H	1:74:A:LEU:HG	4	0.39
(1,645)	1:86:A:LEU:HA	1:49:A:LEU:HA	1	0.39
(1,550)	1:32:B:LEU:HA	1:32:B:LEU:HG	2	0.39
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG21	4	0.39
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG21	4	0.39
(1,368)	1:34:B:GLN:HG2	1:38:B:LYS:HA	9	0.39
(1,367)	1:34:A:GLN:HG2	1:38:A:LYS:HA	9	0.39
(1,189)	1:77:A:GLU:HA	1:87:B:THR:HG22	1	0.39
(1,186)	1:60:B:GLU:HG3	1:61:B:HIS:HA	2	0.39
(1,186)	1:60:B:GLU:HG3	1:61:B:HIS:HA	8	0.39
(1,185)	1:60:A:GLU:HG3	1:61:A:HIS:HA	2	0.39
(1,185)	1:60:A:GLU:HG3	1:61:A:HIS:HA	8	0.39
(1,71)	1:48:A:PHE:HB2	1:9:B:GLU:HB3	5	0.39
(1,66)	1:74:B:LEU:HG	1:62:B:ILE:HG21	2	0.39
(1,20)	1:93:B:LYS:HA	1:109:B:LEU:HG	7	0.39
(1,19)	1:93:A:LYS:HA	1:109:A:LEU:HG	7	0.39
(3,1440)	1:87:B:THR:H	1:77:A:GLU:HG3	8	0.38
(3,1439)	1:87:A:THR:H	1:77:B:GLU:HG3	8	0.38
(3,1382)	1:71:B:ASP:H	1:72:B:LYS:HE2	5	0.38
(3,1381)	1:71:A:ASP:H	1:72:A:LYS:HE2	5	0.38
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG13	7	0.38
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG13	7	0.38
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE2	9	0.38
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE2	9	0.38
(3,960)	1:75:B:SER:H	1:63:B:MET:HE1	2	0.38
(3,959)	1:75:A:SER:H	1:63:A:MET:HE1	2	0.38
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD22	2	0.38
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD22	2	0.38
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	1	0.38
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	1	0.38
(3,798)	1:107:B:PRO:HG3	1:108:B:GLY:HA3	6	0.38
(3,797)	1:107:A:PRO:HG3	1:108:A:GLY:HA3	6	0.38
(3,746)	1:24:B:VAL:HG13	1:25:B:LYS:HG3	1	0.38
(3,746)	1:24:B:VAL:HG12	1:25:B:LYS:HG3	3	0.38
(3,745)	1:24:A:VAL:HG13	1:25:A:LYS:HG3	1	0.38
(3,500)	1:32:B:LEU:HG	1:23:B:SER:HB3	8	0.38
(3,499)	1:32:A:LEU:HG	1:23:A:SER:HB3	8	0.38
(3,493)	1:59:A:ILE:HD13	1:38:A:LYS:HE2	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,220)	1:66:B:LEU:HD12	1:74:B:LEU:HA	10	0.38
(3,208)	1:44:B:ASP:HA	1:9:A:GLU:HG3	1	0.38
(3,208)	1:44:B:ASP:HA	1:9:A:GLU:HG3	7	0.38
(3,180)	1:49:B:LEU:HG	1:48:B:PHE:HB3	10	0.38
(3,179)	1:49:A:LEU:HG	1:48:A:PHE:HB3	10	0.38
(3,146)	1:36:B:GLU:HA	1:25:B:LYS:HE2	7	0.38
(3,88)	1:34:B:GLN:HG3	1:38:B:LYS:HD3	3	0.38
(3,42)	1:58:B:VAL:HG23	1:57:B:LYS:HB2	7	0.38
(3,42)	1:58:B:VAL:HG23	1:57:B:LYS:HB2	10	0.38
(3,41)	1:58:A:VAL:HG23	1:57:A:LYS:HB2	7	0.38
(3,41)	1:58:A:VAL:HG23	1:57:A:LYS:HB2	10	0.38
(1,1746)	1:87:B:THR:H	1:77:A:GLU:HG3	8	0.38
(1,1745)	1:87:A:THR:H	1:77:B:GLU:HG3	8	0.38
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	1	0.38
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	1	0.38
(1,1605)	1:90:A:SER:H	1:13:B:GLU:HG2	5	0.38
(1,1465)	1:35:A:GLY:H	1:72:A:LYS:HB3	8	0.38
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD13	3	0.38
(1,1318)	1:13:B:GLU:H	1:12:B:ILE:HG13	5	0.38
(1,1317)	1:13:A:GLU:H	1:12:A:ILE:HG13	5	0.38
(1,1268)	1:77:B:GLU:H	1:80:B:ILE:HD12	9	0.38
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	3	0.38
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	3	0.38
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG2	5	0.38
(1,1122)	1:84:B:ALA:HA	1:83:B:MET:HG2	6	0.38
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG2	5	0.38
(1,1121)	1:84:A:ALA:HA	1:83:A:MET:HG2	6	0.38
(1,1048)	1:53:B:ASN:HA	1:59:B:ILE:HA	8	0.38
(1,1047)	1:53:A:ASN:HA	1:59:A:ILE:HA	8	0.38
(1,1045)	1:85:A:ARG:HA	1:77:B:GLU:HA	1	0.38
(1,1044)	1:53:B:ASN:HA	1:58:B:VAL:HB	2	0.38
(1,1034)	1:63:B:MET:HE3	1:32:B:LEU:HD13	1	0.38
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD21	2	0.38
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD21	2	0.38
(1,912)	1:66:B:LEU:HD11	1:64:B:GLU:HA	8	0.38
(1,911)	1:66:A:LEU:HD11	1:64:A:GLU:HA	8	0.38
(1,646)	1:86:B:LEU:HA	1:49:B:LEU:HA	1	0.38
(1,348)	1:5:B:MET:HG3	1:4:B:LYS:HE3	8	0.38
(1,347)	1:5:A:MET:HG3	1:4:A:LYS:HE3	8	0.38
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE3	3	0.38
(1,72)	1:48:B:PHE:HB2	1:9:A:GLU:HB3	8	0.38
(1,71)	1:48:A:PHE:HB2	1:9:B:GLU:HB3	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:64:B:GLU:HG2	1:71:B:ASP:HA	6	0.38
(1,49)	1:64:A:GLU:HG2	1:71:A:ASP:HA	6	0.38
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	10	0.37
(4,11)	1:98:A:ASP:HA	1:96:A:GLU:HA	10	0.37
(3,1428)	1:86:B:LEU:H	1:86:B:LEU:HG	10	0.37
(3,1427)	1:86:A:LEU:H	1:86:A:LEU:HG	10	0.37
(3,1382)	1:71:B:ASP:H	1:72:B:LYS:HE2	10	0.37
(3,1381)	1:71:A:ASP:H	1:72:A:LYS:HE2	10	0.37
(3,1366)	1:69:B:ASN:H	1:73:B:GLN:HB2	7	0.37
(3,1365)	1:69:A:ASN:H	1:73:A:GLN:HB2	7	0.37
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD22	4	0.37
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD22	4	0.37
(3,1082)	1:23:B:SER:H	1:29:B:PRO:HB2	9	0.37
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	6	0.37
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	6	0.37
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	2	0.37
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE1	4	0.37
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE1	4	0.37
(3,745)	1:24:A:VAL:HG12	1:25:A:LYS:HG3	3	0.37
(3,740)	1:59:B:ILE:HG23	1:58:B:VAL:HG12	8	0.37
(3,530)	1:67:B:ASP:HB3	1:64:B:GLU:HG3	7	0.37
(3,529)	1:67:A:ASP:HB3	1:64:A:GLU:HG3	7	0.37
(3,485)	1:96:A:GLU:HG3	1:97:A:GLY:H	5	0.37
(3,283)	1:58:A:VAL:HA	1:57:A:LYS:HG3	3	0.37
(3,252)	1:33:B:ASN:HB3	1:72:B:LYS:HA	4	0.37
(3,251)	1:33:A:ASN:HB3	1:72:A:LYS:HA	4	0.37
(3,251)	1:33:A:ASN:HB3	1:72:A:LYS:HA	5	0.37
(3,219)	1:66:A:LEU:HD12	1:74:A:LEU:HA	10	0.37
(3,145)	1:36:A:GLU:HA	1:25:A:LYS:HE2	7	0.37
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG22	2	0.37
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG22	2	0.37
(3,87)	1:34:A:GLN:HG3	1:38:A:LYS:HD3	3	0.37
(3,42)	1:58:B:VAL:HG21	1:57:B:LYS:HB2	1	0.37
(3,42)	1:58:B:VAL:HG22	1:57:B:LYS:HB2	5	0.37
(3,41)	1:58:A:VAL:HG21	1:57:A:LYS:HB2	1	0.37
(3,41)	1:58:A:VAL:HG22	1:57:A:LYS:HB2	5	0.37
(3,13)	1:111:A:GLU:HA	1:111:A:GLU:HG3	5	0.37
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	9	0.37
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	9	0.37
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD13	1	0.37
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD22	9	0.37
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD22	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1466)	1:35:B:GLY:H	1:72:B:LYS:HB3	8	0.37
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	9	0.37
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	9	0.37
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD13	3	0.37
(1,1267)	1:77:A:GLU:H	1:80:A:ILE:HD12	9	0.37
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	10	0.37
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	10	0.37
(1,1214)	1:50:B:LYS:HE3	1:49:B:LEU:HB2	7	0.37
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	5	0.37
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	5	0.37
(1,1043)	1:53:A:ASN:HA	1:58:A:VAL:HB	2	0.37
(1,1028)	1:84:B:ALA:HA	1:86:B:LEU:HG	8	0.37
(1,1027)	1:84:A:ALA:HA	1:86:A:LEU:HG	8	0.37
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD23	1	0.37
(1,923)	1:87:A:THR:HA	1:86:A:LEU:HG	2	0.37
(1,882)	1:81:B:MET:HB3	1:79:B:PHE:HA	1	0.37
(1,742)	1:81:B:MET:HA	1:84:B:ALA:HB1	4	0.37
(1,741)	1:81:A:MET:HA	1:84:A:ALA:HB1	4	0.37
(1,716)	1:46:B:GLN:HG2	1:45:B:LEU:HD23	1	0.37
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	6	0.37
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	6	0.37
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	9	0.37
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	9	0.37
(1,630)	1:84:B:ALA:HA	1:86:B:LEU:HG	8	0.37
(1,629)	1:84:A:ALA:HA	1:86:A:LEU:HG	8	0.37
(1,508)	1:11:B:ASN:HB3	1:15:A:ILE:HG13	9	0.37
(1,507)	1:11:A:ASN:HB3	1:15:B:ILE:HG13	9	0.37
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	8	0.37
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	8	0.37
(1,367)	1:34:A:GLN:HG2	1:38:A:LYS:HA	7	0.37
(1,318)	1:82:B:LEU:HB3	1:80:A:ILE:HD11	8	0.37
(1,317)	1:82:A:LEU:HB3	1:80:B:ILE:HD11	8	0.37
(1,249)	1:36:A:GLU:HB3	1:25:A:LYS:HE2	5	0.37
(1,140)	1:16:B:ILE:HD12	1:13:B:GLU:HG2	1	0.37
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD12	1	0.37
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD12	1	0.37
(1,45)	1:39:A:GLU:HG2	1:44:A:ASP:H	5	0.37
(3,1490)	1:103:B:HIS:H	1:101:B:PRO:HB3	1	0.36
(3,1489)	1:103:A:HIS:H	1:101:A:PRO:HB3	1	0.36
(3,1468)	1:110:B:GLY:H	1:48:B:PHE:HB3	9	0.36
(3,1467)	1:110:A:GLY:H	1:48:A:PHE:HB3	9	0.36
(3,1442)	1:87:B:THR:H	1:16:A:ILE:HD11	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1168)	1:38:B:LYS:H	1:38:B:LYS:HG3	3	0.36
(3,1167)	1:38:A:LYS:H	1:38:A:LYS:HG3	3	0.36
(3,1081)	1:23:A:SER:H	1:29:A:PRO:HB2	9	0.36
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	2	0.36
(3,840)	1:76:B:PHE:H	1:79:B:PHE:HB3	2	0.36
(3,840)	1:76:B:PHE:H	1:79:B:PHE:HB3	10	0.36
(3,839)	1:76:A:PHE:H	1:79:A:PHE:HB3	2	0.36
(3,839)	1:76:A:PHE:H	1:79:A:PHE:HB3	10	0.36
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	7	0.36
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	7	0.36
(3,739)	1:59:A:ILE:HG23	1:58:A:VAL:HG12	8	0.36
(3,725)	1:38:A:LYS:HA	1:42:A:ARG:HD2	7	0.36
(3,638)	1:109:B:LEU:HD11	1:48:B:PHE:HA	9	0.36
(3,637)	1:109:A:LEU:HD11	1:48:A:PHE:HA	9	0.36
(3,631)	1:8:A:LEU:HD13	1:44:B:ASP:HB2	6	0.36
(3,565)	1:111:A:GLU:HB2	1:108:A:GLY:HA2	4	0.36
(3,539)	1:15:A:ILE:HA	1:8:B:LEU:HD22	10	0.36
(3,492)	1:59:B:ILE:HD13	1:52:B:GLU:HG2	1	0.36
(3,491)	1:59:A:ILE:HD13	1:52:A:GLU:HG2	1	0.36
(3,486)	1:96:B:GLU:HG3	1:97:B:GLY:H	5	0.36
(3,437)	1:37:A:PHE:HB2	1:63:A:MET:HE1	8	0.36
(3,329)	1:86:A:LEU:HD11	1:49:A:LEU:HG	3	0.36
(3,284)	1:58:B:VAL:HA	1:57:B:LYS:HG3	3	0.36
(3,260)	1:42:B:ARG:HB2	1:43:B:LYS:HG2	6	0.36
(3,259)	1:42:A:ARG:HB2	1:43:A:LYS:HG2	6	0.36
(3,252)	1:33:B:ASN:HB3	1:72:B:LYS:HA	5	0.36
(3,220)	1:66:B:LEU:HD12	1:74:B:LEU:HA	4	0.36
(3,219)	1:66:A:LEU:HD12	1:74:A:LEU:HA	4	0.36
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG23	4	0.36
(3,14)	1:111:B:GLU:HA	1:111:B:GLU:HG3	5	0.36
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD13	1	0.36
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	4	0.36
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	4	0.36
(1,1213)	1:50:A:LYS:HE3	1:49:A:LEU:HB2	7	0.36
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD23	1	0.36
(1,924)	1:87:B:THR:HA	1:86:B:LEU:HG	2	0.36
(1,924)	1:87:B:THR:HA	1:86:B:LEU:HG	4	0.36
(1,923)	1:87:A:THR:HA	1:86:A:LEU:HG	4	0.36
(1,908)	1:86:B:LEU:HB3	1:9:A:GLU:HG3	6	0.36
(1,907)	1:86:A:LEU:HB3	1:9:B:GLU:HG3	6	0.36
(1,881)	1:81:A:MET:HB3	1:79:A:PHE:HA	1	0.36
(1,810)	1:74:B:LEU:HG	1:38:B:LYS:H	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:74:A:LEU:HG	1:38:A:LYS:H	3	0.36
(1,715)	1:46:A:GLN:HG2	1:45:A:LEU:HD23	1	0.36
(1,368)	1:34:B:GLN:HG2	1:38:B:LYS:HA	7	0.36
(1,250)	1:36:B:GLU:HB3	1:25:B:LYS:HE2	5	0.36
(1,248)	1:63:B:MET:HB2	1:61:B:HIS:HB2	3	0.36
(1,247)	1:63:A:MET:HB2	1:61:A:HIS:HB2	3	0.36
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE3	3	0.36
(1,139)	1:16:A:ILE:HD12	1:13:A:GLU:HG2	1	0.36
(1,72)	1:33:B:ASN:HB3	1:73:B:GLN:HG2	6	0.36
(1,71)	1:33:A:ASN:HB3	1:73:A:GLN:HG2	6	0.36
(1,66)	1:74:B:LEU:HG	1:62:B:ILE:HG23	8	0.36
(1,65)	1:74:A:LEU:HG	1:62:A:ILE:HG23	8	0.36
(1,50)	1:64:B:GLU:HG3	1:71:B:ASP:HA	5	0.36
(1,49)	1:64:A:GLU:HG3	1:71:A:ASP:HA	5	0.36
(1,46)	1:39:B:GLU:HG2	1:44:B:ASP:H	5	0.36
(3,1441)	1:87:A:THR:H	1:16:B:ILE:HD11	3	0.35
(3,1428)	1:86:B:LEU:H	1:86:B:LEU:HG	1	0.35
(3,1406)	1:81:B:MET:H	1:80:B:ILE:HB	7	0.35
(3,1405)	1:81:A:MET:H	1:80:A:ILE:HB	7	0.35
(3,1178)	1:67:B:ASP:H	1:74:B:LEU:HD22	3	0.35
(3,1177)	1:67:A:ASP:H	1:74:A:LEU:HD22	3	0.35
(3,881)	1:30:A:ASP:H	1:31:A:THR:HG21	3	0.35
(3,726)	1:38:B:LYS:HA	1:42:B:ARG:HD2	7	0.35
(3,632)	1:8:B:LEU:HD13	1:44:A:ASP:HB2	6	0.35
(3,566)	1:111:B:GLU:HB2	1:108:B:GLY:HA2	4	0.35
(3,438)	1:37:B:PHE:HB3	1:63:B:MET:HE3	3	0.35
(3,438)	1:37:B:PHE:HB2	1:63:B:MET:HE1	8	0.35
(3,437)	1:37:A:PHE:HB3	1:63:A:MET:HE3	3	0.35
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	4	0.35
(3,330)	1:86:B:LEU:HD11	1:49:B:LEU:HG	3	0.35
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG23	4	0.35
(3,122)	1:84:B:ALA:HB1	1:80:A:ILE:HG12	8	0.35
(3,121)	1:84:A:ALA:HB1	1:80:B:ILE:HG12	8	0.35
(3,42)	1:58:B:VAL:HG23	1:57:B:LYS:HB2	8	0.35
(3,41)	1:58:A:VAL:HG23	1:57:A:LYS:HB2	8	0.35
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG22	2	0.35
(1,1760)	1:24:B:VAL:H	1:25:B:LYS:HG3	3	0.35
(1,1724)	1:81:B:MET:H	1:83:B:MET:HG2	7	0.35
(1,1723)	1:81:A:MET:H	1:83:A:MET:HG2	7	0.35
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD11	10	0.35
(1,1384)	1:18:B:THR:H	1:16:B:ILE:HG13	2	0.35
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD12	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD12	8	0.35
(1,1327)	1:12:A:ILE:H	1:45:B:LEU:HD22	3	0.35
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD13	8	0.35
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD11	9	0.35
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD13	8	0.35
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD11	9	0.35
(1,812)	1:24:B:VAL:HB	1:21:B:GLN:HG3	1	0.35
(1,811)	1:24:A:VAL:HB	1:21:A:GLN:HG3	1	0.35
(1,756)	1:111:B:GLU:HG3	1:108:B:GLY:HA2	2	0.35
(1,755)	1:111:A:GLU:HG3	1:108:A:GLY:HA2	2	0.35
(1,568)	1:42:B:ARG:HA	1:43:B:LYS:HE3	9	0.35
(1,550)	1:32:B:LEU:HA	1:32:B:LEU:HG	7	0.35
(1,549)	1:32:A:LEU:HA	1:32:A:LEU:HG	7	0.35
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD12	7	0.35
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD12	7	0.35
(1,480)	1:63:B:MET:HB2	1:62:B:ILE:HD13	6	0.35
(1,480)	1:63:B:MET:HB2	1:62:B:ILE:HD13	7	0.35
(1,479)	1:63:A:MET:HB2	1:62:A:ILE:HD13	6	0.35
(1,472)	1:79:B:PHE:HB3	1:81:B:MET:HG2	1	0.35
(1,471)	1:79:A:PHE:HB3	1:81:A:MET:HG2	1	0.35
(1,464)	1:79:B:PHE:HB3	1:81:B:MET:HG2	1	0.35
(1,463)	1:79:A:PHE:HB3	1:81:A:MET:HG2	1	0.35
(1,378)	1:34:B:GLN:HG3	1:63:B:MET:H	9	0.35
(1,377)	1:34:A:GLN:HG3	1:63:A:MET:H	9	0.35
(1,368)	1:34:B:GLN:HG2	1:38:B:LYS:HA	1	0.35
(1,368)	1:34:B:GLN:HG2	1:38:B:LYS:HA	10	0.35
(1,367)	1:34:A:GLN:HG2	1:38:A:LYS:HA	1	0.35
(1,367)	1:34:A:GLN:HG2	1:38:A:LYS:HA	10	0.35
(1,248)	1:63:B:MET:HB2	1:61:B:HIS:HB3	1	0.35
(1,247)	1:63:A:MET:HB2	1:61:A:HIS:HB3	1	0.35
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE3	4	0.35
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD13	6	0.35
(1,94)	1:34:B:GLN:HG3	1:63:B:MET:H	9	0.35
(1,93)	1:34:A:GLN:HG3	1:63:A:MET:H	9	0.35
(1,46)	1:39:B:GLU:HG2	1:44:B:ASP:H	6	0.35
(1,45)	1:39:A:GLU:HG2	1:44:A:ASP:H	6	0.35
(3,1448)	1:88:B:TRP:H	1:77:A:GLU:HG3	3	0.34
(3,1428)	1:86:B:LEU:H	1:86:B:LEU:HG	9	0.34
(3,1427)	1:86:A:LEU:H	1:86:A:LEU:HG	1	0.34
(3,1427)	1:86:A:LEU:H	1:86:A:LEU:HG	9	0.34
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD21	2	0.34
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG22	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE2	4	0.34
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE2	5	0.34
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE2	4	0.34
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE2	5	0.34
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD22	5	0.34
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD22	5	0.34
(3,980)	1:9:B:GLU:H	1:5:B:MET:HG3	10	0.34
(3,979)	1:9:A:GLU:H	1:5:A:MET:HG3	10	0.34
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB3	8	0.34
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB3	8	0.34
(3,882)	1:30:B:ASP:H	1:31:B:THR:HG21	3	0.34
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	8	0.34
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE1	10	0.34
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE1	10	0.34
(3,745)	1:24:A:VAL:HG11	1:25:A:LYS:HG3	2	0.34
(3,642)	1:8:B:LEU:HD23	1:15:A:ILE:HD12	6	0.34
(3,641)	1:8:A:LEU:HD23	1:15:B:ILE:HD12	6	0.34
(3,628)	1:48:B:PHE:HB2	1:9:A:GLU:HG3	1	0.34
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE3	5	0.34
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE3	5	0.34
(3,540)	1:15:B:ILE:HA	1:8:A:LEU:HD22	10	0.34
(3,526)	1:76:B:PHE:HB3	1:16:B:ILE:HA	1	0.34
(3,525)	1:76:A:PHE:HB3	1:16:A:ILE:HA	1	0.34
(3,485)	1:96:A:GLU:HG3	1:97:A:GLY:H	1	0.34
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	4	0.34
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG3	3	0.34
(3,330)	1:86:B:LEU:HD13	1:49:B:LEU:HG	10	0.34
(3,180)	1:49:B:LEU:HG	1:48:B:PHE:HB3	9	0.34
(3,179)	1:49:A:LEU:HG	1:48:A:PHE:HB3	9	0.34
(3,132)	1:78:B:GLU:HB2	1:31:B:THR:HA	7	0.34
(3,131)	1:78:A:GLU:HB2	1:31:A:THR:HA	7	0.34
(3,89)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	5	0.34
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE2	10	0.34
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE2	10	0.34
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG22	2	0.34
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	2	0.34
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	2	0.34
(1,1760)	1:24:B:VAL:H	1:25:B:LYS:HG3	9	0.34
(1,1759)	1:24:A:VAL:H	1:25:A:LYS:HG3	3	0.34
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD23	5	0.34
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD23	5	0.34
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD2	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD11	10	0.34
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	3	0.34
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	3	0.34
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	3	0.34
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	3	0.34
(1,1383)	1:18:A:THR:H	1:16:A:ILE:HG13	2	0.34
(1,1328)	1:12:B:ILE:H	1:45:A:LEU:HD22	3	0.34
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD13	6	0.34
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD13	6	0.34
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	5	0.34
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	5	0.34
(1,1228)	1:76:B:PHE:H	1:80:B:ILE:HB	2	0.34
(1,1227)	1:76:A:PHE:H	1:80:A:ILE:HB	2	0.34
(1,973)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	5	0.34
(1,862)	1:25:B:LYS:HD3	1:33:B:ASN:HB2	5	0.34
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	2	0.34
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	10	0.34
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	10	0.34
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	2	0.34
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	2	0.34
(1,567)	1:42:A:ARG:HA	1:43:A:LYS:HE3	9	0.34
(1,528)	1:49:B:LEU:HB3	1:50:B:LYS:HG2	2	0.34
(1,527)	1:49:A:LEU:HB3	1:50:A:LYS:HG2	2	0.34
(1,479)	1:63:A:MET:HB2	1:62:A:ILE:HD13	7	0.34
(1,371)	1:7:A:GLN:HG2	1:44:B:ASP:HB3	5	0.34
(1,268)	1:8:B:LEU:HG	1:15:A:ILE:HB	3	0.34
(1,268)	1:8:B:LEU:HG	1:15:A:ILE:HB	9	0.34
(1,267)	1:8:A:LEU:HG	1:15:B:ILE:HB	3	0.34
(1,267)	1:8:A:LEU:HG	1:15:B:ILE:HB	9	0.34
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD13	6	0.34
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD13	7	0.34
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD13	7	0.34
(1,72)	1:33:B:ASN:HB3	1:73:B:GLN:HG2	7	0.34
(1,71)	1:33:A:ASN:HB3	1:73:A:GLN:HG2	7	0.34
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	7	0.33
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	7	0.33
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB2	4	0.33
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB2	4	0.33
(3,1447)	1:88:A:TRP:H	1:77:B:GLU:HG3	3	0.33
(3,1442)	1:87:B:THR:H	1:16:A:ILE:HD11	10	0.33
(3,1441)	1:87:A:THR:H	1:16:B:ILE:HD11	10	0.33
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD21	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG21	7	0.33
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG21	7	0.33
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG22	10	0.33
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	8	0.33
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD12	2	0.33
(3,746)	1:24:B:VAL:HG11	1:25:B:LYS:HG3	2	0.33
(3,740)	1:59:B:ILE:HG23	1:58:B:VAL:HG12	9	0.33
(3,740)	1:59:B:ILE:HG21	1:58:B:VAL:HG13	10	0.33
(3,739)	1:59:A:ILE:HG23	1:58:A:VAL:HG13	1	0.33
(3,739)	1:59:A:ILE:HG23	1:58:A:VAL:HG12	9	0.33
(3,739)	1:59:A:ILE:HG21	1:58:A:VAL:HG13	10	0.33
(3,674)	1:73:B:GLN:H	1:63:B:MET:HE2	8	0.33
(3,673)	1:73:A:GLN:H	1:63:A:MET:HE2	8	0.33
(3,627)	1:48:A:PHE:HB2	1:9:B:GLU:HG3	1	0.33
(3,530)	1:67:B:ASP:HB3	1:64:B:GLU:HG3	1	0.33
(3,492)	1:59:B:ILE:HD12	1:52:B:GLU:HG3	5	0.33
(3,491)	1:59:A:ILE:HD12	1:52:A:GLU:HG3	5	0.33
(3,486)	1:96:B:GLU:HG3	1:97:B:GLY:H	1	0.33
(3,378)	1:25:B:LYS:HD2	1:32:B:LEU:HA	8	0.33
(3,377)	1:25:A:LYS:HD2	1:32:A:LEU:HA	8	0.33
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG3	3	0.33
(3,329)	1:86:A:LEU:HD13	1:49:A:LEU:HG	10	0.33
(3,252)	1:33:B:ASN:HB2	1:72:B:LYS:HA	1	0.33
(3,207)	1:44:A:ASP:HA	1:9:B:GLU:HG3	1	0.33
(3,132)	1:78:B:GLU:HB3	1:31:B:THR:HA	3	0.33
(3,131)	1:78:A:GLU:HB3	1:31:A:THR:HA	3	0.33
(3,90)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	5	0.33
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG22	6	0.33
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	7	0.33
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	7	0.33
(1,1760)	1:24:B:VAL:H	1:25:B:LYS:HG3	4	0.33
(1,1760)	1:24:B:VAL:H	1:25:B:LYS:HG3	5	0.33
(1,1759)	1:24:A:VAL:H	1:25:A:LYS:HG3	4	0.33
(1,1759)	1:24:A:VAL:H	1:25:A:LYS:HG3	5	0.33
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB1	10	0.33
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB1	10	0.33
(1,1636)	1:65:B:ASP:H	1:62:B:ILE:HG13	1	0.33
(1,1635)	1:65:A:ASP:H	1:62:A:ILE:HG13	1	0.33
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD2	3	0.33
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD13	9	0.33
(1,1556)	1:44:B:ASP:H	1:45:B:LEU:HG	5	0.33
(1,1555)	1:44:A:ASP:H	1:45:A:LEU:HG	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	4	0.33
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	5	0.33
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	9	0.33
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	4	0.33
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	5	0.33
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	4	0.33
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	5	0.33
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	9	0.33
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	4	0.33
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	5	0.33
(1,1401)	1:20:A:HIS:H	1:87:B:THR:HG23	3	0.33
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG22	6	0.33
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG22	6	0.33
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	1	0.33
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	1	0.33
(1,1318)	1:13:B:GLU:H	1:12:B:ILE:HG13	1	0.33
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD2	3	0.33
(1,1228)	1:76:B:PHE:H	1:80:B:ILE:HB	1	0.33
(1,1228)	1:76:B:PHE:H	1:80:B:ILE:HB	4	0.33
(1,1227)	1:76:A:PHE:H	1:80:A:ILE:HB	1	0.33
(1,1227)	1:76:A:PHE:H	1:80:A:ILE:HB	4	0.33
(1,1175)	1:107:A:PRO:HG3	1:105:A:HIS:H	9	0.33
(1,1040)	1:85:B:ARG:HA	1:89:B:ALA:HB1	5	0.33
(1,1039)	1:85:A:ARG:HA	1:89:A:ALA:HB1	5	0.33
(1,974)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	5	0.33
(1,861)	1:25:A:LYS:HD3	1:33:A:ASN:HB2	5	0.33
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	2	0.33
(1,652)	1:93:B:LYS:H	1:92:B:GLU:HB3	3	0.33
(1,651)	1:93:A:LYS:H	1:92:A:GLU:HB3	3	0.33
(1,588)	1:85:B:ARG:HG3	1:87:B:THR:HB	8	0.33
(1,587)	1:85:A:ARG:HG3	1:87:A:THR:HB	8	0.33
(1,540)	1:54:B:LYS:HG3	1:50:B:LYS:HE2	7	0.33
(1,539)	1:54:A:LYS:HG3	1:50:A:LYS:HE2	7	0.33
(1,507)	1:11:A:ASN:HB3	1:15:B:ILE:HG12	8	0.33
(1,396)	1:33:B:ASN:HB3	1:34:B:GLN:HG2	8	0.33
(1,395)	1:33:A:ASN:HB3	1:34:A:GLN:HG2	8	0.33
(1,372)	1:7:B:GLN:HG2	1:44:A:ASP:HB3	5	0.33
(1,298)	1:9:B:GLU:HB2	1:8:B:LEU:HD23	3	0.33
(1,297)	1:9:A:GLU:HB2	1:8:A:LEU:HD23	3	0.33
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE3	4	0.33
(1,224)	1:62:B:ILE:HG23	1:66:B:LEU:HG	3	0.33
(1,223)	1:62:A:ILE:HG23	1:66:A:LEU:HG	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	7	0.33
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	7	0.33
(3,1354)	1:69:B:ASN:H	1:68:B:THR:HG23	5	0.32
(3,1353)	1:69:A:ASN:H	1:68:A:THR:HG23	5	0.32
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG11	1	0.32
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG11	1	0.32
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	8	0.32
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	8	0.32
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD22	10	0.32
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD22	10	0.32
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD12	2	0.32
(3,772)	1:14:B:THR:HG23	1:17:B:ASN:HB3	6	0.32
(3,771)	1:14:A:THR:HG23	1:17:A:ASN:HB3	6	0.32
(3,740)	1:59:B:ILE:HG23	1:58:B:VAL:HG13	1	0.32
(3,672)	1:34:B:GLN:H	1:63:B:MET:HE3	1	0.32
(3,641)	1:8:A:LEU:HD22	1:15:B:ILE:HD12	10	0.32
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE3	2	0.32
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE1	3	0.32
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE2	8	0.32
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE3	2	0.32
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE2	8	0.32
(3,486)	1:96:B:GLU:HG2	1:97:B:GLY:H	3	0.32
(3,437)	1:37:A:PHE:HB2	1:63:A:MET:HE3	2	0.32
(3,251)	1:33:A:ASN:HB2	1:72:A:LYS:HA	1	0.32
(3,42)	1:58:B:VAL:HG23	1:57:B:LYS:HB2	3	0.32
(3,42)	1:58:B:VAL:HG21	1:57:B:LYS:HB2	6	0.32
(3,41)	1:58:A:VAL:HG23	1:57:A:LYS:HB2	3	0.32
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE3	7	0.32
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE3	7	0.32
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG22	6	0.32
(1,1759)	1:24:A:VAL:H	1:25:A:LYS:HG3	9	0.32
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	9	0.32
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	9	0.32
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG12	9	0.32
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD13	9	0.32
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	8	0.32
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	9	0.32
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	8	0.32
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	9	0.32
(1,1401)	1:20:A:HIS:H	1:87:B:THR:HG22	2	0.32
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG22	7	0.32
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD12	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD12	9	0.32
(1,1317)	1:13:A:GLU:H	1:12:A:ILE:HG13	1	0.32
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD2	3	0.32
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	4	0.32
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	4	0.32
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD11	10	0.32
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD11	10	0.32
(1,1200)	1:60:B:GLU:HB2	1:59:B:ILE:HG22	10	0.32
(1,1199)	1:60:A:GLU:HB2	1:59:A:ILE:HG22	10	0.32
(1,1182)	1:81:B:MET:HB3	1:80:A:ILE:HG12	6	0.32
(1,1180)	1:81:B:MET:HB3	1:80:A:ILE:HG12	6	0.32
(1,1178)	1:81:B:MET:HB3	1:80:A:ILE:HG12	6	0.32
(1,1176)	1:107:B:PRO:HG3	1:105:B:HIS:H	9	0.32
(1,1156)	1:32:B:LEU:HG	1:76:B:PHE:HA	8	0.32
(1,1155)	1:32:A:LEU:HG	1:76:A:PHE:HA	8	0.32
(1,994)	1:109:B:LEU:HD11	1:47:B:ASN:HB2	2	0.32
(1,993)	1:109:A:LEU:HD11	1:47:A:ASN:HB2	2	0.32
(1,962)	1:21:B:GLN:HB3	1:22:B:TYR:HB2	7	0.32
(1,961)	1:21:A:GLN:HB3	1:22:A:TYR:HB2	7	0.32
(1,896)	1:81:B:MET:HB3	1:80:A:ILE:HG12	6	0.32
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	4	0.32
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	4	0.32
(1,508)	1:11:B:ASN:HB3	1:15:A:ILE:HG12	8	0.32
(1,395)	1:33:A:ASN:HB3	1:34:A:GLN:HG2	6	0.32
(1,348)	1:5:B:MET:HG2	1:4:B:LYS:HE3	5	0.32
(1,347)	1:5:A:MET:HG2	1:4:A:LYS:HE3	5	0.32
(1,294)	1:81:B:MET:HB3	1:80:A:ILE:HG12	6	0.32
(1,280)	1:19:B:PHE:HB3	1:32:B:LEU:HB2	9	0.32
(1,248)	1:63:B:MET:HB3	1:61:B:HIS:HB3	6	0.32
(1,247)	1:63:A:MET:HB3	1:61:A:HIS:HB3	6	0.32
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG21	7	0.32
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG21	7	0.32
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	6	0.31
(4,11)	1:98:A:ASP:HA	1:96:A:GLU:HA	6	0.31
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB2	6	0.31
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB2	6	0.31
(3,1442)	1:87:B:THR:H	1:16:A:ILE:HD13	1	0.31
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD22	6	0.31
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD22	6	0.31
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG13	6	0.31
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG13	6	0.31
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD11	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	3	0.31
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	3	0.31
(3,881)	1:30:A:ASP:H	1:31:A:THR:HG23	8	0.31
(3,876)	1:30:B:ASP:H	1:29:B:PRO:HG2	5	0.31
(3,875)	1:30:A:ASP:H	1:29:A:PRO:HG2	5	0.31
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	5	0.31
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	5	0.31
(3,725)	1:38:A:LYS:HA	1:42:A:ARG:HD2	1	0.31
(3,671)	1:34:A:GLN:H	1:63:A:MET:HE3	1	0.31
(3,670)	1:74:B:LEU:H	1:63:B:MET:HE2	1	0.31
(3,669)	1:74:A:LEU:H	1:63:A:MET:HE2	1	0.31
(3,664)	1:63:B:MET:HE2	1:72:B:LYS:HA	1	0.31
(3,642)	1:8:B:LEU:HD22	1:15:A:ILE:HD12	10	0.31
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE1	3	0.31
(3,546)	1:33:B:ASN:HA	1:31:B:THR:HG21	6	0.31
(3,545)	1:33:A:ASN:HA	1:31:A:THR:HG21	6	0.31
(3,529)	1:67:A:ASP:HB3	1:64:A:GLU:HG3	1	0.31
(3,504)	1:111:B:GLU:HA	1:107:B:PRO:HB2	2	0.31
(3,503)	1:111:A:GLU:HA	1:107:A:PRO:HB2	2	0.31
(3,485)	1:96:A:GLU:HG2	1:97:A:GLY:H	3	0.31
(3,438)	1:37:B:PHE:HB2	1:63:B:MET:HE3	2	0.31
(3,252)	1:33:B:ASN:HB3	1:72:B:LYS:HA	2	0.31
(3,251)	1:33:A:ASN:HB3	1:72:A:LYS:HA	2	0.31
(3,41)	1:58:A:VAL:HG21	1:57:A:LYS:HB2	6	0.31
(3,6)	1:73:B:GLN:HG3	1:72:B:LYS:HG3	6	0.31
(3,5)	1:73:A:GLN:HG3	1:72:A:LYS:HG3	6	0.31
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE2	4	0.31
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE2	4	0.31
(1,1815)	1:110:A:GLY:H	1:48:A:PHE:HA	9	0.31
(1,1682)	1:68:B:THR:H	1:68:B:THR:HG22	6	0.31
(1,1681)	1:68:A:THR:H	1:68:A:THR:HG22	6	0.31
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG13	4	0.31
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG12	8	0.31
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG13	4	0.31
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG12	8	0.31
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG12	9	0.31
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB1	9	0.31
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD11	2	0.31
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD11	2	0.31
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	8	0.31
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	8	0.31
(1,1402)	1:20:B:HIS:H	1:87:A:THR:HG22	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1402)	1:20:B:HIS:H	1:87:A:THR:HG23	3	0.31
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG22	7	0.31
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	9	0.31
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	6	0.31
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	9	0.31
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	6	0.31
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	6	0.31
(1,1318)	1:11:B:ASN:H	1:12:B:ILE:HG13	10	0.31
(1,1317)	1:11:A:ASN:H	1:12:A:ILE:HG13	10	0.31
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	10	0.31
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	10	0.31
(1,1200)	1:60:B:GLU:HB2	1:59:B:ILE:HG21	7	0.31
(1,1199)	1:60:A:GLU:HB2	1:59:A:ILE:HG21	7	0.31
(1,1181)	1:81:A:MET:HB3	1:80:B:ILE:HG12	6	0.31
(1,1179)	1:81:A:MET:HB3	1:80:B:ILE:HG12	6	0.31
(1,1177)	1:81:A:MET:HB3	1:80:B:ILE:HG12	6	0.31
(1,1082)	1:79:B:PHE:HA	1:83:B:MET:HA	8	0.31
(1,1081)	1:79:A:PHE:HA	1:83:A:MET:HA	8	0.31
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG3	7	0.31
(1,895)	1:81:A:MET:HB3	1:80:B:ILE:HG12	6	0.31
(1,754)	1:111:B:GLU:HG3	1:4:A:LYS:HE3	8	0.31
(1,753)	1:111:A:GLU:HG3	1:4:B:LYS:HE3	8	0.31
(1,528)	1:49:B:LEU:HB2	1:50:B:LYS:HG2	3	0.31
(1,527)	1:49:A:LEU:HB2	1:50:A:LYS:HG2	3	0.31
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD13	5	0.31
(1,396)	1:33:B:ASN:HB3	1:34:B:GLN:HG2	6	0.31
(1,317)	1:82:A:LEU:HB3	1:80:A:ILE:HD13	9	0.31
(1,293)	1:81:A:MET:HB3	1:80:B:ILE:HG12	6	0.31
(1,286)	1:51:B:LYS:H	1:50:B:LYS:HG3	7	0.31
(1,285)	1:51:A:LYS:H	1:50:A:LYS:HG3	7	0.31
(1,279)	1:19:A:PHE:HB3	1:32:A:LEU:HB2	9	0.31
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE2	6	0.31
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE2	6	0.31
(1,49)	1:64:A:GLU:HG3	1:71:A:ASP:HA	1	0.31
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	2	0.3
(3,1457)	1:89:A:ALA:H	1:16:B:ILE:HD12	10	0.3
(3,1442)	1:87:B:THR:H	1:16:A:ILE:HD12	9	0.3
(3,1441)	1:87:A:THR:H	1:16:B:ILE:HD12	9	0.3
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE3	8	0.3
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE3	8	0.3
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD22	5	0.3
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD22	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD11	3	0.3
(3,980)	1:9:B:GLU:H	1:5:B:MET:HG2	6	0.3
(3,882)	1:30:B:ASP:H	1:31:B:THR:HG23	8	0.3
(3,872)	1:6:B:SER:H	1:5:B:MET:HG2	6	0.3
(3,871)	1:6:A:SER:H	1:5:A:MET:HG2	6	0.3
(3,793)	1:107:A:PRO:HG2	1:93:A:LYS:HG3	10	0.3
(3,726)	1:38:B:LYS:HA	1:42:B:ARG:HD2	1	0.3
(3,672)	1:34:B:GLN:H	1:63:B:MET:HE3	4	0.3
(3,671)	1:34:A:GLN:H	1:63:A:MET:HE3	4	0.3
(3,663)	1:63:A:MET:HE2	1:72:A:LYS:HA	1	0.3
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE1	1	0.3
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE1	1	0.3
(3,566)	1:111:B:GLU:HB2	1:108:B:GLY:HA3	9	0.3
(3,565)	1:111:A:GLU:HB2	1:108:A:GLY:HA3	9	0.3
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB2	9	0.3
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB2	9	0.3
(3,251)	1:33:A:ASN:HB3	1:72:A:LYS:HA	6	0.3
(3,226)	1:66:B:LEU:HD13	1:82:B:LEU:HA	9	0.3
(3,225)	1:66:A:LEU:HD13	1:82:A:LEU:HA	9	0.3
(3,200)	1:46:B:GLN:HB3	1:43:B:LYS:HA	1	0.3
(3,199)	1:46:A:GLN:HB3	1:43:A:LYS:HA	1	0.3
(3,188)	1:51:B:LYS:H	1:50:B:LYS:HG3	7	0.3
(3,187)	1:51:A:LYS:H	1:50:A:LYS:HG3	7	0.3
(3,115)	1:75:A:SER:HB3	1:67:A:ASP:HA	1	0.3
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE3	1	0.3
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE3	1	0.3
(1,1816)	1:110:B:GLY:H	1:48:B:PHE:HA	9	0.3
(1,1792)	1:16:B:ILE:H	1:12:B:ILE:HG22	3	0.3
(1,1792)	1:16:B:ILE:H	1:12:B:ILE:HG22	7	0.3
(1,1791)	1:16:A:ILE:H	1:12:A:ILE:HG22	7	0.3
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	1	0.3
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	10	0.3
(1,1652)	1:62:B:ILE:H	1:62:B:ILE:HD11	4	0.3
(1,1651)	1:62:A:ILE:H	1:62:A:ILE:HD11	4	0.3
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB1	9	0.3
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD12	5	0.3
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD11	6	0.3
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD12	5	0.3
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD11	6	0.3
(1,1558)	1:46:B:GLN:H	1:49:B:LEU:HD12	7	0.3
(1,1557)	1:46:A:GLN:H	1:49:A:LEU:HD12	7	0.3
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG22	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG22	7	0.3
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG22	7	0.3
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	6	0.3
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	3	0.3
(1,1328)	1:12:B:ILE:H	1:45:A:LEU:HD23	6	0.3
(1,1328)	1:12:B:ILE:H	1:86:A:LEU:HD22	9	0.3
(1,1327)	1:12:A:ILE:H	1:45:B:LEU:HD23	6	0.3
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	2	0.3
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	2	0.3
(1,1200)	1:60:B:GLU:HB2	1:59:B:ILE:HG21	6	0.3
(1,1199)	1:60:A:GLU:HB2	1:59:A:ILE:HG21	6	0.3
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG23	4	0.3
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG23	4	0.3
(1,1127)	1:16:A:ILE:HG13	1:17:A:ASN:HB2	8	0.3
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD13	5	0.3
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD13	5	0.3
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	3	0.3
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	6	0.3
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	8	0.3
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	3	0.3
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	6	0.3
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	8	0.3
(1,921)	1:87:A:THR:HA	1:13:B:GLU:HG3	7	0.3
(1,813)	1:21:A:GLN:HG2	1:8:B:LEU:HD12	7	0.3
(1,735)	1:5:A:MET:HA	1:10:A:ARG:HA	9	0.3
(1,720)	1:77:B:GLU:HB3	1:68:B:THR:HG23	1	0.3
(1,719)	1:77:A:GLU:HB3	1:68:A:THR:HG23	1	0.3
(1,697)	1:107:A:PRO:HG2	1:93:A:LYS:HG3	10	0.3
(1,626)	1:99:B:GLU:H	1:99:B:GLU:HG3	5	0.3
(1,625)	1:99:A:GLU:H	1:99:A:GLU:HG3	5	0.3
(1,580)	1:34:B:GLN:HG3	1:38:B:LYS:HD3	3	0.3
(1,579)	1:34:A:GLN:HG3	1:38:A:LYS:HD3	3	0.3
(1,546)	1:68:B:THR:H	1:78:B:GLU:HB3	9	0.3
(1,545)	1:107:A:PRO:HB3	1:108:A:GLY:H	9	0.3
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	1	0.3
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	1	0.3
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD11	1	0.3
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD11	1	0.3
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD13	5	0.3
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	1	0.3
(1,318)	1:82:B:LEU:HB3	1:80:B:ILE:HD13	9	0.3
(1,297)	1:58:A:VAL:HG23	1:56:A:GLU:HB3	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:62:B:ILE:HG21	1:63:B:MET:HA	3	0.3
(1,213)	1:62:A:ILE:HG21	1:63:A:MET:HA	3	0.3
(1,50)	1:64:B:GLU:HG3	1:71:B:ASP:HA	1	0.3
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	8	0.29
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	8	0.29
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	2	0.29
(3,1458)	1:89:B:ALA:H	1:16:A:ILE:HD12	10	0.29
(3,1447)	1:88:A:TRP:H	1:77:B:GLU:HG2	5	0.29
(3,1441)	1:87:A:THR:H	1:16:B:ILE:HD13	1	0.29
(3,1428)	1:86:B:LEU:H	1:86:B:LEU:HG	3	0.29
(3,1427)	1:86:A:LEU:H	1:86:A:LEU:HG	3	0.29
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	6	0.29
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	6	0.29
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD12	5	0.29
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD12	5	0.29
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD21	1	0.29
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD23	9	0.29
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD21	1	0.29
(3,1088)	1:23:B:SER:H	1:40:B:LEU:HD22	8	0.29
(3,1087)	1:23:A:SER:H	1:40:A:LEU:HD22	8	0.29
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG12	5	0.29
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG12	5	0.29
(3,979)	1:9:A:GLU:H	1:5:A:MET:HG2	6	0.29
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	1	0.29
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	2	0.29
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	4	0.29
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	1	0.29
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	2	0.29
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	4	0.29
(3,866)	1:52:B:GLU:H	1:51:B:LYS:HG3	3	0.29
(3,865)	1:52:A:GLU:H	1:51:A:LYS:HG3	3	0.29
(3,794)	1:107:B:PRO:HG2	1:93:B:LYS:HG3	10	0.29
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE3	5	0.29
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE3	5	0.29
(3,691)	1:32:A:LEU:HA	1:36:A:GLU:HB2	3	0.29
(3,674)	1:73:B:GLN:H	1:63:B:MET:HE1	9	0.29
(3,673)	1:73:A:GLN:H	1:63:A:MET:HE1	6	0.29
(3,673)	1:73:A:GLN:H	1:63:A:MET:HE1	9	0.29
(3,600)	1:53:B:ASN:HB2	1:46:B:GLN:HG3	5	0.29
(3,600)	1:53:B:ASN:HB2	1:46:B:GLN:HG3	8	0.29
(3,599)	1:53:A:ASN:HB2	1:46:A:GLN:HG3	5	0.29
(3,599)	1:53:A:ASN:HB2	1:46:A:GLN:HG3	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,252)	1:33:B:ASN:HB3	1:72:B:LYS:HA	6	0.29
(1,1852)	1:5:B:MET:H	1:5:B:MET:HG3	7	0.29
(1,1851)	1:5:A:MET:H	1:5:A:MET:HG3	7	0.29
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG22	3	0.29
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG22	7	0.29
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG22	3	0.29
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG22	7	0.29
(1,1791)	1:16:A:ILE:H	1:12:A:ILE:HG22	3	0.29
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	10	0.29
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	1	0.29
(1,1710)	1:79:B:PHE:H	1:74:B:LEU:HD11	2	0.29
(1,1708)	1:79:B:PHE:H	1:80:B:ILE:HG12	7	0.29
(1,1707)	1:79:A:PHE:H	1:80:A:ILE:HG12	7	0.29
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	6	0.29
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	6	0.29
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG13	5	0.29
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG13	5	0.29
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD21	6	0.29
(1,1544)	1:43:B:LYS:H	1:42:B:ARG:HG2	9	0.29
(1,1543)	1:43:A:LYS:H	1:42:A:ARG:HG2	9	0.29
(1,1402)	1:20:B:HIS:H	1:24:B:VAL:HG12	5	0.29
(1,1401)	1:20:A:HIS:H	1:24:A:VAL:HG12	5	0.29
(1,1370)	1:17:B:ASN:H	1:15:B:ILE:HG13	4	0.29
(1,1369)	1:17:A:ASN:H	1:15:A:ILE:HG13	4	0.29
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG22	3	0.29
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	2	0.29
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	2	0.29
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	3	0.29
(1,1327)	1:12:A:ILE:H	1:86:B:LEU:HD22	9	0.29
(1,1317)	1:13:A:GLU:H	1:12:A:ILE:HG13	3	0.29
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD2	5	0.29
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD2	5	0.29
(1,1266)	1:77:B:GLU:H	1:84:A:ALA:HB3	5	0.29
(1,1265)	1:77:A:GLU:H	1:84:B:ALA:HB3	5	0.29
(1,1128)	1:16:B:ILE:HG13	1:17:B:ASN:HB2	8	0.29
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	4	0.29
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	4	0.29
(1,1048)	1:53:B:ASN:HA	1:59:B:ILE:HA	10	0.29
(1,1047)	1:53:A:ASN:HA	1:59:A:ILE:HA	10	0.29
(1,1046)	1:85:B:ARG:HA	1:77:A:GLU:HA	3	0.29
(1,1045)	1:85:A:ARG:HA	1:77:B:GLU:HA	3	0.29
(1,742)	1:81:B:MET:HA	1:84:B:ALA:HB3	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:81:A:MET:HA	1:84:A:ALA:HB3	3	0.29
(1,736)	1:5:B:MET:HA	1:10:B:ARG:HA	9	0.29
(1,698)	1:107:B:PRO:HG2	1:93:B:LYS:HG3	10	0.29
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG21	2	0.29
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG23	3	0.29
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG21	2	0.29
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG23	3	0.29
(1,646)	1:86:B:LEU:HA	1:49:B:LEU:HA	10	0.29
(1,645)	1:86:A:LEU:HA	1:49:A:LEU:HA	10	0.29
(1,545)	1:107:A:PRO:HB3	1:108:A:GLY:H	6	0.29
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	2	0.29
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	3	0.29
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	2	0.29
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	1	0.29
(1,336)	1:41:B:VAL:HG13	1:48:B:PHE:H	3	0.29
(1,217)	1:12:A:ILE:HG23	1:48:B:PHE:HB2	4	0.29
(1,136)	1:16:B:ILE:H	1:16:B:ILE:HD12	4	0.29
(1,135)	1:16:A:ILE:H	1:16:A:ILE:HD12	4	0.29
(1,66)	1:74:B:LEU:HG	1:62:B:ILE:HG23	9	0.29
(1,65)	1:74:A:LEU:HG	1:62:A:ILE:HG23	9	0.29
(1,28)	1:87:B:THR:HG23	1:85:B:ARG:HA	5	0.29
(1,27)	1:87:A:THR:HG23	1:85:A:ARG:HA	5	0.29
(3,1466)	1:110:B:GLY:H	1:108:B:GLY:HA2	4	0.28
(3,1465)	1:110:A:GLY:H	1:108:A:GLY:HA2	4	0.28
(3,1448)	1:88:B:TRP:H	1:77:A:GLU:HG2	5	0.28
(3,1400)	1:90:B:SER:H	1:109:B:LEU:HD12	6	0.28
(3,1399)	1:90:A:SER:H	1:109:A:LEU:HD12	6	0.28
(3,1366)	1:69:B:ASN:H	1:73:B:GLN:HB2	1	0.28
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD21	1	0.28
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD21	1	0.28
(3,1122)	1:26:B:LEU:H	1:32:B:LEU:HD22	4	0.28
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD22	4	0.28
(3,1121)	1:26:A:LEU:H	1:32:A:LEU:HD23	9	0.28
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG12	4	0.28
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG12	4	0.28
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG12	8	0.28
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD12	10	0.28
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	5	0.28
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	5	0.28
(3,692)	1:32:B:LEU:HA	1:36:B:GLU:HB2	3	0.28
(3,674)	1:73:B:GLN:H	1:63:B:MET:HE1	6	0.28
(3,664)	1:63:B:MET:HE1	1:72:B:LYS:HA	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,663)	1:63:A:MET:HE1	1:72:A:LYS:HA	7	0.28
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	9	0.28
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	9	0.28
(3,584)	1:66:B:LEU:HD21	1:67:B:ASP:HA	7	0.28
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE3	7	0.28
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE3	7	0.28
(3,552)	1:25:B:LYS:HD2	1:24:B:VAL:HG12	8	0.28
(3,437)	1:37:A:PHE:HB2	1:63:A:MET:HE3	1	0.28
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB3	3	0.28
(3,320)	1:51:B:LYS:HE2	1:51:B:LYS:H	1	0.28
(3,319)	1:51:A:LYS:HE2	1:51:A:LYS:H	1	0.28
(3,131)	1:78:A:GLU:HB2	1:31:A:THR:HA	4	0.28
(3,116)	1:75:B:SER:HB3	1:67:B:ASP:HA	1	0.28
(3,54)	1:39:B:GLU:HG3	1:43:B:LYS:HD2	1	0.28
(3,53)	1:39:A:GLU:HG3	1:43:A:LYS:HD2	1	0.28
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	2	0.28
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	7	0.28
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	2	0.28
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	7	0.28
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE2	5	0.28
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG21	10	0.28
(1,1792)	1:16:B:ILE:H	1:12:B:ILE:HG21	10	0.28
(1,1791)	1:16:A:ILE:H	1:12:A:ILE:HG21	10	0.28
(1,1784)	1:89:B:ALA:H	1:84:B:ALA:HA	3	0.28
(1,1783)	1:89:A:ALA:H	1:84:A:ALA:HA	3	0.28
(1,1709)	1:79:A:PHE:H	1:74:A:LEU:HD11	2	0.28
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG12	2	0.28
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG12	2	0.28
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD3	7	0.28
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD3	7	0.28
(1,1592)	1:10:B:ARG:H	1:14:B:THR:H	4	0.28
(1,1591)	1:10:A:ARG:H	1:14:A:THR:H	4	0.28
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD21	6	0.28
(1,1496)	1:38:B:LYS:H	1:38:B:LYS:HD2	4	0.28
(1,1495)	1:38:A:LYS:H	1:38:A:LYS:HD2	4	0.28
(1,1414)	1:61:B:HIS:H	1:64:B:GLU:HB3	9	0.28
(1,1413)	1:61:A:HIS:H	1:64:A:GLU:HB3	9	0.28
(1,1378)	1:18:B:THR:H	1:20:B:HIS:H	9	0.28
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG21	10	0.28
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG21	10	0.28
(1,1346)	1:15:B:ILE:H	1:15:B:ILE:HD12	5	0.28
(1,1345)	1:15:A:ILE:H	1:15:A:ILE:HD12	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	10	0.28
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	10	0.28
(1,1318)	1:13:B:GLU:H	1:12:B:ILE:HG13	3	0.28
(1,1292)	1:5:B:MET:H	1:5:B:MET:HG3	7	0.28
(1,1291)	1:5:A:MET:H	1:5:A:MET:HG3	7	0.28
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	7	0.28
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG22	5	0.28
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG22	5	0.28
(1,1136)	1:5:B:MET:HG3	1:4:B:LYS:HE2	9	0.28
(1,1135)	1:5:A:MET:HG3	1:4:A:LYS:HE2	9	0.28
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	2	0.28
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	2	0.28
(1,936)	1:46:B:GLN:HG2	1:45:B:LEU:HD21	9	0.28
(1,935)	1:46:A:GLN:HG2	1:45:A:LEU:HD21	9	0.28
(1,756)	1:111:B:GLU:HG2	1:108:B:GLY:HA3	1	0.28
(1,755)	1:111:A:GLU:HG2	1:108:A:GLY:HA3	1	0.28
(1,634)	1:89:B:ALA:H	1:84:B:ALA:HA	3	0.28
(1,633)	1:89:A:ALA:H	1:84:A:ALA:HA	3	0.28
(1,546)	1:107:B:PRO:HB3	1:108:B:GLY:H	6	0.28
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	7	0.28
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	3	0.28
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	7	0.28
(1,348)	1:5:B:MET:HG3	1:4:B:LYS:HE2	9	0.28
(1,347)	1:5:A:MET:HG3	1:4:A:LYS:HE2	9	0.28
(1,336)	1:41:B:VAL:HG12	1:48:B:PHE:H	2	0.28
(1,335)	1:41:A:VAL:HG13	1:48:A:PHE:H	3	0.28
(1,328)	1:66:B:LEU:HD21	1:67:B:ASP:HA	7	0.28
(1,298)	1:58:B:VAL:HG23	1:56:B:GLU:HB3	8	0.28
(1,189)	1:77:A:GLU:HA	1:87:B:THR:HG22	4	0.28
(1,166)	1:41:B:VAL:HB	1:37:B:PHE:HB3	3	0.28
(1,165)	1:41:A:VAL:HB	1:37:A:PHE:HB3	3	0.28
(1,118)	1:66:B:LEU:HG	1:62:B:ILE:HD12	5	0.28
(1,117)	1:66:A:LEU:HG	1:62:A:ILE:HD12	5	0.28
(1,82)	1:46:B:GLN:HG3	1:5:A:MET:H	6	0.28
(4,260)	1:113:B:THR:H	1:107:B:PRO:HA	7	0.27
(4,259)	1:113:A:THR:H	1:107:A:PRO:HA	7	0.27
(3,1382)	1:71:B:ASP:H	1:72:B:LYS:HE2	4	0.27
(3,1381)	1:71:A:ASP:H	1:72:A:LYS:HE2	4	0.27
(3,1365)	1:69:A:ASN:H	1:73:A:GLN:HB2	1	0.27
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	7	0.27
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	7	0.27
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG13	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG11	2	0.27
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG12	8	0.27
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG11	10	0.27
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD12	10	0.27
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	2	0.27
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	2	0.27
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	9	0.27
(3,802)	1:29:B:PRO:HD2	1:30:B:ASP:HB2	10	0.27
(3,801)	1:29:A:PRO:HD2	1:30:A:ASP:HB2	10	0.27
(3,726)	1:38:B:LYS:HA	1:42:B:ARG:HD2	5	0.27
(3,692)	1:32:B:LEU:HA	1:36:B:GLU:HB2	7	0.27
(3,691)	1:32:A:LEU:HA	1:36:A:GLU:HB2	7	0.27
(3,583)	1:66:A:LEU:HD21	1:67:A:ASP:HA	7	0.27
(3,551)	1:25:A:LYS:HD2	1:24:A:VAL:HG12	8	0.27
(3,438)	1:37:B:PHE:HB2	1:63:B:MET:HE3	1	0.27
(3,438)	1:37:B:PHE:HB2	1:63:B:MET:HE2	6	0.27
(3,437)	1:37:A:PHE:HB2	1:63:A:MET:HE2	6	0.27
(3,378)	1:25:B:LYS:HD2	1:32:B:LEU:HA	9	0.27
(3,378)	1:25:B:LYS:HD2	1:32:B:LEU:HA	10	0.27
(3,377)	1:25:A:LYS:HD2	1:32:A:LEU:HA	10	0.27
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	1	0.27
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB3	3	0.27
(3,245)	1:7:A:GLN:HG2	1:18:B:THR:HB	5	0.27
(3,206)	1:44:B:ASP:HA	1:6:A:SER:HB3	2	0.27
(3,132)	1:78:B:GLU:HB2	1:31:B:THR:HA	4	0.27
(3,33)	1:87:A:THR:HG23	1:88:A:TRP:HA	8	0.27
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	9	0.27
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	10	0.27
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	9	0.27
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	10	0.27
(1,1858)	1:108:B:GLY:H	1:111:B:GLU:HA	4	0.27
(1,1857)	1:108:A:GLY:H	1:111:A:GLU:HA	4	0.27
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE2	5	0.27
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG21	10	0.27
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG23	5	0.27
(1,1815)	1:110:A:GLY:H	1:48:A:PHE:HA	3	0.27
(1,1804)	1:109:B:LEU:H	1:113:B:THR:H	2	0.27
(1,1776)	1:87:B:THR:H	1:83:B:MET:HE1	5	0.27
(1,1775)	1:87:A:THR:H	1:83:A:MET:HE1	5	0.27
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	3	0.27
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	3	0.27
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG13	3	0.27
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG13	3	0.27
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD13	8	0.27
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD13	8	0.27
(1,1592)	1:10:B:ARG:H	1:14:B:THR:H	9	0.27
(1,1591)	1:10:A:ARG:H	1:14:A:THR:H	9	0.27
(1,1377)	1:18:A:THR:H	1:20:A:HIS:H	9	0.27
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG23	5	0.27
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG23	5	0.27
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	7	0.27
(1,1200)	1:60:B:GLU:HB2	1:59:B:ILE:HG22	5	0.27
(1,1199)	1:60:A:GLU:HB2	1:59:A:ILE:HG22	5	0.27
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	1	0.27
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	10	0.27
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	1	0.27
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	10	0.27
(1,814)	1:21:B:GLN:HG2	1:8:A:LEU:HD12	7	0.27
(1,810)	1:68:B:THR:H	1:74:B:LEU:HG	8	0.27
(1,809)	1:68:A:THR:H	1:74:A:LEU:HG	8	0.27
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	1	0.27
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	1	0.27
(1,672)	1:8:B:LEU:HG	1:15:A:ILE:H	5	0.27
(1,568)	1:42:B:ARG:HA	1:54:B:LYS:HE3	10	0.27
(1,567)	1:42:A:ARG:HA	1:54:A:LYS:HE3	10	0.27
(1,414)	1:63:B:MET:HB2	1:59:B:ILE:HG21	6	0.27
(1,413)	1:63:A:MET:HB2	1:59:A:ILE:HG21	6	0.27
(1,335)	1:41:A:VAL:HG12	1:48:A:PHE:H	2	0.27
(1,327)	1:66:A:LEU:HD21	1:67:A:ASP:HA	7	0.27
(1,261)	1:8:A:LEU:HG	1:40:B:LEU:HG	3	0.27
(1,226)	1:12:B:ILE:HG21	1:80:B:ILE:HB	7	0.27
(1,225)	1:12:A:ILE:HG21	1:80:A:ILE:HB	7	0.27
(1,218)	1:12:B:ILE:HG23	1:48:A:PHE:HB2	4	0.27
(1,190)	1:77:B:GLU:HA	1:87:A:THR:HG22	4	0.27
(1,166)	1:41:B:VAL:HB	1:37:B:PHE:HB3	1	0.27
(1,165)	1:41:A:VAL:HB	1:37:A:PHE:HB3	1	0.27
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	10	0.27
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	10	0.27
(1,124)	1:45:B:LEU:HG	1:9:A:GLU:HA	5	0.27
(1,95)	1:7:A:GLN:HG2	1:18:B:THR:HB	5	0.27
(1,74)	1:48:B:PHE:HB3	1:86:B:LEU:HG	4	0.27
(1,73)	1:48:A:PHE:HB3	1:86:A:LEU:HG	4	0.27
(1,1)	1:101:A:PRO:HB2	1:104:A:HIS:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	4	0.26
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	4	0.26
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	9	0.26
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	9	0.26
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD22	1	0.26
(3,1481)	1:102:A:GLY:H	1:104:A:HIS:HB2	5	0.26
(3,1474)	1:100:B:GLY:H	1:98:B:ASP:HA	7	0.26
(3,1473)	1:100:A:GLY:H	1:98:A:ASP:HA	7	0.26
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD23	2	0.26
(3,1088)	1:23:B:SER:H	1:40:B:LEU:HD21	9	0.26
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG12	3	0.26
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG13	1	0.26
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG11	2	0.26
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG12	3	0.26
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG11	10	0.26
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	9	0.26
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	9	0.26
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	1	0.26
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	9	0.26
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	1	0.26
(3,725)	1:38:A:LYS:HA	1:42:A:ARG:HD2	5	0.26
(3,602)	1:46:B:GLN:HG3	1:4:A:LYS:HE3	5	0.26
(3,539)	1:15:A:ILE:HA	1:8:B:LEU:HD23	7	0.26
(3,500)	1:32:B:LEU:HG	1:23:B:SER:HB3	1	0.26
(3,378)	1:25:B:LYS:HD3	1:32:B:LEU:HA	1	0.26
(3,377)	1:25:A:LYS:HD3	1:32:A:LEU:HA	1	0.26
(3,370)	1:85:B:ARG:HG2	1:77:A:GLU:HG2	8	0.26
(3,369)	1:85:A:ARG:HG2	1:77:B:GLU:HG2	8	0.26
(3,246)	1:7:B:GLN:HG2	1:18:A:THR:HB	5	0.26
(3,205)	1:44:A:ASP:HA	1:6:B:SER:HB3	2	0.26
(3,188)	1:51:B:LYS:H	1:50:B:LYS:HG3	5	0.26
(3,187)	1:51:A:LYS:H	1:50:A:LYS:HG3	5	0.26
(3,34)	1:87:B:THR:HG23	1:88:B:TRP:HA	8	0.26
(3,14)	1:111:B:GLU:HA	1:111:B:GLU:HG2	2	0.26
(3,13)	1:111:A:GLU:HA	1:111:A:GLU:HG2	2	0.26
(2,4)	1:74:A:LEU:N	1:32:A:LEU:O	3	0.26
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG23	5	0.26
(1,1816)	1:110:B:GLY:H	1:48:B:PHE:HA	3	0.26
(1,1803)	1:109:A:LEU:H	1:113:A:THR:H	2	0.26
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	7	0.26
(1,1674)	1:66:B:LEU:H	1:62:B:ILE:HG12	3	0.26
(1,1673)	1:66:A:LEU:H	1:62:A:ILE:HG12	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB2	5	0.26
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB2	5	0.26
(1,1421)	1:22:A:TYR:H	1:36:A:GLU:HG3	9	0.26
(1,1414)	1:21:B:GLN:H	1:29:B:PRO:HB2	10	0.26
(1,1413)	1:21:A:GLN:H	1:29:A:PRO:HB2	10	0.26
(1,1318)	1:11:B:ASN:H	1:12:B:ILE:HG13	4	0.26
(1,1317)	1:11:A:ASN:H	1:12:A:ILE:HG13	4	0.26
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	2	0.26
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	2	0.26
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	2	0.26
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	2	0.26
(1,1275)	1:48:A:PHE:H	1:45:A:LEU:HG	7	0.26
(1,1194)	1:47:B:ASN:HB3	1:111:B:GLU:HB3	2	0.26
(1,1193)	1:47:A:ASN:HB3	1:111:A:GLU:HB3	2	0.26
(1,1182)	1:81:B:MET:HB2	1:80:B:ILE:HG13	3	0.26
(1,1181)	1:81:A:MET:HB2	1:80:A:ILE:HG13	3	0.26
(1,1180)	1:81:B:MET:HB2	1:80:B:ILE:HG13	3	0.26
(1,1179)	1:81:A:MET:HB2	1:80:A:ILE:HG13	3	0.26
(1,1178)	1:81:B:MET:HB2	1:80:B:ILE:HG13	3	0.26
(1,1177)	1:81:A:MET:HB2	1:80:A:ILE:HG13	3	0.26
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	5	0.26
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	9	0.26
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	5	0.26
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	9	0.26
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	3	0.26
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	3	0.26
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	1	0.26
(1,948)	1:46:B:GLN:HB2	1:53:B:ASN:HA	10	0.26
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	1	0.26
(1,947)	1:46:A:GLN:HB2	1:53:A:ASN:HA	10	0.26
(1,896)	1:81:B:MET:HB2	1:80:B:ILE:HG13	3	0.26
(1,895)	1:81:A:MET:HB2	1:80:A:ILE:HG13	3	0.26
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	4	0.26
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	4	0.26
(1,686)	1:42:B:ARG:HA	1:59:B:ILE:HG22	1	0.26
(1,685)	1:42:A:ARG:HA	1:59:A:ILE:HG22	1	0.26
(1,671)	1:8:A:LEU:HG	1:15:B:ILE:H	5	0.26
(1,330)	1:66:B:LEU:HD13	1:84:B:ALA:H	2	0.26
(1,329)	1:66:A:LEU:HD13	1:84:A:ALA:H	2	0.26
(1,294)	1:81:B:MET:HB2	1:80:B:ILE:HG13	3	0.26
(1,293)	1:81:A:MET:HB2	1:80:A:ILE:HG13	3	0.26
(1,262)	1:8:B:LEU:HG	1:40:A:LEU:HG	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:60:A:GLU:HG2	1:61:A:HIS:HA	10	0.26
(1,123)	1:45:A:LEU:HG	1:9:B:GLU:HA	5	0.26
(1,96)	1:7:B:GLN:HG2	1:18:A:THR:HB	5	0.26
(1,2)	1:101:B:PRO:HB2	1:104:B:HIS:HA	4	0.26
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD22	1	0.25
(3,1482)	1:102:B:GLY:H	1:104:B:HIS:HB2	5	0.25
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD23	2	0.25
(3,1087)	1:23:A:SER:H	1:40:A:LEU:HD21	9	0.25
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG11	9	0.25
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB3	10	0.25
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB3	10	0.25
(3,904)	1:72:B:LYS:H	1:72:B:LYS:HD2	7	0.25
(3,903)	1:72:A:LYS:H	1:72:A:LYS:HD2	7	0.25
(3,872)	1:6:B:SER:H	1:5:B:MET:HG2	9	0.25
(3,872)	1:6:B:SER:H	1:5:B:MET:HG3	10	0.25
(3,871)	1:6:A:SER:H	1:5:A:MET:HG2	9	0.25
(3,871)	1:6:A:SER:H	1:5:A:MET:HG3	10	0.25
(3,839)	1:76:A:PHE:H	1:79:A:PHE:HB3	1	0.25
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	4	0.25
(3,671)	1:34:A:GLN:H	1:63:A:MET:HE3	10	0.25
(3,601)	1:46:A:GLN:HG3	1:4:B:LYS:HE3	5	0.25
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG2	10	0.25
(3,540)	1:15:B:ILE:HA	1:8:A:LEU:HD23	7	0.25
(3,499)	1:32:A:LEU:HG	1:23:A:SER:HB3	1	0.25
(3,378)	1:25:B:LYS:HD3	1:32:B:LEU:HA	6	0.25
(3,377)	1:25:A:LYS:HD3	1:32:A:LEU:HA	6	0.25
(3,377)	1:25:A:LYS:HD2	1:32:A:LEU:HA	9	0.25
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	1	0.25
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB2	1	0.25
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB2	1	0.25
(3,96)	1:19:B:PHE:HA	1:8:A:LEU:HD11	5	0.25
(3,92)	1:7:B:GLN:HG2	1:6:B:SER:HB3	9	0.25
(3,91)	1:7:A:GLN:HG2	1:6:A:SER:HB3	9	0.25
(3,51)	1:39:A:GLU:HG3	1:43:A:LYS:HE2	1	0.25
(3,34)	1:87:B:THR:HG23	1:88:B:TRP:HA	10	0.25
(3,33)	1:87:A:THR:HG23	1:88:A:TRP:HA	10	0.25
(2,64)	1:82:A:LEU:H	1:78:A:GLU:O	7	0.25
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	2	0.25
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG13	7	0.25
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG13	7	0.25
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD3	1	0.25
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD3	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1422)	1:22:B:TYR:H	1:36:B:GLU:HG3	9	0.25
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	8	0.25
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	8	0.25
(1,1328)	1:12:B:ILE:H	1:86:A:LEU:HD12	5	0.25
(1,1327)	1:12:A:ILE:H	1:86:B:LEU:HD12	5	0.25
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	10	0.25
(1,1276)	1:48:B:PHE:H	1:45:B:LEU:HG	7	0.25
(1,1180)	1:81:B:MET:HB3	1:80:A:ILE:HG12	10	0.25
(1,1179)	1:81:A:MET:HB3	1:80:B:ILE:HG12	10	0.25
(1,1178)	1:81:B:MET:HB3	1:80:A:ILE:HG12	10	0.25
(1,1177)	1:81:A:MET:HB3	1:80:B:ILE:HG12	10	0.25
(1,988)	1:48:B:PHE:HB3	1:109:B:LEU:H	9	0.25
(1,987)	1:48:A:PHE:HB3	1:109:A:LEU:H	9	0.25
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	1	0.25
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	4	0.25
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	1	0.25
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	4	0.25
(1,896)	1:81:B:MET:HB3	1:80:A:ILE:HG12	10	0.25
(1,895)	1:81:A:MET:HB3	1:80:B:ILE:HG12	10	0.25
(1,892)	1:81:B:MET:HB3	1:66:B:LEU:HG	3	0.25
(1,890)	1:81:B:MET:HB3	1:66:B:LEU:HG	3	0.25
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	3	0.25
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	3	0.25
(1,603)	1:18:A:THR:HG21	1:21:A:GLN:HG2	7	0.25
(1,560)	1:16:B:ILE:HB	1:12:B:ILE:HB	8	0.25
(1,559)	1:16:A:ILE:HB	1:12:A:ILE:HB	8	0.25
(1,400)	1:63:B:MET:HB3	1:72:B:LYS:HE2	8	0.25
(1,186)	1:60:B:GLU:HG2	1:61:B:HIS:HA	10	0.25
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	10	0.24
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	10	0.24
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	5	0.24
(4,11)	1:98:A:ASP:HA	1:96:A:GLU:HA	2	0.24
(4,11)	1:98:A:ASP:HA	1:96:A:GLU:HA	5	0.24
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG11	9	0.24
(3,920)	1:47:B:ASN:H	1:46:B:GLN:HB2	7	0.24
(3,919)	1:47:A:ASN:H	1:46:A:GLN:HB2	7	0.24
(3,872)	1:6:B:SER:H	1:5:B:MET:HG2	4	0.24
(3,871)	1:6:A:SER:H	1:5:A:MET:HG2	4	0.24
(3,840)	1:76:B:PHE:H	1:79:B:PHE:HB3	1	0.24
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD22	4	0.24
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD22	4	0.24
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,692)	1:32:B:LEU:HA	1:36:B:GLU:HB2	2	0.24
(3,691)	1:32:A:LEU:HA	1:36:A:GLU:HB2	2	0.24
(3,672)	1:34:B:GLN:H	1:63:B:MET:HE3	10	0.24
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG2	10	0.24
(3,479)	1:111:A:GLU:HG2	1:109:A:LEU:HB3	3	0.24
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	6	0.24
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	6	0.24
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG3	6	0.24
(3,320)	1:51:B:LYS:HE2	1:51:B:LYS:H	5	0.24
(3,319)	1:51:A:LYS:HE2	1:51:A:LYS:H	5	0.24
(3,95)	1:19:A:PHE:HA	1:8:B:LEU:HD11	5	0.24
(3,52)	1:39:B:GLU:HG3	1:43:B:LYS:HE2	1	0.24
(3,16)	1:101:B:PRO:HG2	1:102:B:GLY:HA2	1	0.24
(3,15)	1:101:A:PRO:HG2	1:102:A:GLY:HA2	1	0.24
(3,14)	1:111:B:GLU:HA	1:111:B:GLU:HG2	3	0.24
(3,14)	1:111:B:GLU:HA	1:111:B:GLU:HG2	10	0.24
(3,13)	1:111:A:GLU:HA	1:111:A:GLU:HG2	3	0.24
(3,13)	1:111:A:GLU:HA	1:111:A:GLU:HG2	10	0.24
(2,64)	1:82:A:LEU:H	1:78:A:GLU:O	1	0.24
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG22	4	0.24
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG22	4	0.24
(1,1791)	1:16:A:ILE:H	1:12:A:ILE:HG21	1	0.24
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	2	0.24
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	5	0.24
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	5	0.24
(1,1759)	1:24:A:VAL:H	1:25:A:LYS:HG3	10	0.24
(1,1735)	1:82:A:LEU:H	1:86:A:LEU:H	4	0.24
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG13	6	0.24
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG13	6	0.24
(1,1432)	1:23:B:SER:H	1:21:B:GLN:H	2	0.24
(1,1432)	1:23:B:SER:H	1:21:B:GLN:H	5	0.24
(1,1431)	1:23:A:SER:H	1:21:A:GLN:H	2	0.24
(1,1431)	1:23:A:SER:H	1:21:A:GLN:H	5	0.24
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	7	0.24
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	7	0.24
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	10	0.24
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	4	0.24
(1,1184)	1:56:B:GLU:HB2	1:57:B:LYS:HD3	2	0.24
(1,1183)	1:56:A:GLU:HB2	1:57:A:LYS:HD3	2	0.24
(1,1116)	1:84:B:ALA:HA	1:86:B:LEU:HD23	3	0.24
(1,1115)	1:84:A:ALA:HA	1:86:A:LEU:HD23	3	0.24
(1,1114)	1:66:B:LEU:H	1:66:B:LEU:HA	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:66:A:LEU:H	1:66:A:LEU:HA	7	0.24
(1,1046)	1:53:B:ASN:HA	1:38:B:LYS:HA	6	0.24
(1,1045)	1:53:A:ASN:HA	1:38:A:LYS:HA	6	0.24
(1,1028)	1:84:B:ALA:HA	1:86:B:LEU:HG	10	0.24
(1,1027)	1:84:A:ALA:HA	1:86:A:LEU:HG	10	0.24
(1,991)	1:8:A:LEU:HD21	1:48:B:PHE:HB2	9	0.24
(1,980)	1:48:B:PHE:HB3	1:45:B:LEU:HD22	4	0.24
(1,979)	1:48:A:PHE:HB3	1:45:A:LEU:HD22	4	0.24
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	2	0.24
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	9	0.24
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	2	0.24
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	9	0.24
(1,891)	1:81:A:MET:HB3	1:66:A:LEU:HG	3	0.24
(1,889)	1:81:A:MET:HB3	1:66:A:LEU:HG	3	0.24
(1,806)	1:74:B:LEU:HG	1:73:B:GLN:HG2	7	0.24
(1,806)	1:74:B:LEU:HG	1:73:B:GLN:HG2	9	0.24
(1,756)	1:111:B:GLU:HG2	1:108:B:GLY:HA3	9	0.24
(1,755)	1:111:A:GLU:HG2	1:108:A:GLY:HA3	9	0.24
(1,745)	1:111:A:GLU:HG2	1:109:A:LEU:HB3	3	0.24
(1,630)	1:84:B:ALA:HA	1:86:B:LEU:HG	10	0.24
(1,629)	1:84:A:ALA:HA	1:86:A:LEU:HG	10	0.24
(1,604)	1:18:B:THR:HG21	1:21:B:GLN:HG2	7	0.24
(1,399)	1:63:A:MET:HB3	1:72:A:LYS:HE2	8	0.24
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD12	4	0.24
(1,390)	1:36:B:GLU:HA	1:40:B:LEU:HD11	6	0.24
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD12	4	0.24
(1,338)	1:41:B:VAL:HG11	1:42:B:ARG:HA	3	0.24
(1,337)	1:41:A:VAL:HG11	1:42:A:ARG:HA	3	0.24
(1,318)	1:82:B:LEU:HB3	1:80:B:ILE:HD11	6	0.24
(1,317)	1:82:A:LEU:HB3	1:80:A:ILE:HD11	6	0.24
(1,224)	1:62:B:ILE:HG23	1:66:B:LEU:HG	2	0.24
(1,223)	1:62:A:ILE:HG23	1:66:A:LEU:HG	2	0.24
(1,185)	1:60:A:GLU:HG2	1:61:A:HIS:HA	7	0.24
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD12	4	0.24
(1,180)	1:36:B:GLU:HA	1:40:B:LEU:HD11	6	0.24
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD12	4	0.24
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	2	0.24
(1,118)	1:66:B:LEU:HG	1:62:B:ILE:HD12	6	0.24
(1,117)	1:66:A:LEU:HG	1:62:A:ILE:HD12	6	0.24
(1,81)	1:46:A:GLN:HG3	1:5:B:MET:H	6	0.24
(4,64)	1:32:B:LEU:HG	1:31:B:THR:HB	7	0.23
(4,63)	1:32:A:LEU:HG	1:31:A:THR:HB	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	1	0.23
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	2	0.23
(4,11)	1:98:A:ASP:HA	1:96:A:GLU:HA	1	0.23
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG3	8	0.23
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG3	8	0.23
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	1	0.23
(3,1086)	1:23:B:SER:H	1:24:B:VAL:HG12	7	0.23
(3,1085)	1:23:A:SER:H	1:24:A:VAL:HG12	7	0.23
(3,960)	1:75:B:SER:H	1:63:B:MET:HE1	7	0.23
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD22	7	0.23
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD22	7	0.23
(3,882)	1:30:B:ASP:H	1:31:B:THR:HG21	4	0.23
(3,881)	1:30:A:ASP:H	1:31:A:THR:HG21	4	0.23
(3,860)	1:74:B:LEU:H	1:74:B:LEU:HD22	1	0.23
(3,859)	1:74:A:LEU:H	1:74:A:LEU:HD22	1	0.23
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB3	5	0.23
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB3	7	0.23
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB3	5	0.23
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB3	7	0.23
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	8	0.23
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	8	0.23
(3,627)	1:48:A:PHE:HB2	1:9:B:GLU:HG2	4	0.23
(3,602)	1:46:B:GLN:HG3	1:4:A:LYS:HE3	2	0.23
(3,601)	1:46:A:GLN:HG3	1:4:B:LYS:HE2	10	0.23
(3,584)	1:66:B:LEU:HD22	1:67:B:ASP:HA	10	0.23
(3,583)	1:66:A:LEU:HD22	1:67:A:ASP:HA	10	0.23
(3,540)	1:15:B:ILE:HA	1:8:A:LEU:HD11	8	0.23
(3,539)	1:15:A:ILE:HA	1:8:B:LEU:HD11	8	0.23
(3,526)	1:76:B:PHE:HB2	1:16:B:ILE:HA	7	0.23
(3,525)	1:76:A:PHE:HB2	1:16:A:ILE:HA	7	0.23
(3,480)	1:111:B:GLU:HG2	1:109:B:LEU:HB3	3	0.23
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG3	6	0.23
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG3	8	0.23
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB2	6	0.23
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB2	6	0.23
(3,226)	1:66:B:LEU:HD12	1:82:B:LEU:HA	6	0.23
(3,225)	1:66:A:LEU:HD12	1:82:A:LEU:HA	6	0.23
(3,164)	1:13:B:GLU:HB3	1:14:B:THR:HG21	5	0.23
(3,164)	1:13:B:GLU:HB3	1:14:B:THR:HG21	10	0.23
(3,163)	1:13:A:GLU:HB3	1:14:A:THR:HG21	5	0.23
(3,163)	1:13:A:GLU:HB3	1:14:A:THR:HG21	10	0.23
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG23	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG23	10	0.23
(3,34)	1:87:B:THR:HG21	1:88:B:TRP:HA	6	0.23
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE3	8	0.23
(1,1818)	1:16:B:ILE:H	1:12:B:ILE:HG21	1	0.23
(1,1817)	1:16:A:ILE:H	1:12:A:ILE:HG21	1	0.23
(1,1792)	1:16:B:ILE:H	1:12:B:ILE:HG21	1	0.23
(1,1760)	1:24:B:VAL:H	1:25:B:LYS:HG3	10	0.23
(1,1736)	1:82:B:LEU:H	1:86:B:LEU:H	4	0.23
(1,1736)	1:82:B:LEU:H	1:86:B:LEU:H	7	0.23
(1,1735)	1:82:A:LEU:H	1:86:A:LEU:H	7	0.23
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB3	3	0.23
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB3	3	0.23
(1,1576)	1:49:B:LEU:H	1:49:B:LEU:HD22	6	0.23
(1,1575)	1:49:A:LEU:H	1:49:A:LEU:HD22	6	0.23
(1,1561)	1:44:A:ASP:H	1:40:A:LEU:HD22	6	0.23
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	10	0.23
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	10	0.23
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	10	0.23
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	10	0.23
(1,1374)	1:17:B:ASN:H	1:13:B:GLU:HA	3	0.23
(1,1374)	1:17:B:ASN:H	1:13:B:GLU:HA	6	0.23
(1,1373)	1:17:A:ASN:H	1:13:A:GLU:HA	6	0.23
(1,1368)	1:16:B:ILE:H	1:12:B:ILE:HG21	1	0.23
(1,1367)	1:16:A:ILE:H	1:12:A:ILE:HG21	1	0.23
(1,1332)	1:12:B:ILE:H	1:14:B:THR:H	5	0.23
(1,1331)	1:12:A:ILE:H	1:14:A:THR:H	5	0.23
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD2	2	0.23
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	3	0.23
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	3	0.23
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	4	0.23
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	9	0.23
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	9	0.23
(1,1176)	1:107:B:PRO:HG2	1:109:B:LEU:H	3	0.23
(1,1048)	1:53:B:ASN:HA	1:59:B:ILE:HA	3	0.23
(1,1048)	1:53:B:ASN:HA	1:59:B:ILE:HA	5	0.23
(1,1047)	1:53:A:ASN:HA	1:59:A:ILE:HA	3	0.23
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	5	0.23
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	6	0.23
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	5	0.23
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	6	0.23
(1,861)	1:25:A:LYS:HD2	1:43:A:LYS:HE3	6	0.23
(1,805)	1:74:A:LEU:HG	1:73:A:GLN:HG2	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:74:A:LEU:HG	1:73:A:GLN:HG2	9	0.23
(1,746)	1:111:B:GLU:HG2	1:109:B:LEU:HB3	3	0.23
(1,694)	1:74:B:LEU:HG	1:78:B:GLU:HG2	2	0.23
(1,693)	1:74:A:LEU:HG	1:78:A:GLU:HG2	2	0.23
(1,688)	1:107:B:PRO:HG2	1:109:B:LEU:H	3	0.23
(1,396)	1:33:B:ASN:HB3	1:34:B:GLN:HG2	7	0.23
(1,395)	1:33:A:ASN:HB3	1:34:A:GLN:HG2	7	0.23
(1,389)	1:36:A:GLU:HA	1:40:A:LEU:HD11	6	0.23
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG2	2	0.23
(1,356)	1:54:B:LYS:HA	1:42:B:ARG:HG2	6	0.23
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG2	2	0.23
(1,355)	1:54:A:LYS:HA	1:42:A:ARG:HG2	6	0.23
(1,338)	1:41:B:VAL:HG12	1:42:B:ARG:HA	1	0.23
(1,328)	1:66:B:LEU:HD22	1:67:B:ASP:HA	10	0.23
(1,327)	1:66:A:LEU:HD22	1:67:A:ASP:HA	10	0.23
(1,272)	1:12:B:ILE:H	1:8:B:LEU:HG	10	0.23
(1,271)	1:12:A:ILE:H	1:8:A:LEU:HG	10	0.23
(1,190)	1:77:B:GLU:HA	1:87:A:THR:HG21	10	0.23
(1,189)	1:77:A:GLU:HA	1:87:B:THR:HG21	10	0.23
(1,186)	1:60:B:GLU:HG2	1:61:B:HIS:HA	7	0.23
(1,186)	1:60:B:GLU:HG2	1:61:B:HIS:HA	9	0.23
(1,185)	1:60:A:GLU:HG2	1:61:A:HIS:HA	9	0.23
(1,179)	1:36:A:GLU:HA	1:40:A:LEU:HD11	6	0.23
(1,174)	1:78:B:GLU:HB3	1:32:B:LEU:HB2	8	0.23
(1,173)	1:78:A:GLU:HB3	1:32:A:LEU:HB2	8	0.23
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG22	5	0.23
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG22	5	0.23
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	2	0.23
(4,260)	1:113:B:THR:H	1:107:B:PRO:HA	3	0.22
(4,259)	1:113:A:THR:H	1:107:A:PRO:HA	3	0.22
(4,62)	1:25:B:LYS:HA	1:21:B:GLN:HA	8	0.22
(4,61)	1:25:A:LYS:HA	1:21:A:GLN:HA	8	0.22
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	4	0.22
(4,11)	1:98:A:ASP:HA	1:96:A:GLU:HA	4	0.22
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	2	0.22
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	6	0.22
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	10	0.22
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	1	0.22
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	6	0.22
(3,959)	1:75:A:SER:H	1:63:A:MET:HE1	7	0.22
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE3	2	0.22
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE3	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,674)	1:73:B:GLN:H	1:63:B:MET:HE3	4	0.22
(3,673)	1:73:A:GLN:H	1:63:A:MET:HE3	4	0.22
(3,670)	1:74:B:LEU:H	1:63:B:MET:HE1	10	0.22
(3,669)	1:74:A:LEU:H	1:63:A:MET:HE1	10	0.22
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	2	0.22
(3,602)	1:46:B:GLN:HG3	1:4:A:LYS:HE2	10	0.22
(3,378)	1:25:B:LYS:HD2	1:32:B:LEU:HA	4	0.22
(3,377)	1:25:A:LYS:HD2	1:32:A:LEU:HA	4	0.22
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG3	8	0.22
(3,320)	1:51:B:LYS:HE3	1:51:B:LYS:H	8	0.22
(3,319)	1:51:A:LYS:HE3	1:51:A:LYS:H	8	0.22
(3,199)	1:46:A:GLN:HB3	1:43:A:LYS:HA	4	0.22
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG22	1	0.22
(3,140)	1:41:B:VAL:HB	1:59:B:ILE:HG23	3	0.22
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG22	1	0.22
(3,132)	1:78:B:GLU:HB2	1:31:B:THR:HA	10	0.22
(3,131)	1:78:A:GLU:HB2	1:31:A:THR:HA	9	0.22
(3,131)	1:78:A:GLU:HB2	1:31:A:THR:HA	10	0.22
(3,88)	1:34:B:GLN:HG2	1:38:B:LYS:HD2	4	0.22
(3,33)	1:87:A:THR:HG21	1:88:A:TRP:HA	6	0.22
(3,6)	1:73:B:GLN:HG3	1:72:B:LYS:HG3	4	0.22
(3,5)	1:73:A:GLN:HG3	1:72:A:LYS:HG3	4	0.22
(2,86)	1:94:A:MET:H	1:90:A:SER:O	5	0.22
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE3	8	0.22
(1,1815)	1:110:A:GLY:H	1:48:A:PHE:HA	4	0.22
(1,1684)	1:68:B:THR:H	1:74:B:LEU:HD23	4	0.22
(1,1683)	1:68:A:THR:H	1:74:A:LEU:HD23	4	0.22
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD3	2	0.22
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD3	2	0.22
(1,1562)	1:44:B:ASP:H	1:40:B:LEU:HD22	6	0.22
(1,1500)	1:44:B:ASP:H	1:40:B:LEU:HD22	6	0.22
(1,1499)	1:44:A:ASP:H	1:40:A:LEU:HD22	6	0.22
(1,1466)	1:35:B:GLY:H	1:72:B:LYS:HB3	9	0.22
(1,1436)	1:23:B:SER:H	1:19:B:PHE:H	9	0.22
(1,1373)	1:17:A:ASN:H	1:13:A:GLU:HA	3	0.22
(1,1369)	1:17:A:ASN:H	1:15:A:ILE:HG13	9	0.22
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD2	2	0.22
(1,1200)	1:60:B:GLU:HB2	1:59:B:ILE:HG21	9	0.22
(1,1199)	1:60:A:GLU:HB2	1:59:A:ILE:HG21	9	0.22
(1,1175)	1:107:A:PRO:HG2	1:109:A:LEU:H	3	0.22
(1,1047)	1:53:A:ASN:HA	1:59:A:ILE:HA	5	0.22
(1,1009)	1:8:A:LEU:HD11	1:41:B:VAL:HA	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:8:B:LEU:HD21	1:48:A:PHE:HB2	9	0.22
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	7	0.22
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	7	0.22
(1,862)	1:25:B:LYS:HD2	1:43:B:LYS:HE3	6	0.22
(1,806)	1:74:B:LEU:HG	1:73:B:GLN:HG2	5	0.22
(1,805)	1:74:A:LEU:HG	1:73:A:GLN:HG2	5	0.22
(1,687)	1:107:A:PRO:HG2	1:109:A:LEU:H	3	0.22
(1,660)	1:7:B:GLN:HG2	1:8:B:LEU:HG	9	0.22
(1,659)	1:7:A:GLN:HG2	1:8:A:LEU:HG	9	0.22
(1,554)	1:76:B:PHE:HB3	1:80:B:ILE:HG12	8	0.22
(1,553)	1:76:A:PHE:HB3	1:80:A:ILE:HG12	8	0.22
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	9	0.22
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	9	0.22
(1,453)	1:7:A:GLN:HB2	1:10:A:ARG:HB2	9	0.22
(1,400)	1:63:B:MET:HB3	1:72:B:LYS:HE2	3	0.22
(1,338)	1:41:B:VAL:HG12	1:42:B:ARG:HA	8	0.22
(1,338)	1:41:B:VAL:HG13	1:42:B:ARG:HA	9	0.22
(1,337)	1:41:A:VAL:HG12	1:42:A:ARG:HA	1	0.22
(1,337)	1:41:A:VAL:HG12	1:42:A:ARG:HA	8	0.22
(1,337)	1:41:A:VAL:HG13	1:42:A:ARG:HA	9	0.22
(1,286)	1:51:B:LYS:H	1:50:B:LYS:HG2	10	0.22
(1,285)	1:51:A:LYS:H	1:50:A:LYS:HG2	10	0.22
(1,233)	1:46:A:GLN:HA	1:4:B:LYS:HE2	9	0.22
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	1	0.22
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	1	0.22
(1,139)	1:16:A:ILE:HD12	1:13:A:GLU:HG2	4	0.22
(1,28)	1:87:B:THR:HG23	1:85:B:ARG:HA	8	0.22
(1,27)	1:87:A:THR:HG23	1:85:A:ARG:HA	8	0.22
(1,24)	1:96:B:GLU:HA	1:107:B:PRO:HD2	3	0.22
(4,260)	1:113:B:THR:H	1:107:B:PRO:HA	5	0.21
(4,259)	1:113:A:THR:H	1:107:A:PRO:HA	5	0.21
(4,61)	1:25:A:LYS:HA	1:21:A:GLN:HA	10	0.21
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	3	0.21
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	10	0.21
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	3	0.21
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	10	0.21
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	4	0.21
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	4	0.21
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	3	0.21
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	2	0.21
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	3	0.21
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1050)	1:19:B:PHE:H	1:8:A:LEU:HD11	2	0.21
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD22	8	0.21
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD21	9	0.21
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD22	8	0.21
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD21	9	0.21
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE2	6	0.21
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE2	6	0.21
(3,642)	1:8:B:LEU:HD23	1:15:A:ILE:HD11	7	0.21
(3,641)	1:8:A:LEU:HD23	1:15:B:ILE:HD11	7	0.21
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	2	0.21
(3,628)	1:48:B:PHE:HB2	1:9:A:GLU:HG2	4	0.21
(3,601)	1:46:A:GLN:HG3	1:4:B:LYS:HE3	2	0.21
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE2	10	0.21
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE2	10	0.21
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG3	1	0.21
(3,552)	1:25:B:LYS:HD2	1:24:B:VAL:HG11	9	0.21
(3,546)	1:33:B:ASN:HA	1:31:B:THR:HG23	3	0.21
(3,545)	1:33:A:ASN:HA	1:31:A:THR:HG23	3	0.21
(3,526)	1:76:B:PHE:HB2	1:16:B:ILE:HA	4	0.21
(3,525)	1:76:A:PHE:HB2	1:16:A:ILE:HA	4	0.21
(3,486)	1:96:B:GLU:HG2	1:97:B:GLY:H	8	0.21
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	2	0.21
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG3	1	0.21
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG3	1	0.21
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB2	2	0.21
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB2	2	0.21
(3,330)	1:86:B:LEU:HD23	1:49:B:LEU:HG	7	0.21
(3,329)	1:86:A:LEU:HD23	1:49:A:LEU:HG	7	0.21
(3,200)	1:46:B:GLN:HB3	1:43:B:LYS:HA	4	0.21
(3,188)	1:51:B:LYS:H	1:50:B:LYS:HG2	10	0.21
(3,187)	1:51:A:LYS:H	1:50:A:LYS:HG2	10	0.21
(3,168)	1:39:B:GLU:HA	1:39:B:GLU:HB2	3	0.21
(3,139)	1:41:A:VAL:HB	1:59:A:ILE:HG23	3	0.21
(3,132)	1:78:B:GLU:HB2	1:31:B:THR:HA	9	0.21
(3,106)	1:38:B:LYS:HG2	1:34:B:GLN:HA	8	0.21
(3,105)	1:38:A:LYS:HG2	1:34:A:GLN:HA	8	0.21
(3,91)	1:7:A:GLN:HG2	1:6:A:SER:HB3	6	0.21
(3,87)	1:34:A:GLN:HG2	1:38:A:LYS:HD2	4	0.21
(3,34)	1:87:B:THR:HG21	1:88:B:TRP:HA	4	0.21
(3,33)	1:87:A:THR:HG21	1:88:A:TRP:HA	4	0.21
(1,1853)	1:109:A:LEU:H	1:13:B:GLU:HG3	9	0.21
(1,1816)	1:110:B:GLY:H	1:48:B:PHE:HA	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1772)	1:87:B:THR:H	1:80:A:ILE:HB	4	0.21
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	3	0.21
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	10	0.21
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	3	0.21
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	10	0.21
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB2	8	0.21
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB2	8	0.21
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD3	9	0.21
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD3	9	0.21
(1,1484)	1:37:B:PHE:H	1:32:B:LEU:HD22	1	0.21
(1,1483)	1:37:A:PHE:H	1:32:A:LEU:HD22	1	0.21
(1,1465)	1:35:A:GLY:H	1:72:A:LYS:HB3	9	0.21
(1,1436)	1:23:B:SER:H	1:19:B:PHE:H	4	0.21
(1,1435)	1:23:A:SER:H	1:19:A:PHE:H	1	0.21
(1,1435)	1:23:A:SER:H	1:19:A:PHE:H	4	0.21
(1,1435)	1:23:A:SER:H	1:19:A:PHE:H	9	0.21
(1,1370)	1:17:B:ASN:H	1:15:B:ILE:HG13	9	0.21
(1,1370)	1:17:B:ASN:H	1:15:B:ILE:HG13	10	0.21
(1,1369)	1:17:A:ASN:H	1:15:A:ILE:HG13	10	0.21
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD2	4	0.21
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	6	0.21
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	6	0.21
(1,1180)	1:81:B:MET:HB2	1:80:A:ILE:HG12	2	0.21
(1,1178)	1:81:B:MET:HB2	1:80:A:ILE:HG12	2	0.21
(1,992)	1:8:B:LEU:HD23	1:48:A:PHE:HB2	3	0.21
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	8	0.21
(1,978)	1:57:B:LYS:HA	1:57:B:LYS:H	10	0.21
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	8	0.21
(1,977)	1:57:A:LYS:HA	1:57:A:LYS:H	10	0.21
(1,896)	1:81:B:MET:HB2	1:80:A:ILE:HG12	2	0.21
(1,766)	1:59:B:ILE:HD12	1:59:B:ILE:HB	4	0.21
(1,765)	1:59:A:ILE:HD12	1:59:A:ILE:HB	4	0.21
(1,660)	1:7:B:GLN:HG2	1:8:B:LEU:HG	5	0.21
(1,659)	1:7:A:GLN:HG2	1:8:A:LEU:HG	5	0.21
(1,626)	1:96:B:GLU:HG2	1:97:B:GLY:H	8	0.21
(1,596)	1:85:B:ARG:HG3	1:62:B:ILE:HG22	9	0.21
(1,595)	1:85:A:ARG:HG3	1:62:A:ILE:HG22	9	0.21
(1,544)	1:5:B:MET:H	1:4:B:LYS:HG3	1	0.21
(1,543)	1:5:A:MET:H	1:4:A:LYS:HG3	1	0.21
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	10	0.21
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	10	0.21
(1,456)	1:7:B:GLN:HB3	1:9:B:GLU:HG2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:7:A:GLN:HB3	1:9:A:GLU:HG2	8	0.21
(1,454)	1:7:B:GLN:HB2	1:10:B:ARG:HB2	9	0.21
(1,399)	1:63:A:MET:HB3	1:72:A:LYS:HE2	3	0.21
(1,368)	1:34:B:GLN:HG2	1:38:B:LYS:HA	2	0.21
(1,367)	1:34:A:GLN:HG2	1:38:A:LYS:HA	2	0.21
(1,248)	1:63:B:MET:HB3	1:61:B:HIS:HB3	4	0.21
(1,234)	1:46:B:GLN:HA	1:4:A:LYS:HE2	9	0.21
(1,140)	1:16:B:ILE:HD12	1:13:B:GLU:HG2	4	0.21
(1,74)	1:48:B:PHE:HB3	1:86:B:LEU:HG	7	0.21
(1,73)	1:48:A:PHE:HB3	1:86:A:LEU:HG	7	0.21
(1,23)	1:96:A:GLU:HA	1:107:A:PRO:HD2	3	0.21
(4,62)	1:25:B:LYS:HA	1:21:B:GLN:HA	10	0.2
(3,1442)	1:87:B:THR:H	1:16:A:ILE:HD11	8	0.2
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	8	0.2
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	8	0.2
(3,1284)	1:57:B:LYS:H	1:58:B:VAL:HG23	3	0.2
(3,1283)	1:57:A:LYS:H	1:58:A:VAL:HG23	3	0.2
(3,1162)	1:37:B:PHE:H	1:40:B:LEU:HD12	10	0.2
(3,1161)	1:37:A:PHE:H	1:40:A:LEU:HD12	10	0.2
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	4	0.2
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	4	0.2
(3,1049)	1:19:A:PHE:H	1:8:B:LEU:HD11	2	0.2
(3,872)	1:6:B:SER:H	1:5:B:MET:HG2	8	0.2
(3,871)	1:6:A:SER:H	1:5:A:MET:HG2	8	0.2
(3,840)	1:76:B:PHE:H	1:79:B:PHE:HB3	6	0.2
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD11	1	0.2
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD13	3	0.2
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD11	1	0.2
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD13	3	0.2
(3,801)	1:29:A:PRO:HD2	1:30:A:ASP:HB2	7	0.2
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	8	0.2
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	8	0.2
(3,606)	1:66:B:LEU:HA	1:78:B:GLU:HG3	7	0.2
(3,605)	1:66:A:LEU:HA	1:78:A:GLU:HG3	7	0.2
(3,601)	1:46:A:GLN:HG3	1:4:B:LYS:HE2	9	0.2
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE1	6	0.2
(3,580)	1:82:B:LEU:HB3	1:83:B:MET:HE3	9	0.2
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE1	6	0.2
(3,566)	1:111:B:GLU:HB2	1:108:B:GLY:HA2	7	0.2
(3,565)	1:111:A:GLU:HB2	1:108:A:GLY:HA2	7	0.2
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG2	4	0.2
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG3	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG2	4	0.2
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG3	7	0.2
(3,551)	1:25:A:LYS:HD2	1:24:A:VAL:HG11	9	0.2
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG23	9	0.2
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG23	9	0.2
(3,485)	1:96:A:GLU:HG2	1:97:A:GLY:H	8	0.2
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	2	0.2
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	10	0.2
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	10	0.2
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB2	10	0.2
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB2	10	0.2
(3,167)	1:39:A:GLU:HA	1:39:A:GLU:HB2	3	0.2
(3,92)	1:7:B:GLN:HG2	1:6:B:SER:HB3	6	0.2
(2,64)	1:82:A:LEU:H	1:78:A:GLU:O	4	0.2
(2,64)	1:82:A:LEU:H	1:78:A:GLU:O	10	0.2
(1,1854)	1:109:B:LEU:H	1:13:A:GLU:HG3	9	0.2
(1,1771)	1:87:A:THR:H	1:80:B:ILE:HB	4	0.2
(1,1770)	1:87:B:THR:H	1:82:B:LEU:HD12	8	0.2
(1,1769)	1:87:A:THR:H	1:82:A:LEU:HD12	8	0.2
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	8	0.2
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD3	5	0.2
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD3	5	0.2
(1,1608)	1:80:B:ILE:H	1:80:B:ILE:HG12	7	0.2
(1,1607)	1:80:A:ILE:H	1:80:A:ILE:HG12	7	0.2
(1,1606)	1:80:B:ILE:H	1:78:B:GLU:HG3	2	0.2
(1,1605)	1:80:A:ILE:H	1:78:A:GLU:HG3	2	0.2
(1,1594)	1:10:B:ARG:H	1:8:B:LEU:HD13	4	0.2
(1,1593)	1:10:A:ARG:H	1:8:A:LEU:HD13	4	0.2
(1,1517)	1:40:A:LEU:H	1:25:A:LYS:HD3	1	0.2
(1,1436)	1:23:B:SER:H	1:19:B:PHE:H	1	0.2
(1,1422)	1:22:B:TYR:H	1:36:B:GLU:HG3	3	0.2
(1,1421)	1:22:A:TYR:H	1:36:A:GLU:HG3	3	0.2
(1,1402)	1:20:B:HIS:H	1:8:A:LEU:HD21	6	0.2
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	1	0.2
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD2	4	0.2
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD13	3	0.2
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD11	1	0.2
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD13	3	0.2
(1,1252)	1:6:B:SER:H	1:10:B:ARG:H	6	0.2
(1,1251)	1:6:A:SER:H	1:10:A:ARG:H	6	0.2
(1,1196)	1:98:B:ASP:HA	1:95:B:HIS:HB3	7	0.2
(1,1195)	1:98:A:ASP:HA	1:95:A:HIS:HB3	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:31:B:THR:HG21	1:71:B:ASP:HB3	6	0.2
(1,1053)	1:31:A:THR:HG21	1:71:A:ASP:HB3	6	0.2
(1,1048)	1:53:B:ASN:HA	1:59:B:ILE:HA	7	0.2
(1,1047)	1:53:A:ASN:HA	1:59:A:ILE:HA	7	0.2
(1,1010)	1:8:B:LEU:HD13	1:41:A:VAL:HA	6	0.2
(1,1010)	1:8:B:LEU:HD11	1:41:A:VAL:HA	7	0.2
(1,962)	1:21:B:GLN:HB3	1:22:B:TYR:HB2	1	0.2
(1,961)	1:21:A:GLN:HB3	1:22:A:TYR:HB2	1	0.2
(1,821)	1:46:A:GLN:HG3	1:50:A:LYS:HE3	10	0.2
(1,806)	1:74:B:LEU:HG	1:34:B:GLN:HB2	2	0.2
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG12	5	0.2
(1,756)	1:111:B:GLU:HG3	1:108:B:GLY:HA2	5	0.2
(1,736)	1:5:B:MET:HA	1:10:B:ARG:HA	1	0.2
(1,735)	1:5:A:MET:HA	1:10:A:ARG:HA	1	0.2
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	8	0.2
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	8	0.2
(1,640)	1:66:B:LEU:HA	1:78:B:GLU:HG3	7	0.2
(1,639)	1:66:A:LEU:HA	1:78:A:GLU:HG3	7	0.2
(1,625)	1:96:A:GLU:HG2	1:97:A:GLY:H	8	0.2
(1,549)	1:32:A:LEU:HA	1:36:A:GLU:HB2	9	0.2
(1,368)	1:34:B:GLN:HG2	1:38:B:LYS:HA	8	0.2
(1,367)	1:34:A:GLN:HG2	1:38:A:LYS:HA	8	0.2
(1,338)	1:41:B:VAL:HG12	1:42:B:ARG:HA	4	0.2
(1,338)	1:41:B:VAL:HG11	1:42:B:ARG:HA	7	0.2
(1,337)	1:41:A:VAL:HG12	1:42:A:ARG:HA	4	0.2
(1,337)	1:41:A:VAL:HG11	1:42:A:ARG:HA	7	0.2
(1,247)	1:63:A:MET:HB3	1:61:A:HIS:HB3	4	0.2
(1,166)	1:41:B:VAL:HB	1:37:B:PHE:HB3	4	0.2
(1,165)	1:41:A:VAL:HB	1:37:A:PHE:HB3	4	0.2
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	5	0.2
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	6	0.2
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	6	0.2
(4,62)	1:25:B:LYS:HA	1:21:B:GLN:HA	4	0.19
(4,61)	1:25:A:LYS:HA	1:21:A:GLN:HA	4	0.19
(4,61)	1:25:A:LYS:HA	1:21:A:GLN:HA	7	0.19
(3,1479)	1:100:A:GLY:H	1:99:A:GLU:HB2	5	0.19
(3,1458)	1:89:B:ALA:H	1:16:A:ILE:HD13	9	0.19
(3,1457)	1:89:A:ALA:H	1:16:B:ILE:HD13	9	0.19
(3,1364)	1:69:B:ASN:H	1:68:B:THR:HB	8	0.19
(3,1363)	1:69:A:ASN:H	1:68:A:THR:HB	8	0.19
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG11	6	0.19
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG11	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG3	3	0.19
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG2	9	0.19
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG3	3	0.19
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG2	9	0.19
(3,1168)	1:38:B:LYS:H	1:38:B:LYS:HG3	8	0.19
(3,1167)	1:38:A:LYS:H	1:38:A:LYS:HG3	8	0.19
(3,864)	1:74:B:LEU:H	1:31:B:THR:HB	1	0.19
(3,863)	1:74:A:LEU:H	1:31:A:THR:HB	1	0.19
(3,860)	1:74:B:LEU:H	1:74:B:LEU:HD22	7	0.19
(3,859)	1:74:A:LEU:H	1:74:A:LEU:HD22	7	0.19
(3,839)	1:76:A:PHE:H	1:79:A:PHE:HB3	6	0.19
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD22	6	0.19
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD22	6	0.19
(3,802)	1:29:B:PRO:HD2	1:30:B:ASP:HB2	7	0.19
(3,602)	1:46:B:GLN:HG3	1:4:A:LYS:HE2	9	0.19
(3,579)	1:82:A:LEU:HB3	1:83:A:MET:HE3	9	0.19
(3,566)	1:111:B:GLU:HB2	1:108:B:GLY:HA3	1	0.19
(3,565)	1:111:A:GLU:HB2	1:108:A:GLY:HA3	1	0.19
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG3	3	0.19
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG3	7	0.19
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG3	3	0.19
(3,504)	1:111:B:GLU:HA	1:107:B:PRO:HB2	10	0.19
(3,503)	1:111:A:GLU:HA	1:107:A:PRO:HB2	10	0.19
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG3	5	0.19
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG3	5	0.19
(3,180)	1:49:B:LEU:HG	1:48:B:PHE:HB3	6	0.19
(3,179)	1:49:A:LEU:HG	1:48:A:PHE:HB3	6	0.19
(3,92)	1:7:B:GLN:HG2	1:6:B:SER:HB3	5	0.19
(3,88)	1:34:B:GLN:HG2	1:38:B:LYS:HD2	6	0.19
(3,87)	1:34:A:GLN:HG2	1:38:A:LYS:HD2	6	0.19
(3,86)	1:7:B:GLN:HG3	1:7:B:GLN:HA	2	0.19
(3,85)	1:7:A:GLN:HG3	1:7:A:GLN:HA	2	0.19
(3,34)	1:87:B:THR:HG23	1:88:B:TRP:HA	2	0.19
(3,33)	1:87:A:THR:HG23	1:88:A:TRP:HA	2	0.19
(3,6)	1:73:B:GLN:HG3	1:72:B:LYS:HG3	7	0.19
(3,5)	1:73:A:GLN:HG3	1:72:A:LYS:HG3	7	0.19
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	8	0.19
(1,1653)	1:63:A:MET:H	1:62:A:ILE:HG13	1	0.19
(1,1592)	1:10:B:ARG:H	1:14:B:THR:H	6	0.19
(1,1592)	1:10:B:ARG:H	1:14:B:THR:H	8	0.19
(1,1591)	1:10:A:ARG:H	1:14:A:THR:H	6	0.19
(1,1591)	1:10:A:ARG:H	1:14:A:THR:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:49:B:LEU:H	1:49:B:LEU:HD23	8	0.19
(1,1558)	1:46:B:GLN:H	1:49:B:LEU:HD13	2	0.19
(1,1557)	1:46:A:GLN:H	1:49:A:LEU:HD13	2	0.19
(1,1518)	1:40:B:LEU:H	1:25:B:LYS:HD3	1	0.19
(1,1432)	1:23:B:SER:H	1:21:B:GLN:H	8	0.19
(1,1431)	1:23:A:SER:H	1:21:A:GLN:H	8	0.19
(1,1401)	1:20:A:HIS:H	1:8:B:LEU:HD21	6	0.19
(1,1390)	1:10:B:ARG:H	1:5:B:MET:H	3	0.19
(1,1389)	1:10:A:ARG:H	1:5:A:MET:H	3	0.19
(1,1384)	1:18:B:THR:H	1:16:B:ILE:HG13	9	0.19
(1,1374)	1:17:B:ASN:H	1:13:B:GLU:HA	1	0.19
(1,1373)	1:17:A:ASN:H	1:13:A:GLU:HA	1	0.19
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	6	0.19
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	6	0.19
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD11	1	0.19
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD11	4	0.19
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	1	0.19
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	1	0.19
(1,1276)	1:48:B:PHE:H	1:45:B:LEU:HG	2	0.19
(1,1275)	1:48:A:PHE:H	1:45:A:LEU:HG	2	0.19
(1,1180)	1:81:B:MET:HB2	1:80:A:ILE:HG12	9	0.19
(1,1179)	1:81:A:MET:HB2	1:80:B:ILE:HG12	2	0.19
(1,1179)	1:81:A:MET:HB2	1:80:B:ILE:HG12	9	0.19
(1,1178)	1:81:B:MET:HB2	1:80:A:ILE:HG12	9	0.19
(1,1177)	1:81:A:MET:HB2	1:80:B:ILE:HG12	2	0.19
(1,1177)	1:81:A:MET:HB2	1:80:B:ILE:HG12	9	0.19
(1,1009)	1:8:A:LEU:HD13	1:41:B:VAL:HA	6	0.19
(1,991)	1:8:A:LEU:HD23	1:48:B:PHE:HB2	3	0.19
(1,980)	1:48:B:PHE:HB3	1:45:B:LEU:HD21	3	0.19
(1,979)	1:48:A:PHE:HB3	1:45:A:LEU:HD21	3	0.19
(1,896)	1:81:B:MET:HB2	1:80:A:ILE:HG12	9	0.19
(1,895)	1:81:A:MET:HB2	1:80:B:ILE:HG12	2	0.19
(1,895)	1:81:A:MET:HB2	1:80:B:ILE:HG12	9	0.19
(1,822)	1:46:B:GLN:HG3	1:50:B:LYS:HE3	10	0.19
(1,805)	1:74:A:LEU:HG	1:34:A:GLN:HB2	2	0.19
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG12	5	0.19
(1,755)	1:111:A:GLU:HG3	1:108:A:GLY:HA2	5	0.19
(1,550)	1:32:B:LEU:HA	1:32:B:LEU:HG	8	0.19
(1,550)	1:32:B:LEU:HA	1:36:B:GLU:HB2	9	0.19
(1,549)	1:32:A:LEU:HA	1:32:A:LEU:HG	8	0.19
(1,489)	1:37:A:PHE:HB2	1:74:A:LEU:HD11	3	0.19
(1,480)	1:36:B:GLU:HB2	1:31:B:THR:HG23	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:36:A:GLU:HB2	1:31:A:THR:HG23	4	0.19
(1,368)	1:34:B:GLN:HG3	1:38:B:LYS:HA	4	0.19
(1,367)	1:34:A:GLN:HG3	1:38:A:LYS:HA	4	0.19
(1,338)	1:41:B:VAL:HG11	1:42:B:ARG:HA	10	0.19
(1,337)	1:41:A:VAL:HG11	1:42:A:ARG:HA	10	0.19
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	5	0.19
(1,137)	1:16:A:ILE:HD12	1:93:B:LYS:HE3	4	0.19
(1,124)	1:45:B:LEU:HG	1:9:A:GLU:HA	2	0.19
(4,62)	1:25:B:LYS:HA	1:21:B:GLN:HA	7	0.18
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD22	2	0.18
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD22	2	0.18
(3,1480)	1:100:B:GLY:H	1:99:B:GLU:HB2	5	0.18
(3,1441)	1:87:A:THR:H	1:16:B:ILE:HD11	8	0.18
(3,1382)	1:71:B:ASP:H	1:72:B:LYS:HE3	2	0.18
(3,1381)	1:71:A:ASP:H	1:72:A:LYS:HE3	2	0.18
(3,1280)	1:57:B:LYS:H	1:57:B:LYS:HD3	5	0.18
(3,1279)	1:57:A:LYS:H	1:57:A:LYS:HD3	5	0.18
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG2	1	0.18
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG3	5	0.18
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG2	1	0.18
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG3	5	0.18
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	7	0.18
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	8	0.18
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	9	0.18
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	7	0.18
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	9	0.18
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	5	0.18
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	5	0.18
(3,1022)	1:14:B:THR:H	1:17:B:ASN:HB3	1	0.18
(3,958)	1:75:B:SER:H	1:74:B:LEU:HD22	1	0.18
(3,957)	1:75:A:SER:H	1:74:A:LEU:HD22	1	0.18
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD12	10	0.18
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD12	10	0.18
(3,768)	1:72:B:LYS:HE3	1:72:B:LYS:HA	7	0.18
(3,767)	1:72:A:LYS:HE3	1:72:A:LYS:HA	7	0.18
(3,674)	1:73:B:GLN:H	1:63:B:MET:HE3	10	0.18
(3,673)	1:73:A:GLN:H	1:63:A:MET:HE3	10	0.18
(3,660)	1:72:B:LYS:HB3	1:64:B:GLU:HA	6	0.18
(3,660)	1:72:B:LYS:HB3	1:64:B:GLU:HA	7	0.18
(3,659)	1:72:A:LYS:HB3	1:64:A:GLU:HA	6	0.18
(3,659)	1:72:A:LYS:HB3	1:64:A:GLU:HA	7	0.18
(3,602)	1:46:B:GLN:HG3	1:4:A:LYS:HE3	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,530)	1:67:B:ASP:HB3	1:64:B:GLU:HG3	2	0.18
(3,529)	1:67:A:ASP:HB3	1:64:A:GLU:HG3	2	0.18
(3,502)	1:32:B:LEU:HA	1:32:B:LEU:HG	9	0.18
(3,350)	1:71:B:ASP:HA	1:67:B:ASP:HB3	7	0.18
(3,320)	1:51:B:LYS:HE2	1:51:B:LYS:H	10	0.18
(3,155)	1:34:A:GLN:HA	1:34:A:GLN:HG3	5	0.18
(3,91)	1:7:A:GLN:HG2	1:6:A:SER:HB3	5	0.18
(3,52)	1:39:B:GLU:HG3	1:43:B:LYS:HE3	7	0.18
(3,33)	1:87:A:THR:HG21	1:88:A:TRP:HA	7	0.18
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	5	0.18
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	6	0.18
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	5	0.18
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	6	0.18
(2,86)	1:94:A:MET:H	1:90:A:SER:O	8	0.18
(2,79)	1:91:A:HIS:N	1:87:A:THR:O	8	0.18
(2,64)	1:82:A:LEU:H	1:78:A:GLU:O	5	0.18
(2,64)	1:82:A:LEU:H	1:78:A:GLU:O	9	0.18
(2,42)	1:53:A:ASN:H	1:50:A:LYS:O	6	0.18
(2,26)	1:22:A:TYR:H	1:18:A:THR:O	1	0.18
(1,1735)	1:82:A:LEU:H	1:86:A:LEU:H	1	0.18
(1,1654)	1:63:B:MET:H	1:62:B:ILE:HG13	1	0.18
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB1	1	0.18
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB1	1	0.18
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD3	6	0.18
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD3	6	0.18
(1,1582)	1:50:B:LYS:H	1:86:B:LEU:HD13	10	0.18
(1,1581)	1:50:A:LYS:H	1:86:A:LEU:HD13	10	0.18
(1,1575)	1:49:A:LEU:H	1:49:A:LEU:HD23	8	0.18
(1,1436)	1:23:B:SER:H	1:19:B:PHE:H	7	0.18
(1,1435)	1:23:A:SER:H	1:19:A:PHE:H	7	0.18
(1,1431)	1:23:A:SER:H	1:21:A:GLN:H	9	0.18
(1,1414)	1:21:B:GLN:H	1:29:B:PRO:HB2	8	0.18
(1,1413)	1:21:A:GLN:H	1:29:A:PRO:HB2	8	0.18
(1,1383)	1:18:A:THR:H	1:16:A:ILE:HG13	9	0.18
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD12	2	0.18
(1,1326)	1:13:B:GLU:H	1:16:B:ILE:HD13	7	0.18
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD12	2	0.18
(1,1325)	1:13:A:GLU:H	1:16:A:ILE:HD13	7	0.18
(1,1306)	1:10:B:ARG:H	1:45:A:LEU:HD22	10	0.18
(1,1305)	1:10:A:ARG:H	1:45:B:LEU:HD22	10	0.18
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD11	4	0.18
(1,1180)	1:81:B:MET:HB2	1:80:B:ILE:HG13	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:81:A:MET:HB2	1:80:A:ILE:HG13	4	0.18
(1,1178)	1:81:B:MET:HB2	1:80:B:ILE:HG13	4	0.18
(1,1177)	1:81:A:MET:HB2	1:80:A:ILE:HG13	4	0.18
(1,994)	1:109:B:LEU:HD13	1:47:B:ASN:HB3	6	0.18
(1,962)	1:21:B:GLN:HB2	1:22:B:TYR:HB2	4	0.18
(1,961)	1:21:A:GLN:HB2	1:22:A:TYR:HB2	4	0.18
(1,896)	1:81:B:MET:HB2	1:80:B:ILE:HG13	4	0.18
(1,895)	1:81:A:MET:HB2	1:80:A:ILE:HG13	4	0.18
(1,864)	1:25:B:LYS:HD2	1:39:B:GLU:HB3	10	0.18
(1,828)	1:71:B:ASP:HA	1:67:B:ASP:HB3	7	0.18
(1,681)	1:37:A:PHE:HB3	1:63:A:MET:H	10	0.18
(1,490)	1:37:B:PHE:HB2	1:74:B:LEU:HD11	3	0.18
(1,486)	1:63:B:MET:HB2	1:38:B:LYS:HG3	3	0.18
(1,485)	1:63:A:MET:HB2	1:38:A:LYS:HG3	3	0.18
(1,396)	1:33:B:ASN:HB3	1:34:B:GLN:HG2	2	0.18
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG23	2	0.18
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG22	6	0.18
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG23	2	0.18
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG22	6	0.18
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	8	0.18
(1,138)	1:16:B:ILE:HD12	1:93:A:LYS:HE3	4	0.18
(1,123)	1:45:A:LEU:HG	1:9:B:GLU:HA	2	0.18
(4,260)	1:113:B:THR:H	1:107:B:PRO:HA	2	0.17
(4,259)	1:113:A:THR:H	1:107:A:PRO:HA	2	0.17
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	2	0.17
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	1	0.17
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	2	0.17
(4,112)	1:76:B:PHE:H	1:31:B:THR:H	1	0.17
(4,111)	1:76:A:PHE:H	1:31:A:THR:H	1	0.17
(4,62)	1:25:B:LYS:HA	1:21:B:GLN:HA	1	0.17
(3,1479)	1:100:A:GLY:H	1:99:A:GLU:HB2	2	0.17
(3,1284)	1:57:B:LYS:H	1:58:B:VAL:HG21	6	0.17
(3,1283)	1:57:A:LYS:H	1:58:A:VAL:HG21	6	0.17
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG3	10	0.17
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG3	10	0.17
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	10	0.17
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	3	0.17
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	8	0.17
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	10	0.17
(3,1021)	1:14:A:THR:H	1:17:A:ASN:HB3	1	0.17
(3,1010)	1:12:B:ILE:H	1:11:B:ASN:HB3	7	0.17
(3,1009)	1:12:A:ILE:H	1:11:A:ASN:HB3	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,904)	1:72:B:LYS:H	1:72:B:LYS:HD3	2	0.17
(3,903)	1:72:A:LYS:H	1:72:A:LYS:HD3	2	0.17
(3,828)	1:32:B:LEU:H	1:32:B:LEU:HD22	5	0.17
(3,827)	1:32:A:LEU:H	1:32:A:LEU:HD22	5	0.17
(3,802)	1:29:B:PRO:HD2	1:30:B:ASP:HB2	8	0.17
(3,801)	1:29:A:PRO:HD2	1:30:A:ASP:HB2	8	0.17
(3,775)	1:32:A:LEU:HG	1:63:A:MET:HE3	9	0.17
(3,713)	1:50:A:LYS:HE3	1:47:A:ASN:HA	10	0.17
(3,638)	1:109:B:LEU:HD12	1:48:B:PHE:HA	3	0.17
(3,637)	1:109:A:LEU:HD12	1:48:A:PHE:HA	3	0.17
(3,600)	1:53:B:ASN:HB2	1:46:B:GLN:HG3	3	0.17
(3,599)	1:53:A:ASN:HB2	1:46:A:GLN:HG3	3	0.17
(3,564)	1:78:B:GLU:HB3	1:74:B:LEU:HB3	3	0.17
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG2	5	0.17
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG2	5	0.17
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG21	4	0.17
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG21	4	0.17
(3,501)	1:32:A:LEU:HA	1:32:A:LEU:HG	9	0.17
(3,378)	1:25:B:LYS:HD3	1:32:B:LEU:HA	2	0.17
(3,349)	1:71:A:ASP:HA	1:67:A:ASP:HB3	7	0.17
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG2	7	0.17
(3,319)	1:51:A:LYS:HE2	1:51:A:LYS:H	10	0.17
(3,208)	1:44:B:ASP:HA	1:9:A:GLU:HG2	4	0.17
(3,156)	1:34:B:GLN:HA	1:34:B:GLN:HG3	5	0.17
(3,131)	1:78:A:GLU:HB2	1:31:A:THR:HA	2	0.17
(3,86)	1:7:B:GLN:HG3	1:7:B:GLN:HA	7	0.17
(3,85)	1:7:A:GLN:HG3	1:7:A:GLN:HA	7	0.17
(3,80)	1:59:B:ILE:HB	1:38:B:LYS:HG3	3	0.17
(3,79)	1:59:A:ILE:HB	1:38:A:LYS:HG3	3	0.17
(3,51)	1:39:A:GLU:HG3	1:43:A:LYS:HE3	7	0.17
(3,34)	1:87:B:THR:HG21	1:88:B:TRP:HA	1	0.17
(3,34)	1:87:B:THR:HG21	1:88:B:TRP:HA	7	0.17
(3,34)	1:87:B:THR:HG21	1:88:B:TRP:HA	9	0.17
(3,33)	1:87:A:THR:HG21	1:88:A:TRP:HA	1	0.17
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	1	0.17
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	1	0.17
(2,80)	1:91:A:HIS:H	1:87:A:THR:O	3	0.17
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	2	0.17
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	3	0.17
(2,42)	1:53:A:ASN:H	1:50:A:LYS:O	2	0.17
(1,1838)	1:103:B:HIS:H	1:104:B:HIS:HB2	3	0.17
(1,1775)	1:87:A:THR:H	1:83:A:MET:HE1	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:22:B:TYR:H	1:24:B:VAL:H	6	0.17
(1,1757)	1:22:A:TYR:H	1:24:A:VAL:H	6	0.17
(1,1736)	1:82:B:LEU:H	1:86:B:LEU:H	1	0.17
(1,1736)	1:82:B:LEU:H	1:86:B:LEU:H	5	0.17
(1,1735)	1:82:A:LEU:H	1:86:A:LEU:H	5	0.17
(1,1724)	1:81:B:MET:H	1:78:B:GLU:HG2	1	0.17
(1,1723)	1:81:A:MET:H	1:78:A:GLU:HG2	1	0.17
(1,1644)	1:65:B:ASP:H	1:63:B:MET:HG3	10	0.17
(1,1643)	1:65:A:ASP:H	1:63:A:MET:HG3	10	0.17
(1,1530)	1:42:B:ARG:H	1:49:B:LEU:HD12	7	0.17
(1,1529)	1:42:A:ARG:H	1:49:A:LEU:HD12	7	0.17
(1,1496)	1:38:B:LYS:H	1:38:B:LYS:HD2	2	0.17
(1,1432)	1:23:B:SER:H	1:21:B:GLN:H	9	0.17
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG22	3	0.17
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG22	3	0.17
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	1	0.17
(1,1356)	1:16:B:ILE:H	1:87:A:THR:HA	4	0.17
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	4	0.17
(1,1270)	1:48:B:PHE:H	1:51:B:LYS:HE2	9	0.17
(1,1266)	1:77:B:GLU:H	1:84:A:ALA:HB2	3	0.17
(1,1265)	1:77:A:GLU:H	1:84:B:ALA:HB2	3	0.17
(1,1194)	1:47:B:ASN:HB2	1:111:B:GLU:HB3	10	0.17
(1,1193)	1:47:A:ASN:HB2	1:111:A:GLU:HB3	10	0.17
(1,1156)	1:32:B:LEU:HG	1:76:B:PHE:HA	1	0.17
(1,1155)	1:32:A:LEU:HG	1:76:A:PHE:HA	1	0.17
(1,1154)	1:32:B:LEU:HG	1:36:B:GLU:HG2	7	0.17
(1,1153)	1:32:A:LEU:HG	1:36:A:GLU:HG2	7	0.17
(1,1152)	1:32:B:LEU:HG	1:74:B:LEU:HG	2	0.17
(1,1151)	1:32:A:LEU:HG	1:74:A:LEU:HG	2	0.17
(1,1093)	1:13:A:GLU:HA	1:86:B:LEU:HD21	1	0.17
(1,993)	1:109:A:LEU:HD13	1:47:A:ASN:HB3	6	0.17
(1,894)	1:78:B:GLU:HB3	1:74:B:LEU:HB3	3	0.17
(1,863)	1:25:A:LYS:HD2	1:39:A:GLU:HB3	10	0.17
(1,831)	1:76:A:PHE:HB2	1:88:B:TRP:HB2	6	0.17
(1,827)	1:71:A:ASP:HA	1:67:A:ASP:HB3	7	0.17
(1,806)	1:74:B:LEU:HG	1:73:B:GLN:HG2	4	0.17
(1,805)	1:74:A:LEU:HG	1:73:A:GLN:HG2	4	0.17
(1,682)	1:37:B:PHE:HB3	1:63:B:MET:H	3	0.17
(1,682)	1:37:B:PHE:HB3	1:63:B:MET:H	10	0.17
(1,546)	1:107:B:PRO:HB2	1:108:B:GLY:H	10	0.17
(1,545)	1:107:A:PRO:HB2	1:108:A:GLY:H	10	0.17
(1,526)	1:49:B:LEU:HB2	1:46:B:GLN:HB3	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:49:A:LEU:HB2	1:46:A:GLN:HB3	5	0.17
(1,439)	1:10:A:ARG:HG3	1:11:A:ASN:HB2	9	0.17
(1,395)	1:33:A:ASN:HB3	1:34:A:GLN:HG2	2	0.17
(1,338)	1:41:B:VAL:HG13	1:42:B:ARG:HA	2	0.17
(1,338)	1:41:B:VAL:HG12	1:42:B:ARG:HA	5	0.17
(1,337)	1:41:A:VAL:HG13	1:42:A:ARG:HA	2	0.17
(1,337)	1:41:A:VAL:HG12	1:42:A:ARG:HA	5	0.17
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	4	0.17
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	4	0.17
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	8	0.17
(1,123)	1:45:A:LEU:HG	1:9:B:GLU:HA	10	0.17
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	1	0.16
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	9	0.16
(4,61)	1:25:A:LYS:HA	1:21:A:GLN:HA	1	0.16
(3,1480)	1:100:B:GLY:H	1:99:B:GLU:HB2	2	0.16
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG12	2	0.16
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	1	0.16
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	3	0.16
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	1	0.16
(3,864)	1:74:B:LEU:H	1:31:B:THR:HB	5	0.16
(3,864)	1:74:B:LEU:H	1:31:B:THR:HB	10	0.16
(3,863)	1:74:A:LEU:H	1:31:A:THR:HB	5	0.16
(3,863)	1:74:A:LEU:H	1:31:A:THR:HB	10	0.16
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	8	0.16
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	8	0.16
(3,776)	1:32:B:LEU:HG	1:63:B:MET:HE3	9	0.16
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB1	3	0.16
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB1	4	0.16
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB1	3	0.16
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB1	4	0.16
(3,714)	1:50:B:LYS:HE3	1:47:B:ASN:HA	10	0.16
(3,692)	1:32:B:LEU:HA	1:36:B:GLU:HB2	6	0.16
(3,691)	1:32:A:LEU:HA	1:36:A:GLU:HB2	6	0.16
(3,679)	1:85:A:ARG:HG2	1:85:A:ARG:HA	1	0.16
(3,601)	1:46:A:GLN:HG3	1:4:B:LYS:HE3	3	0.16
(3,563)	1:78:A:GLU:HB3	1:74:A:LEU:HB3	3	0.16
(3,546)	1:33:B:ASN:HA	1:31:B:THR:HG22	8	0.16
(3,545)	1:33:A:ASN:HA	1:31:A:THR:HG22	8	0.16
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG23	6	0.16
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG23	6	0.16
(3,377)	1:25:A:LYS:HD3	1:32:A:LEU:HA	2	0.16
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG2	7	0.16
(3,346)	1:5:B:MET:H	1:4:B:LYS:HG3	9	0.16
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG3	4	0.16
(3,345)	1:5:A:MET:H	1:4:A:LYS:HG3	9	0.16
(3,329)	1:86:A:LEU:HD21	1:49:A:LEU:HG	4	0.16
(3,320)	1:51:B:LYS:HE2	1:51:B:LYS:H	4	0.16
(3,320)	1:51:B:LYS:HE2	1:51:B:LYS:H	6	0.16
(3,320)	1:51:B:LYS:HE2	1:51:B:LYS:H	7	0.16
(3,319)	1:51:A:LYS:HE2	1:51:A:LYS:H	4	0.16
(3,266)	1:42:B:ARG:HB2	1:43:B:LYS:H	6	0.16
(3,266)	1:42:B:ARG:HB2	1:43:B:LYS:H	8	0.16
(3,265)	1:42:A:ARG:HB2	1:43:A:LYS:H	2	0.16
(3,265)	1:42:A:ARG:HB2	1:43:A:LYS:H	6	0.16
(3,265)	1:42:A:ARG:HB2	1:43:A:LYS:H	8	0.16
(3,207)	1:44:A:ASP:HA	1:9:B:GLU:HG2	4	0.16
(3,156)	1:34:B:GLN:HA	1:34:B:GLN:HG3	9	0.16
(3,132)	1:78:B:GLU:HB2	1:31:B:THR:HA	2	0.16
(3,50)	1:78:B:GLU:HG2	1:77:B:GLU:H	6	0.16
(3,33)	1:87:A:THR:HG21	1:88:A:TRP:HA	9	0.16
(3,14)	1:111:B:GLU:HA	1:111:B:GLU:HG3	1	0.16
(3,13)	1:111:A:GLU:HA	1:111:A:GLU:HG3	1	0.16
(3,13)	1:111:A:GLU:HA	1:111:A:GLU:HG3	9	0.16
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	4	0.16
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	8	0.16
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	4	0.16
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	8	0.16
(3,6)	1:73:B:GLN:HG3	1:72:B:LYS:HG2	1	0.16
(2,64)	1:82:A:LEU:H	1:78:A:GLU:O	2	0.16
(2,62)	1:81:A:MET:H	1:77:A:GLU:O	8	0.16
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	7	0.16
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	9	0.16
(2,42)	1:53:A:ASN:H	1:50:A:LYS:O	9	0.16
(2,3)	1:74:A:LEU:H	1:32:A:LEU:O	3	0.16
(2,2)	1:32:A:LEU:N	1:74:A:LEU:O	8	0.16
(1,1837)	1:103:A:HIS:H	1:104:A:HIS:HB2	3	0.16
(1,1834)	1:94:B:MET:H	1:90:B:SER:H	10	0.16
(1,1833)	1:94:A:MET:H	1:90:A:SER:H	10	0.16
(1,1776)	1:87:B:THR:H	1:83:B:MET:HE1	2	0.16
(1,1700)	1:71:B:ASP:H	1:72:B:LYS:HG3	5	0.16
(1,1699)	1:71:A:ASP:H	1:72:A:LYS:HG3	5	0.16
(1,1698)	1:71:B:ASP:H	1:63:B:MET:HE1	2	0.16
(1,1697)	1:71:A:ASP:H	1:63:A:MET:HE1	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1614)	1:85:B:ARG:H	1:85:B:ARG:HD3	8	0.16
(1,1613)	1:85:A:ARG:H	1:85:A:ARG:HD3	8	0.16
(1,1540)	1:42:B:ARG:H	1:40:B:LEU:H	3	0.16
(1,1495)	1:38:A:LYS:H	1:38:A:LYS:HD2	2	0.16
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	4	0.16
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	5	0.16
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	4	0.16
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	5	0.16
(1,1269)	1:48:A:PHE:H	1:51:A:LYS:HE2	9	0.16
(1,1200)	1:60:B:GLU:HB2	1:59:B:ILE:HG21	4	0.16
(1,1199)	1:60:A:GLU:HB2	1:59:A:ILE:HG21	4	0.16
(1,1181)	1:58:A:VAL:HG21	1:56:A:GLU:HB2	9	0.16
(1,1135)	1:57:A:LYS:HE3	1:60:A:GLU:HG3	10	0.16
(1,893)	1:78:A:GLU:HB3	1:74:A:LEU:HB3	3	0.16
(1,832)	1:76:B:PHE:HB2	1:88:A:TRP:HB2	6	0.16
(1,806)	1:74:B:LEU:HG	1:73:B:GLN:HG2	10	0.16
(1,805)	1:74:A:LEU:HG	1:73:A:GLN:HG2	10	0.16
(1,773)	1:82:A:LEU:HA	1:80:B:ILE:HG13	7	0.16
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	4	0.16
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	4	0.16
(1,681)	1:37:A:PHE:HB3	1:63:A:MET:H	3	0.16
(1,594)	1:85:B:ARG:HG3	1:82:B:LEU:HG	3	0.16
(1,593)	1:85:A:ARG:HG3	1:82:A:LEU:HG	3	0.16
(1,592)	1:85:B:ARG:HG3	1:66:B:LEU:HG	9	0.16
(1,591)	1:85:A:ARG:HG3	1:66:A:LEU:HG	9	0.16
(1,440)	1:10:B:ARG:HG3	1:11:B:ASN:HB2	9	0.16
(1,404)	1:99:B:GLU:HB2	1:98:B:ASP:HB2	2	0.16
(1,403)	1:99:A:GLU:HB2	1:98:A:ASP:HB2	2	0.16
(1,297)	1:58:A:VAL:HG21	1:56:A:GLU:HB2	9	0.16
(1,293)	1:58:A:VAL:HG21	1:56:A:GLU:HB2	9	0.16
(1,166)	1:41:B:VAL:HB	1:37:B:PHE:HB3	2	0.16
(1,166)	1:41:B:VAL:HB	1:37:B:PHE:HB3	7	0.16
(1,166)	1:41:B:VAL:HB	1:37:B:PHE:HB3	9	0.16
(1,165)	1:41:A:VAL:HB	1:37:A:PHE:HB3	2	0.16
(1,165)	1:41:A:VAL:HB	1:37:A:PHE:HB3	7	0.16
(1,165)	1:41:A:VAL:HB	1:37:A:PHE:HB3	9	0.16
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	3	0.16
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	3	0.16
(1,139)	1:16:A:ILE:HD13	1:13:A:GLU:HB3	8	0.16
(1,124)	1:45:B:LEU:HG	1:9:A:GLU:HA	8	0.16
(1,124)	1:45:B:LEU:HG	1:9:A:GLU:HA	10	0.16
(1,123)	1:45:A:LEU:HG	1:9:B:GLU:HA	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:45:A:LEU:HG	1:9:B:GLU:HA	9	0.16
(4,255)	1:73:A:GLN:H	1:67:A:ASP:H	8	0.15
(4,2)	1:98:B:ASP:HA	1:95:B:HIS:HA	10	0.15
(4,1)	1:98:A:ASP:HA	1:95:A:HIS:HA	10	0.15
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD22	7	0.15
(3,1447)	1:88:A:TRP:H	1:77:B:GLU:HG3	8	0.15
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG12	2	0.15
(3,1245)	1:50:A:LYS:H	1:41:A:VAL:HG13	3	0.15
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG3	2	0.15
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG2	4	0.15
(3,1208)	1:42:B:ARG:H	1:43:B:LYS:HG3	7	0.15
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG3	2	0.15
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG2	4	0.15
(3,1207)	1:42:A:ARG:H	1:43:A:LYS:HG3	7	0.15
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	5	0.15
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	9	0.15
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	9	0.15
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB3	8	0.15
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB1	10	0.15
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB3	8	0.15
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB1	10	0.15
(3,680)	1:85:B:ARG:HG2	1:85:B:ARG:HA	1	0.15
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	6	0.15
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	6	0.15
(3,564)	1:78:B:GLU:HB3	1:74:B:LEU:HB3	8	0.15
(3,563)	1:78:A:GLU:HB3	1:74:A:LEU:HB3	8	0.15
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG2	8	0.15
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG2	8	0.15
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG21	3	0.15
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG21	3	0.15
(3,530)	1:67:B:ASP:HB3	1:64:B:GLU:HG3	10	0.15
(3,529)	1:67:A:ASP:HB3	1:64:A:GLU:HG3	10	0.15
(3,330)	1:86:B:LEU:HD21	1:49:B:LEU:HG	4	0.15
(3,319)	1:51:A:LYS:HE2	1:51:A:LYS:H	6	0.15
(3,319)	1:51:A:LYS:HE2	1:51:A:LYS:H	7	0.15
(3,266)	1:42:B:ARG:HB2	1:43:B:LYS:H	2	0.15
(3,206)	1:44:B:ASP:HA	1:6:A:SER:HB3	8	0.15
(3,155)	1:34:A:GLN:HA	1:34:A:GLN:HG3	9	0.15
(3,86)	1:7:B:GLN:HG3	1:7:B:GLN:HA	8	0.15
(3,85)	1:7:A:GLN:HG3	1:7:A:GLN:HA	8	0.15
(3,80)	1:59:B:ILE:HB	1:38:B:LYS:HG2	7	0.15
(3,79)	1:59:A:ILE:HB	1:38:A:LYS:HG2	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,54)	1:39:B:GLU:HG3	1:43:B:LYS:HD3	7	0.15
(3,53)	1:39:A:GLU:HG3	1:43:A:LYS:HD3	7	0.15
(3,14)	1:111:B:GLU:HA	1:111:B:GLU:HG3	9	0.15
(3,12)	1:98:B:ASP:H	1:98:B:ASP:HA	3	0.15
(3,11)	1:98:A:ASP:H	1:98:A:ASP:HA	3	0.15
(3,5)	1:73:A:GLN:HG3	1:72:A:LYS:HG2	1	0.15
(2,86)	1:94:A:MET:H	1:90:A:SER:O	3	0.15
(1,1757)	1:84:A:ALA:H	1:86:A:LEU:H	5	0.15
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	7	0.15
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	7	0.15
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB2	2	0.15
(1,1592)	1:10:B:ARG:H	1:14:B:THR:H	10	0.15
(1,1591)	1:10:A:ARG:H	1:14:A:THR:H	10	0.15
(1,1540)	1:42:B:ARG:H	1:40:B:LEU:H	6	0.15
(1,1539)	1:42:A:ARG:H	1:40:A:LEU:H	3	0.15
(1,1432)	1:23:B:SER:H	1:21:B:GLN:H	3	0.15
(1,1431)	1:23:A:SER:H	1:21:A:GLN:H	3	0.15
(1,1328)	1:12:B:ILE:H	1:86:A:LEU:HD21	10	0.15
(1,1327)	1:12:A:ILE:H	1:86:B:LEU:HD21	10	0.15
(1,1308)	1:10:B:ARG:H	1:10:B:ARG:HD2	6	0.15
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	7	0.15
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	9	0.15
(1,1259)	1:47:A:ASN:H	1:9:B:GLU:HB3	10	0.15
(1,1182)	1:58:B:VAL:HG21	1:56:B:GLU:HB2	9	0.15
(1,1180)	1:81:B:MET:HB3	1:80:A:ILE:HG12	5	0.15
(1,1178)	1:81:B:MET:HB3	1:80:A:ILE:HG12	5	0.15
(1,1136)	1:57:B:LYS:HE3	1:60:B:GLU:HG3	10	0.15
(1,1100)	1:24:B:VAL:HG12	1:22:B:TYR:HB2	3	0.15
(1,1099)	1:24:A:VAL:HG12	1:22:A:TYR:HB2	3	0.15
(1,1040)	1:85:B:ARG:HA	1:89:B:ALA:HB1	8	0.15
(1,1039)	1:85:A:ARG:HA	1:89:A:ALA:HB1	8	0.15
(1,980)	1:86:B:LEU:HD23	1:48:B:PHE:HB3	2	0.15
(1,980)	1:86:B:LEU:HD22	1:48:B:PHE:HB3	8	0.15
(1,979)	1:86:A:LEU:HD23	1:48:A:PHE:HB3	2	0.15
(1,962)	1:21:B:GLN:HB2	1:22:B:TYR:HB2	10	0.15
(1,961)	1:21:A:GLN:HB2	1:22:A:TYR:HB2	10	0.15
(1,896)	1:81:B:MET:HB3	1:80:A:ILE:HG12	5	0.15
(1,894)	1:78:B:GLU:HB3	1:74:B:LEU:HB3	8	0.15
(1,893)	1:78:A:GLU:HB3	1:74:A:LEU:HB3	8	0.15
(1,822)	1:46:B:GLN:HG3	1:50:B:LYS:HE2	9	0.15
(1,821)	1:46:A:GLN:HG3	1:50:A:LYS:HE2	9	0.15
(1,806)	1:74:B:LEU:HG	1:73:B:GLN:HG2	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:111:B:GLU:HA	1:50:B:LYS:HB3	1	0.15
(1,795)	1:111:A:GLU:HA	1:50:A:LYS:HB3	1	0.15
(1,774)	1:82:B:LEU:HA	1:80:A:ILE:HG13	7	0.15
(1,694)	1:74:B:LEU:HG	1:78:B:GLU:HG3	10	0.15
(1,693)	1:74:A:LEU:HG	1:78:A:GLU:HG3	10	0.15
(1,614)	1:36:B:GLU:HA	1:25:B:LYS:HD3	1	0.15
(1,613)	1:36:A:GLU:HA	1:25:A:LYS:HD3	1	0.15
(1,546)	1:107:B:PRO:HB3	1:108:B:GLY:H	7	0.15
(1,545)	1:107:A:PRO:HB3	1:108:A:GLY:H	7	0.15
(1,458)	1:111:B:GLU:HA	1:50:B:LYS:HB3	1	0.15
(1,457)	1:111:A:GLU:HA	1:50:A:LYS:HB3	1	0.15
(1,456)	1:7:B:GLN:HB3	1:9:B:GLU:HG2	5	0.15
(1,455)	1:7:A:GLN:HB3	1:9:A:GLU:HG2	5	0.15
(1,387)	1:7:A:GLN:HA	1:8:A:LEU:HD23	1	0.15
(1,330)	1:66:B:LEU:HD11	1:84:B:ALA:H	4	0.15
(1,329)	1:66:A:LEU:HD11	1:84:A:ALA:H	4	0.15
(1,298)	1:58:B:VAL:HG21	1:56:B:GLU:HB2	9	0.15
(1,294)	1:58:B:VAL:HG21	1:56:B:GLU:HB2	9	0.15
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG23	10	0.15
(1,152)	1:37:B:PHE:HA	1:42:B:ARG:H	9	0.15
(1,151)	1:37:A:PHE:HA	1:42:A:ARG:H	9	0.15
(1,140)	1:16:B:ILE:HD13	1:13:B:GLU:HB3	8	0.15
(1,138)	1:16:B:ILE:HD12	1:93:A:LYS:HE3	1	0.15
(1,124)	1:45:B:LEU:HG	1:9:A:GLU:HA	9	0.15
(1,55)	1:13:A:GLU:HG2	1:109:B:LEU:HD11	2	0.15
(4,256)	1:73:B:GLN:H	1:67:B:ASP:H	8	0.14
(4,236)	1:81:B:MET:H	1:81:A:MET:H	8	0.14
(4,235)	1:81:A:MET:H	1:81:B:MET:H	8	0.14
(4,118)	1:33:B:ASN:H	1:26:B:LEU:H	5	0.14
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	5	0.14
(4,117)	1:33:A:ASN:H	1:26:A:LEU:H	9	0.14
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD23	3	0.14
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD23	3	0.14
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD22	7	0.14
(3,1448)	1:88:B:TRP:H	1:77:A:GLU:HG3	8	0.14
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	5	0.14
(3,1246)	1:50:B:LYS:H	1:41:B:VAL:HG13	3	0.14
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	5	0.14
(3,980)	1:9:B:GLU:H	1:5:B:MET:HG2	4	0.14
(3,979)	1:9:A:GLU:H	1:5:A:MET:HG2	4	0.14
(3,872)	1:6:B:SER:H	1:5:B:MET:HG2	5	0.14
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB2	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB3	1	0.14
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB3	2	0.14
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB2	6	0.14
(3,722)	1:31:B:THR:HG21	1:73:B:GLN:HB3	9	0.14
(3,721)	1:31:A:THR:HG21	1:73:A:GLN:HB3	9	0.14
(3,692)	1:32:B:LEU:HA	1:36:B:GLU:HB2	5	0.14
(3,691)	1:32:A:LEU:HA	1:36:A:GLU:HB2	5	0.14
(3,680)	1:85:B:ARG:HG2	1:85:B:ARG:HA	4	0.14
(3,679)	1:85:A:ARG:HG2	1:85:A:ARG:HA	4	0.14
(3,640)	1:8:B:LEU:HD21	1:83:A:MET:HG2	1	0.14
(3,639)	1:8:A:LEU:HD21	1:83:B:MET:HG2	1	0.14
(3,564)	1:78:B:GLU:HB2	1:74:B:LEU:HB3	6	0.14
(3,563)	1:78:A:GLU:HB2	1:74:A:LEU:HB3	6	0.14
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG22	10	0.14
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG22	10	0.14
(3,366)	1:85:B:ARG:HG3	1:77:A:GLU:HA	3	0.14
(3,339)	1:57:A:LYS:HG2	1:56:A:GLU:HB3	8	0.14
(3,205)	1:44:A:ASP:HA	1:6:B:SER:HB3	8	0.14
(3,164)	1:13:B:GLU:HB3	1:14:B:THR:HG21	4	0.14
(3,163)	1:13:A:GLU:HB3	1:14:A:THR:HG21	4	0.14
(3,154)	1:34:B:GLN:HA	1:59:B:ILE:HG21	7	0.14
(3,153)	1:34:A:GLN:HA	1:59:A:ILE:HG21	7	0.14
(3,92)	1:7:B:GLN:HG2	1:6:B:SER:HB3	10	0.14
(3,91)	1:7:A:GLN:HG2	1:6:A:SER:HB3	10	0.14
(3,86)	1:7:B:GLN:HG3	1:7:B:GLN:HA	3	0.14
(3,85)	1:7:A:GLN:HG3	1:7:A:GLN:HA	3	0.14
(3,49)	1:78:A:GLU:HG2	1:77:A:GLU:H	6	0.14
(2,82)	1:92:A:GLU:H	1:88:A:TRP:O	8	0.14
(2,79)	1:91:A:HIS:N	1:87:A:THR:O	5	0.14
(2,79)	1:91:A:HIS:N	1:87:A:THR:O	10	0.14
(2,61)	1:81:A:MET:N	1:77:A:GLU:O	8	0.14
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	5	0.14
(2,26)	1:22:A:TYR:H	1:18:A:THR:O	2	0.14
(2,26)	1:22:A:TYR:H	1:18:A:THR:O	7	0.14
(2,26)	1:22:A:TYR:H	1:18:A:THR:O	10	0.14
(2,4)	1:74:A:LEU:N	1:32:A:LEU:O	9	0.14
(1,1854)	1:5:B:MET:H	1:9:B:GLU:HG2	7	0.14
(1,1853)	1:5:A:MET:H	1:9:A:GLU:HG2	7	0.14
(1,1758)	1:84:B:ALA:H	1:86:B:LEU:H	5	0.14
(1,1706)	1:78:B:GLU:H	1:67:B:ASP:HA	10	0.14
(1,1705)	1:78:A:GLU:H	1:67:A:ASP:HA	10	0.14
(1,1700)	1:71:B:ASP:H	1:72:B:LYS:HG3	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1699)	1:71:A:ASP:H	1:72:A:LYS:HG3	8	0.14
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	5	0.14
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB2	2	0.14
(1,1610)	1:80:B:ILE:H	1:80:B:ILE:HD13	3	0.14
(1,1609)	1:80:A:ILE:H	1:80:A:ILE:HD13	3	0.14
(1,1540)	1:42:B:ARG:H	1:40:B:LEU:H	1	0.14
(1,1540)	1:42:B:ARG:H	1:40:B:LEU:H	2	0.14
(1,1539)	1:42:A:ARG:H	1:40:A:LEU:H	1	0.14
(1,1539)	1:42:A:ARG:H	1:40:A:LEU:H	2	0.14
(1,1539)	1:42:A:ARG:H	1:40:A:LEU:H	6	0.14
(1,1431)	1:23:A:SER:H	1:21:A:GLN:H	10	0.14
(1,1414)	1:61:B:HIS:H	1:64:B:GLU:HB3	7	0.14
(1,1413)	1:61:A:HIS:H	1:64:A:GLU:HB3	7	0.14
(1,1378)	1:18:B:THR:H	1:20:B:HIS:H	5	0.14
(1,1377)	1:18:A:THR:H	1:20:A:HIS:H	5	0.14
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG22	4	0.14
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG23	5	0.14
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG22	4	0.14
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG23	5	0.14
(1,1328)	1:12:B:ILE:H	1:45:A:LEU:HD21	7	0.14
(1,1327)	1:12:A:ILE:H	1:45:B:LEU:HD22	7	0.14
(1,1307)	1:10:A:ARG:H	1:10:A:ARG:HD2	6	0.14
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	7	0.14
(1,1269)	1:48:A:PHE:H	1:4:B:LYS:HE3	4	0.14
(1,1260)	1:47:B:ASN:H	1:9:A:GLU:HB3	10	0.14
(1,1179)	1:81:A:MET:HB3	1:80:B:ILE:HG12	5	0.14
(1,1177)	1:81:A:MET:HB3	1:80:B:ILE:HG12	5	0.14
(1,1098)	1:59:B:ILE:HG22	1:42:B:ARG:HD3	8	0.14
(1,1094)	1:13:B:GLU:HA	1:86:A:LEU:HD21	1	0.14
(1,979)	1:86:A:LEU:HD22	1:48:A:PHE:HB3	8	0.14
(1,962)	1:21:B:GLN:HB3	1:22:B:TYR:HB2	6	0.14
(1,961)	1:21:A:GLN:HB3	1:22:A:TYR:HB2	6	0.14
(1,895)	1:81:A:MET:HB3	1:80:B:ILE:HG12	5	0.14
(1,894)	1:78:B:GLU:HB2	1:74:B:LEU:HB3	6	0.14
(1,893)	1:78:A:GLU:HB2	1:74:A:LEU:HB3	6	0.14
(1,805)	1:74:A:LEU:HG	1:73:A:GLN:HG2	6	0.14
(1,759)	1:99:A:GLU:HG3	1:99:A:GLU:HA	4	0.14
(1,742)	1:4:B:LYS:HA	1:4:B:LYS:HG2	7	0.14
(1,741)	1:4:A:LYS:HA	1:4:A:LYS:HG2	7	0.14
(1,682)	1:37:B:PHE:HB3	1:63:B:MET:H	5	0.14
(1,681)	1:37:A:PHE:HB3	1:63:A:MET:H	5	0.14
(1,580)	1:34:B:GLN:HG2	1:38:B:LYS:HD2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:33:B:ASN:HB2	1:34:B:GLN:HG2	10	0.14
(1,395)	1:33:A:ASN:HB2	1:34:A:GLN:HG2	10	0.14
(1,388)	1:7:B:GLN:HA	1:8:B:LEU:HD23	1	0.14
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG23	10	0.14
(1,56)	1:13:B:GLU:HG2	1:109:A:LEU:HD11	2	0.14
(1,37)	1:58:A:VAL:HG13	1:53:A:ASN:HA	6	0.14
(1,27)	1:58:A:VAL:HG13	1:53:A:ASN:HA	6	0.14
(4,64)	1:32:B:LEU:HG	1:31:B:THR:HB	1	0.13
(4,63)	1:32:A:LEU:HG	1:31:A:THR:HB	1	0.13
(4,62)	1:25:B:LYS:HA	1:21:B:GLN:HA	2	0.13
(4,62)	1:25:B:LYS:HA	1:21:B:GLN:HA	5	0.13
(4,61)	1:25:A:LYS:HA	1:21:A:GLN:HA	2	0.13
(3,1490)	1:103:B:HIS:H	1:101:B:PRO:HB2	6	0.13
(3,1489)	1:103:A:HIS:H	1:101:A:PRO:HB2	6	0.13
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD21	9	0.13
(3,1466)	1:110:B:GLY:H	1:108:B:GLY:HA2	10	0.13
(3,1465)	1:110:A:GLY:H	1:108:A:GLY:HA2	10	0.13
(3,1423)	1:84:A:ALA:H	1:80:B:ILE:HG22	7	0.13
(3,1382)	1:71:B:ASP:H	1:72:B:LYS:HE3	8	0.13
(3,1381)	1:71:A:ASP:H	1:72:A:LYS:HE3	8	0.13
(3,1380)	1:70:B:ALA:H	1:74:B:LEU:HD23	3	0.13
(3,1379)	1:70:A:ALA:H	1:74:A:LEU:HD23	3	0.13
(3,1363)	1:69:A:ASN:H	1:68:A:THR:HB	2	0.13
(3,1344)	1:66:B:LEU:H	1:66:B:LEU:HG	7	0.13
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	2	0.13
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	2	0.13
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	5	0.13
(3,1284)	1:57:B:LYS:H	1:58:B:VAL:HG22	5	0.13
(3,1283)	1:57:A:LYS:H	1:58:A:VAL:HG22	5	0.13
(3,871)	1:6:A:SER:H	1:5:A:MET:HG2	5	0.13
(3,864)	1:74:B:LEU:H	1:31:B:THR:HB	4	0.13
(3,780)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	5	0.13
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB3	1	0.13
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB3	2	0.13
(3,758)	1:86:B:LEU:HA	1:89:B:ALA:HB1	9	0.13
(3,757)	1:86:A:LEU:HA	1:89:A:ALA:HB1	9	0.13
(3,734)	1:77:B:GLU:HA	1:80:B:ILE:HG23	7	0.13
(3,733)	1:77:A:GLU:HA	1:80:A:ILE:HG23	7	0.13
(3,692)	1:32:B:LEU:HA	1:36:B:GLU:HB2	8	0.13
(3,691)	1:32:A:LEU:HA	1:36:A:GLU:HB2	8	0.13
(3,600)	1:53:B:ASN:HB2	1:46:B:GLN:HG3	9	0.13
(3,599)	1:53:A:ASN:HB2	1:46:A:GLN:HG3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,590)	1:87:B:THR:HA	1:87:B:THR:HG23	3	0.13
(3,590)	1:87:B:THR:HA	1:87:B:THR:HG22	8	0.13
(3,589)	1:87:A:THR:HA	1:87:A:THR:HG23	3	0.13
(3,589)	1:87:A:THR:HA	1:87:A:THR:HG22	8	0.13
(3,560)	1:34:B:GLN:HB2	1:63:B:MET:HG2	9	0.13
(3,559)	1:34:A:GLN:HB2	1:63:A:MET:HG2	9	0.13
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG23	1	0.13
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG23	8	0.13
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG23	1	0.13
(3,365)	1:85:A:ARG:HG3	1:77:B:GLU:HA	3	0.13
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB3	4	0.13
(3,340)	1:57:B:LYS:HG3	1:56:B:GLU:HB3	5	0.13
(3,340)	1:57:B:LYS:HG2	1:56:B:GLU:HB3	8	0.13
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB3	4	0.13
(3,339)	1:57:A:LYS:HG3	1:56:A:GLU:HB3	5	0.13
(3,266)	1:42:B:ARG:HB2	1:43:B:LYS:H	10	0.13
(3,265)	1:42:A:ARG:HB2	1:43:A:LYS:H	10	0.13
(3,80)	1:59:B:ILE:HB	1:38:B:LYS:HG2	10	0.13
(3,79)	1:59:A:ILE:HB	1:38:A:LYS:HG2	10	0.13
(3,64)	1:29:B:PRO:HA	1:24:B:VAL:HG21	9	0.13
(3,6)	1:73:B:GLN:HG3	1:72:B:LYS:HG2	5	0.13
(3,5)	1:73:A:GLN:HG3	1:72:A:LYS:HG2	5	0.13
(2,76)	1:89:A:ALA:H	1:85:A:ARG:O	5	0.13
(2,62)	1:81:A:MET:H	1:77:A:GLU:O	7	0.13
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	6	0.13
(2,42)	1:53:A:ASN:H	1:50:A:LYS:O	8	0.13
(2,21)	1:20:A:HIS:N	1:16:A:ILE:O	5	0.13
(2,4)	1:74:A:LEU:N	1:32:A:LEU:O	6	0.13
(1,1858)	1:110:B:GLY:H	1:111:B:GLU:HA	1	0.13
(1,1857)	1:110:A:GLY:H	1:111:A:GLU:HA	1	0.13
(1,1838)	1:73:B:GLN:H	1:72:B:LYS:HE3	6	0.13
(1,1776)	1:87:B:THR:H	1:83:B:MET:HE3	4	0.13
(1,1775)	1:87:A:THR:H	1:83:A:MET:HE3	4	0.13
(1,1770)	1:87:B:THR:H	1:82:B:LEU:HD13	2	0.13
(1,1769)	1:87:A:THR:H	1:82:A:LEU:HD13	2	0.13
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	2	0.13
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	5	0.13
(1,1652)	1:62:B:ILE:H	1:62:B:ILE:HD13	5	0.13
(1,1651)	1:62:A:ILE:H	1:62:A:ILE:HD13	5	0.13
(1,1496)	1:38:B:LYS:H	1:38:B:LYS:HD3	5	0.13
(1,1432)	1:23:B:SER:H	1:21:B:GLN:H	10	0.13
(1,1377)	1:18:A:THR:H	1:20:A:HIS:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1375)	1:17:A:ASN:H	1:12:A:ILE:HG21	10	0.13
(1,1370)	1:17:B:ASN:H	1:15:B:ILE:HG13	7	0.13
(1,1369)	1:17:A:ASN:H	1:15:A:ILE:HG13	7	0.13
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	1	0.13
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	1	0.13
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	9	0.13
(1,1276)	1:48:B:PHE:H	1:45:B:LEU:HG	5	0.13
(1,1275)	1:48:A:PHE:H	1:45:A:LEU:HG	5	0.13
(1,1097)	1:59:A:ILE:HG22	1:42:A:ARG:HD3	8	0.13
(1,1048)	1:53:B:ASN:HA	1:59:B:ILE:HA	9	0.13
(1,1047)	1:53:A:ASN:HA	1:59:A:ILE:HA	9	0.13
(1,806)	1:74:B:LEU:HG	1:73:B:GLN:HG2	1	0.13
(1,760)	1:99:B:GLU:HG3	1:99:B:GLU:HA	4	0.13
(1,760)	1:99:B:GLU:HG3	1:99:B:GLU:HA	8	0.13
(1,714)	1:21:B:GLN:HG3	1:40:B:LEU:HB2	5	0.13
(1,689)	1:107:A:PRO:HG3	1:112:A:GLY:HA3	7	0.13
(1,596)	1:85:B:ARG:HG3	1:62:B:ILE:HG22	6	0.13
(1,595)	1:85:A:ARG:HG3	1:62:A:ILE:HG22	6	0.13
(1,579)	1:34:A:GLN:HG2	1:38:A:LYS:HD2	4	0.13
(1,507)	1:11:A:ASN:HB3	1:15:B:ILE:HG13	5	0.13
(1,378)	1:34:B:GLN:HG3	1:63:B:MET:H	6	0.13
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG23	3	0.13
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG23	3	0.13
(1,140)	1:16:B:ILE:HD13	1:13:B:GLU:HG2	10	0.13
(1,139)	1:16:A:ILE:HD13	1:13:A:GLU:HG2	10	0.13
(1,137)	1:16:A:ILE:HD12	1:93:B:LYS:HE3	1	0.13
(1,94)	1:34:B:GLN:HG3	1:63:B:MET:H	6	0.13
(1,38)	1:58:B:VAL:HG13	1:53:B:ASN:HA	6	0.13
(1,28)	1:58:B:VAL:HG13	1:53:B:ASN:HA	6	0.13
(4,232)	1:79:B:PHE:H	1:80:B:ILE:HB	7	0.12
(4,231)	1:79:A:PHE:H	1:80:A:ILE:HB	7	0.12
(4,111)	1:76:A:PHE:H	1:31:A:THR:H	4	0.12
(4,61)	1:25:A:LYS:HA	1:21:A:GLN:HA	5	0.12
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD21	9	0.12
(3,1486)	1:73:B:GLN:H	1:74:B:LEU:HD22	10	0.12
(3,1479)	1:100:A:GLY:H	1:99:A:GLU:HB3	8	0.12
(3,1448)	1:88:B:TRP:H	1:77:A:GLU:HG3	1	0.12
(3,1364)	1:69:B:ASN:H	1:68:B:THR:HB	2	0.12
(3,1343)	1:66:A:LEU:H	1:66:A:LEU:HG	7	0.12
(3,1180)	1:67:B:ASP:H	1:72:B:LYS:HE3	6	0.12
(3,1179)	1:67:A:ASP:H	1:72:A:LYS:HE3	6	0.12
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	6	0.12
(3,1143)	1:33:A:ASN:H	1:32:A:LEU:HD23	7	0.12
(3,1124)	1:31:B:THR:H	1:23:B:SER:HA	7	0.12
(3,1123)	1:31:A:THR:H	1:23:A:SER:HA	7	0.12
(3,863)	1:74:A:LEU:H	1:31:A:THR:HB	4	0.12
(3,779)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	5	0.12
(3,680)	1:85:B:ARG:HG2	1:85:B:ARG:HA	7	0.12
(3,679)	1:85:A:ARG:HG2	1:85:A:ARG:HA	7	0.12
(3,664)	1:63:B:MET:HE1	1:72:B:LYS:HA	2	0.12
(3,663)	1:63:A:MET:HE1	1:72:A:LYS:HA	2	0.12
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	1	0.12
(3,630)	1:48:B:PHE:HB2	1:45:B:LEU:HA	10	0.12
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	10	0.12
(3,628)	1:48:B:PHE:HB2	1:9:A:GLU:HG3	6	0.12
(3,627)	1:48:A:PHE:HB2	1:9:B:GLU:HG3	6	0.12
(3,622)	1:36:B:GLU:HA	1:36:B:GLU:HB3	10	0.12
(3,621)	1:36:A:GLU:HA	1:36:A:GLU:HB3	10	0.12
(3,590)	1:87:B:THR:HA	1:87:B:THR:HG23	9	0.12
(3,589)	1:87:A:THR:HA	1:87:A:THR:HG23	9	0.12
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG23	8	0.12
(3,506)	1:74:B:LEU:HG	1:66:B:LEU:HB2	3	0.12
(3,505)	1:74:A:LEU:HG	1:66:A:LEU:HB2	3	0.12
(3,406)	1:5:B:MET:H	1:5:B:MET:HB2	2	0.12
(3,334)	1:86:B:LEU:HD13	1:48:B:PHE:HB3	3	0.12
(3,88)	1:34:B:GLN:HG2	1:38:B:LYS:HD2	2	0.12
(3,87)	1:34:A:GLN:HG2	1:38:A:LYS:HD2	2	0.12
(2,84)	1:93:A:LYS:H	1:89:A:ALA:O	8	0.12
(2,63)	1:82:A:LEU:N	1:78:A:GLU:O	1	0.12
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	4	0.12
(2,26)	1:22:A:TYR:H	1:18:A:THR:O	8	0.12
(2,21)	1:20:A:HIS:N	1:16:A:ILE:O	2	0.12
(2,2)	1:32:A:LEU:N	1:74:A:LEU:O	5	0.12
(1,1854)	1:5:B:MET:H	1:9:B:GLU:HG3	1	0.12
(1,1853)	1:5:A:MET:H	1:9:A:GLU:HG3	1	0.12
(1,1837)	1:73:A:GLN:H	1:72:A:LYS:HE3	6	0.12
(1,1834)	1:94:B:MET:H	1:90:B:SER:H	4	0.12
(1,1833)	1:94:A:MET:H	1:90:A:SER:H	4	0.12
(1,1700)	1:71:B:ASP:H	1:72:B:LYS:HG3	3	0.12
(1,1699)	1:71:A:ASP:H	1:72:A:LYS:HG3	3	0.12
(1,1696)	1:71:B:ASP:H	1:64:B:GLU:HG2	4	0.12
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	2	0.12
(1,1650)	1:68:B:THR:H	1:70:B:ALA:HB2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1649)	1:68:A:THR:H	1:70:A:ALA:HB2	4	0.12
(1,1530)	1:42:B:ARG:H	1:59:B:ILE:HD12	6	0.12
(1,1529)	1:42:A:ARG:H	1:59:A:ILE:HD12	6	0.12
(1,1495)	1:38:A:LYS:H	1:38:A:LYS:HD3	5	0.12
(1,1452)	1:45:B:LEU:H	1:40:B:LEU:HD12	1	0.12
(1,1451)	1:45:A:LEU:H	1:40:A:LEU:HD12	1	0.12
(1,1402)	1:20:B:HIS:H	1:87:A:THR:HG23	9	0.12
(1,1378)	1:18:B:THR:H	1:20:B:HIS:H	3	0.12
(1,1376)	1:17:B:ASN:H	1:12:B:ILE:HG21	10	0.12
(1,1270)	1:48:B:PHE:H	1:4:A:LYS:HE3	4	0.12
(1,1266)	1:77:B:GLU:H	1:84:A:ALA:HB1	7	0.12
(1,1150)	1:32:B:LEU:HG	1:40:B:LEU:HB2	3	0.12
(1,1149)	1:32:A:LEU:HG	1:40:A:LEU:HB2	3	0.12
(1,1100)	1:24:B:VAL:HG11	1:22:B:TYR:HB2	9	0.12
(1,1099)	1:24:A:VAL:HG11	1:22:A:TYR:HB2	9	0.12
(1,974)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	2	0.12
(1,973)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	2	0.12
(1,962)	1:21:B:GLN:HB2	1:22:B:TYR:HB2	2	0.12
(1,961)	1:21:A:GLN:HB2	1:22:A:TYR:HB2	2	0.12
(1,805)	1:74:A:LEU:HG	1:73:A:GLN:HG2	1	0.12
(1,759)	1:99:A:GLU:HG3	1:99:A:GLU:HA	8	0.12
(1,742)	1:81:B:MET:HA	1:84:B:ALA:HB2	9	0.12
(1,741)	1:81:A:MET:HA	1:84:A:ALA:HB2	9	0.12
(1,713)	1:21:A:GLN:HG3	1:40:A:LEU:HB2	5	0.12
(1,690)	1:107:B:PRO:HG3	1:112:B:GLY:HA3	7	0.12
(1,646)	1:86:B:LEU:HA	1:49:B:LEU:HA	5	0.12
(1,645)	1:86:A:LEU:HA	1:49:A:LEU:HA	5	0.12
(1,579)	1:34:A:GLN:HG2	1:38:A:LYS:HD2	6	0.12
(1,508)	1:11:B:ASN:HB3	1:15:A:ILE:HG13	5	0.12
(1,377)	1:34:A:GLN:HG3	1:63:A:MET:H	6	0.12
(1,372)	1:34:B:GLN:HG3	1:72:B:LYS:HE2	2	0.12
(1,371)	1:34:A:GLN:HG3	1:72:A:LYS:HE2	2	0.12
(1,286)	1:51:B:LYS:H	1:50:B:LYS:HG2	6	0.12
(1,285)	1:51:A:LYS:H	1:50:A:LYS:HG2	6	0.12
(1,156)	1:37:B:PHE:HA	1:59:B:ILE:HG22	8	0.12
(1,155)	1:37:A:PHE:HA	1:59:A:ILE:HG22	8	0.12
(1,116)	1:49:B:LEU:HG	1:45:B:LEU:H	6	0.12
(1,115)	1:49:A:LEU:HG	1:45:A:LEU:H	6	0.12
(1,93)	1:34:A:GLN:HG3	1:63:A:MET:H	6	0.12
(1,64)	1:74:B:LEU:HG	1:66:B:LEU:HB2	3	0.12
(1,63)	1:74:A:LEU:HG	1:66:A:LEU:HB2	3	0.12
(1,46)	1:39:B:GLU:HG2	1:44:B:ASP:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:39:A:GLU:HG2	1:44:A:ASP:H	4	0.12
(4,236)	1:81:B:MET:H	1:81:A:MET:H	7	0.11
(4,235)	1:81:A:MET:H	1:81:B:MET:H	7	0.11
(4,232)	1:79:B:PHE:H	1:80:B:ILE:HB	8	0.11
(4,231)	1:79:A:PHE:H	1:80:A:ILE:HB	8	0.11
(4,112)	1:76:B:PHE:H	1:31:B:THR:H	4	0.11
(4,64)	1:32:B:LEU:HG	1:31:B:THR:HB	2	0.11
(4,64)	1:32:B:LEU:HG	1:31:B:THR:HB	5	0.11
(4,63)	1:32:A:LEU:HG	1:31:A:THR:HB	2	0.11
(4,63)	1:32:A:LEU:HG	1:31:A:THR:HB	5	0.11
(4,10)	1:21:B:GLN:HA	1:17:B:ASN:HA	7	0.11
(4,9)	1:21:A:GLN:HA	1:17:A:ASN:HA	7	0.11
(3,1485)	1:73:A:GLN:H	1:74:A:LEU:HD22	10	0.11
(3,1480)	1:100:B:GLY:H	1:99:B:GLU:HB3	8	0.11
(3,1468)	1:110:B:GLY:H	1:48:B:PHE:HB2	3	0.11
(3,1467)	1:110:A:GLY:H	1:48:A:PHE:HB2	3	0.11
(3,1448)	1:88:B:TRP:H	1:77:A:GLU:HG2	4	0.11
(3,1429)	1:86:A:LEU:H	1:82:A:LEU:HD12	7	0.11
(3,1424)	1:84:B:ALA:H	1:80:A:ILE:HG22	7	0.11
(3,1382)	1:71:B:ASP:H	1:72:B:LYS:HE3	3	0.11
(3,1381)	1:71:A:ASP:H	1:72:A:LYS:HE3	3	0.11
(3,1344)	1:66:B:LEU:H	1:66:B:LEU:HG	1	0.11
(3,1343)	1:66:A:LEU:H	1:66:A:LEU:HG	1	0.11
(3,1319)	1:67:A:ASP:H	1:68:A:THR:H	1	0.11
(3,1279)	1:57:A:LYS:H	1:57:A:LYS:HD3	6	0.11
(3,1159)	1:82:A:LEU:H	1:84:A:ALA:H	2	0.11
(3,1144)	1:33:B:ASN:H	1:32:B:LEU:HD23	7	0.11
(3,948)	1:75:B:SER:H	1:78:B:GLU:H	7	0.11
(3,947)	1:75:A:SER:H	1:78:A:GLU:H	7	0.11
(3,942)	1:48:B:PHE:H	1:50:B:LYS:H	9	0.11
(3,822)	1:5:B:MET:HB3	1:7:B:GLN:H	10	0.11
(3,712)	1:11:B:ASN:HB2	1:8:B:LEU:HA	3	0.11
(3,711)	1:11:A:ASN:HB2	1:8:A:LEU:HA	3	0.11
(3,629)	1:48:A:PHE:HB2	1:45:A:LEU:HA	1	0.11
(3,590)	1:87:B:THR:HA	1:87:B:THR:HG22	10	0.11
(3,538)	1:15:B:ILE:HA	1:15:B:ILE:HG23	5	0.11
(3,537)	1:15:A:ILE:HA	1:15:A:ILE:HG23	5	0.11
(3,492)	1:59:B:ILE:HD11	1:52:B:GLU:HG2	8	0.11
(3,491)	1:59:A:ILE:HD11	1:52:A:GLU:HG2	8	0.11
(3,474)	1:77:B:GLU:HB2	1:76:B:PHE:HB2	7	0.11
(3,473)	1:77:A:GLU:HB2	1:76:A:PHE:HB2	7	0.11
(3,405)	1:5:A:MET:H	1:5:A:MET:HB2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,378)	1:25:B:LYS:HD3	1:32:B:LEU:HA	5	0.11
(3,333)	1:86:A:LEU:HD13	1:48:A:PHE:HB3	3	0.11
(3,246)	1:7:B:GLN:HG2	1:18:A:THR:HB	4	0.11
(3,220)	1:66:B:LEU:HD13	1:74:B:LEU:HA	5	0.11
(3,219)	1:66:A:LEU:HD13	1:74:A:LEU:HA	5	0.11
(3,200)	1:46:B:GLN:HB3	1:43:B:LYS:HA	10	0.11
(3,188)	1:51:B:LYS:H	1:50:B:LYS:HG2	6	0.11
(3,187)	1:51:A:LYS:H	1:50:A:LYS:HG2	6	0.11
(3,156)	1:34:B:GLN:HA	1:34:B:GLN:HG3	10	0.11
(3,155)	1:34:A:GLN:HA	1:34:A:GLN:HG3	10	0.11
(3,80)	1:59:B:ILE:HB	1:38:B:LYS:HG2	4	0.11
(3,79)	1:59:A:ILE:HB	1:38:A:LYS:HG2	4	0.11
(2,84)	1:93:A:LYS:H	1:89:A:ALA:O	3	0.11
(2,66)	1:83:A:MET:H	1:79:A:PHE:O	4	0.11
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	10	0.11
(2,42)	1:53:A:ASN:H	1:50:A:LYS:O	1	0.11
(2,42)	1:53:A:ASN:H	1:50:A:LYS:O	4	0.11
(2,42)	1:53:A:ASN:H	1:50:A:LYS:O	5	0.11
(2,21)	1:20:A:HIS:N	1:16:A:ILE:O	7	0.11
(2,4)	1:74:A:LEU:N	1:32:A:LEU:O	8	0.11
(2,2)	1:32:A:LEU:N	1:74:A:LEU:O	3	0.11
(1,1791)	1:93:A:LYS:H	1:109:A:LEU:HD22	2	0.11
(1,1760)	1:24:B:VAL:H	1:25:B:LYS:HG3	2	0.11
(1,1759)	1:24:A:VAL:H	1:25:A:LYS:HG3	2	0.11
(1,1736)	1:82:B:LEU:H	1:86:B:LEU:H	2	0.11
(1,1735)	1:82:A:LEU:H	1:86:A:LEU:H	2	0.11
(1,1700)	1:71:B:ASP:H	1:72:B:LYS:HG3	10	0.11
(1,1699)	1:71:A:ASP:H	1:72:A:LYS:HG3	10	0.11
(1,1695)	1:71:A:ASP:H	1:64:A:GLU:HG2	4	0.11
(1,1446)	1:24:B:VAL:H	1:25:B:LYS:HG3	2	0.11
(1,1445)	1:24:A:VAL:H	1:25:A:LYS:HG3	2	0.11
(1,1438)	1:24:B:VAL:H	1:25:B:LYS:HG3	2	0.11
(1,1437)	1:24:A:VAL:H	1:25:A:LYS:HG3	2	0.11
(1,1436)	1:23:B:SER:H	1:19:B:PHE:H	10	0.11
(1,1401)	1:20:A:HIS:H	1:87:B:THR:HG23	9	0.11
(1,1384)	1:18:B:THR:H	1:16:B:ILE:HG13	3	0.11
(1,1383)	1:18:A:THR:H	1:16:A:ILE:HG13	3	0.11
(1,1369)	1:17:A:ASN:H	1:15:A:ILE:HG13	8	0.11
(1,1304)	1:9:B:GLU:H	1:11:B:ASN:H	8	0.11
(1,1303)	1:9:A:GLU:H	1:11:A:ASN:H	8	0.11
(1,1296)	1:8:B:LEU:H	1:12:B:ILE:HD12	9	0.11
(1,1295)	1:8:A:LEU:H	1:12:A:ILE:HD12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:48:B:PHE:H	1:45:B:LEU:HG	10	0.11
(1,1275)	1:48:A:PHE:H	1:45:A:LEU:HG	10	0.11
(1,1146)	1:32:B:LEU:HG	1:31:B:THR:HG23	6	0.11
(1,1145)	1:32:A:LEU:HG	1:31:A:THR:HG23	6	0.11
(1,1100)	1:24:B:VAL:HG12	1:22:B:TYR:HB2	7	0.11
(1,1099)	1:24:A:VAL:HG12	1:22:A:TYR:HB2	7	0.11
(1,1054)	1:31:B:THR:HG21	1:71:B:ASP:HB2	2	0.11
(1,1028)	1:84:B:ALA:HA	1:86:B:LEU:HG	1	0.11
(1,1028)	1:84:B:ALA:HA	1:86:B:LEU:HG	6	0.11
(1,1027)	1:84:A:ALA:HA	1:86:A:LEU:HG	1	0.11
(1,1027)	1:84:A:ALA:HA	1:86:A:LEU:HG	6	0.11
(1,950)	1:86:B:LEU:HA	1:88:B:TRP:HB3	3	0.11
(1,949)	1:86:A:LEU:HA	1:88:A:TRP:HB3	3	0.11
(1,922)	1:87:B:THR:HA	1:13:A:GLU:HG2	2	0.11
(1,630)	1:84:B:ALA:HA	1:86:B:LEU:HG	1	0.11
(1,630)	1:84:B:ALA:HA	1:86:B:LEU:HG	6	0.11
(1,629)	1:84:A:ALA:HA	1:86:A:LEU:HG	1	0.11
(1,629)	1:84:A:ALA:HA	1:86:A:LEU:HG	6	0.11
(1,622)	1:21:B:GLN:HA	1:17:B:ASN:HA	7	0.11
(1,621)	1:21:A:GLN:HA	1:17:A:ASN:HA	7	0.11
(1,580)	1:34:B:GLN:HG2	1:38:B:LYS:HD2	6	0.11
(1,480)	1:63:B:MET:HB2	1:62:B:ILE:HD12	3	0.11
(1,479)	1:63:A:MET:HB2	1:62:A:ILE:HD12	3	0.11
(1,378)	1:34:B:GLN:HG3	1:63:B:MET:H	1	0.11
(1,110)	1:7:B:GLN:HG3	1:15:A:ILE:HG12	8	0.11
(1,109)	1:7:A:GLN:HG3	1:15:B:ILE:HG12	8	0.11
(1,96)	1:7:B:GLN:HG2	1:18:A:THR:HB	4	0.11
(1,94)	1:34:B:GLN:HG3	1:63:B:MET:H	1	0.11
(4,236)	1:81:B:MET:H	1:81:A:MET:H	10	0.1
(4,235)	1:81:A:MET:H	1:81:B:MET:H	10	0.1
(4,112)	1:76:B:PHE:H	1:31:B:THR:H	8	0.1
(4,111)	1:76:A:PHE:H	1:31:A:THR:H	8	0.1
(4,53)	1:84:A:ALA:HA	1:76:B:PHE:HA	7	0.1
(4,12)	1:98:B:ASP:HA	1:96:B:GLU:HA	3	0.1
(3,1447)	1:88:A:TRP:H	1:77:B:GLU:HG3	1	0.1
(3,1432)	1:86:B:LEU:H	1:16:A:ILE:HD11	3	0.1
(3,1430)	1:86:B:LEU:H	1:82:B:LEU:HD12	7	0.1
(3,1343)	1:66:A:LEU:H	1:66:A:LEU:HG	8	0.1
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	1	0.1
(3,1320)	1:67:B:ASP:H	1:68:B:THR:H	9	0.1
(3,1280)	1:57:B:LYS:H	1:57:B:LYS:HD3	6	0.1
(3,1160)	1:82:B:LEU:H	1:84:B:ALA:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,942)	1:48:B:PHE:H	1:50:B:LYS:H	1	0.1
(3,942)	1:48:B:PHE:H	1:50:B:LYS:H	2	0.1
(3,941)	1:48:A:PHE:H	1:50:A:LYS:H	1	0.1
(3,941)	1:48:A:PHE:H	1:50:A:LYS:H	2	0.1
(3,941)	1:48:A:PHE:H	1:50:A:LYS:H	9	0.1
(3,821)	1:5:A:MET:HB3	1:7:A:GLN:H	10	0.1
(3,777)	1:21:A:GLN:HG2	1:32:A:LEU:HD21	6	0.1
(3,659)	1:72:A:LYS:HB3	1:64:A:GLU:HA	9	0.1
(3,589)	1:87:A:THR:HA	1:87:A:THR:HG22	10	0.1
(3,377)	1:25:A:LYS:HD3	1:32:A:LEU:HA	5	0.1
(3,265)	1:42:A:ARG:HB3	1:43:A:LYS:H	5	0.1
(3,225)	1:66:A:LEU:HD21	1:82:A:LEU:HA	8	0.1
(3,200)	1:46:B:GLN:HB3	1:43:B:LYS:HA	5	0.1
(3,199)	1:46:A:GLN:HB3	1:43:A:LYS:HA	10	0.1
(3,147)	1:60:A:GLU:HG3	1:56:A:GLU:H	3	0.1
(2,76)	1:89:A:ALA:H	1:85:A:ARG:O	1	0.1
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	1	0.1
(2,58)	1:66:A:LEU:H	1:62:A:ILE:O	8	0.1
(2,37)	1:42:A:ARG:N	1:38:A:LYS:O	7	0.1
(2,26)	1:22:A:TYR:H	1:18:A:THR:O	4	0.1
(2,2)	1:32:A:LEU:N	1:74:A:LEU:O	4	0.1
(2,2)	1:32:A:LEU:N	1:74:A:LEU:O	7	0.1
(1,1792)	1:93:B:LYS:H	1:109:B:LEU:HD22	2	0.1
(1,1770)	1:87:B:THR:H	1:82:B:LEU:HD13	6	0.1
(1,1769)	1:87:A:THR:H	1:82:A:LEU:HD13	6	0.1
(1,1769)	1:87:A:THR:H	1:82:A:LEU:HD11	9	0.1
(1,1692)	1:67:B:ASP:H	1:68:B:THR:H	1	0.1
(1,1691)	1:67:A:ASP:H	1:68:A:THR:H	1	0.1
(1,1540)	1:42:B:ARG:H	1:40:B:LEU:H	5	0.1
(1,1495)	1:38:A:LYS:H	1:38:A:LYS:HD3	1	0.1
(1,1435)	1:23:A:SER:H	1:19:A:PHE:H	10	0.1
(1,1370)	1:17:B:ASN:H	1:15:B:ILE:HG13	8	0.1
(1,1368)	1:93:B:LYS:H	1:109:B:LEU:HD22	2	0.1
(1,1367)	1:93:A:LYS:H	1:109:A:LEU:HD22	2	0.1
(1,1355)	1:16:A:ILE:H	1:87:B:THR:HA	2	0.1
(1,1284)	1:75:B:SER:H	1:32:B:LEU:HB2	7	0.1
(1,1283)	1:75:A:SER:H	1:32:A:LEU:HB2	7	0.1
(1,1100)	1:24:B:VAL:HG11	1:22:B:TYR:HB2	2	0.1
(1,1099)	1:24:A:VAL:HG11	1:22:A:TYR:HB2	2	0.1
(1,1098)	1:59:B:ILE:HG23	1:42:B:ARG:HD2	10	0.1
(1,1097)	1:59:A:ILE:HG23	1:42:A:ARG:HD2	10	0.1
(1,1053)	1:31:A:THR:HG21	1:71:A:ASP:HB2	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,961)	1:21:A:GLN:HB2	1:22:A:TYR:HB2	9	0.1
(1,715)	1:21:A:GLN:HG2	1:32:A:LEU:HD21	6	0.1
(1,684)	1:42:B:ARG:HA	1:50:B:LYS:HA	8	0.1
(1,683)	1:42:A:ARG:HA	1:50:A:LYS:HA	8	0.1
(1,377)	1:34:A:GLN:HG3	1:63:A:MET:H	1	0.1
(1,93)	1:34:A:GLN:HG3	1:63:A:MET:H	1	0.1

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

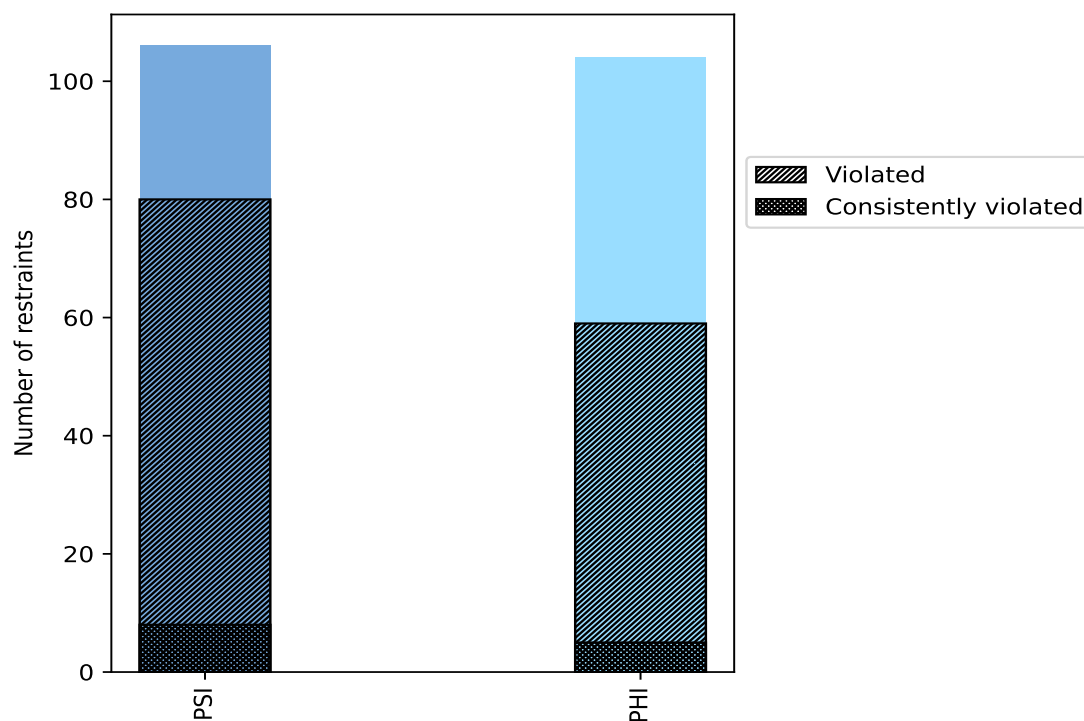
10.1 Summary of dihedral-angle violations [i](#)

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	106	50.5	80	75.5	38.1	8	7.5	3.8
PHI	104	49.5	59	56.7	28.1	5	4.8	2.4
Total	210	100.0	139	66.2	66.2	13	6.2	6.2

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

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



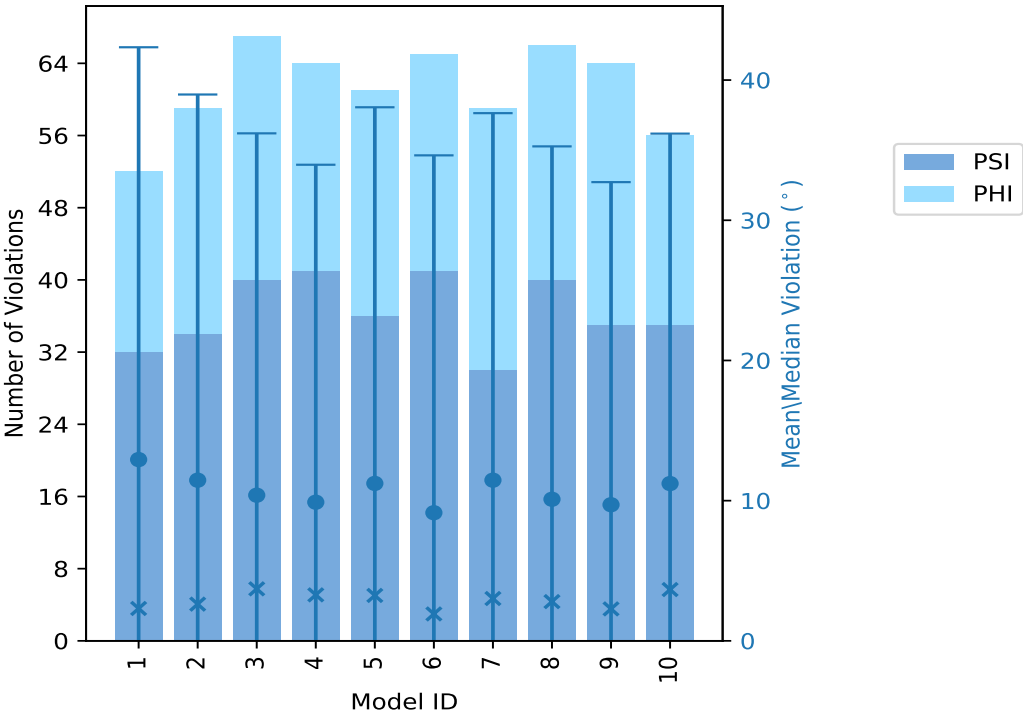
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	32	20	52	12.93	146.94	29.41	2.31
2	34	25	59	11.46	141.66	27.51	2.62
3	40	27	67	10.39	158.81	25.81	3.71
4	41	23	64	9.89	129.05	24.07	3.28
5	36	25	61	11.23	145.76	26.83	3.24
6	41	24	65	9.14	153.85	25.49	1.92
7	30	29	59	11.46	124.72	26.18	3.02
8	40	26	66	10.1	129.25	25.17	2.8
9	35	29	64	9.71	124.0	23.01	2.28
10	35	21	56	11.22	123.27	24.96	3.66

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

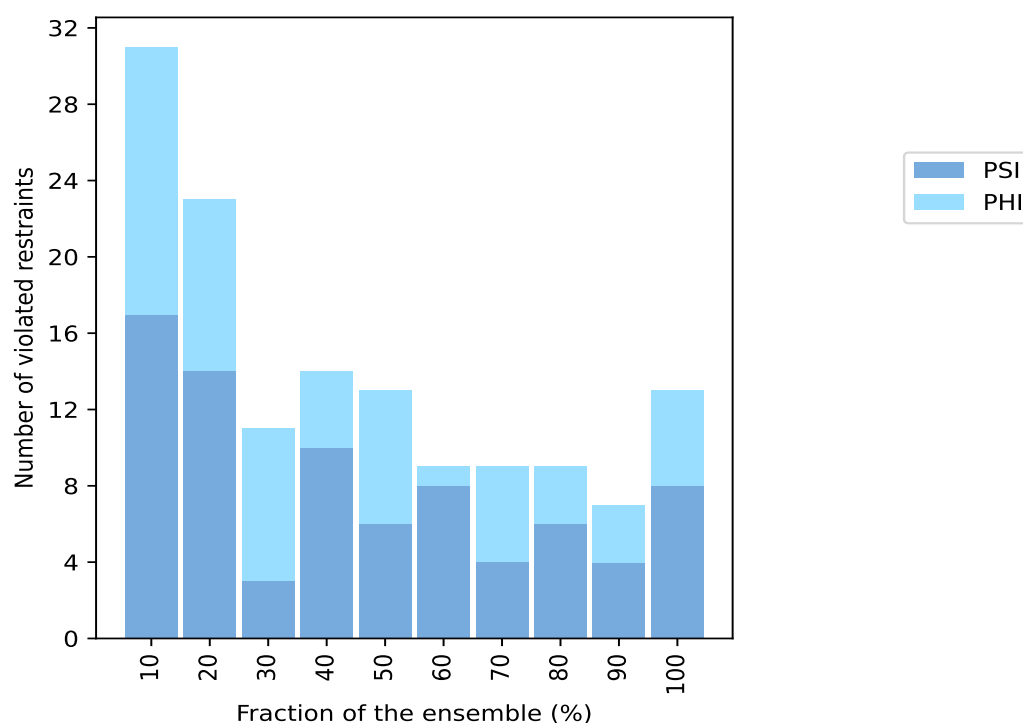
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
17	14	31	1	10.0
14	9	23	2	20.0
3	8	11	3	30.0
10	4	14	4	40.0
6	7	13	5	50.0
8	1	9	6	60.0
4	5	9	7	70.0
6	3	9	8	80.0
4	3	7	9	90.0
8	5	13	10	100.0

¹ Number of models with violations

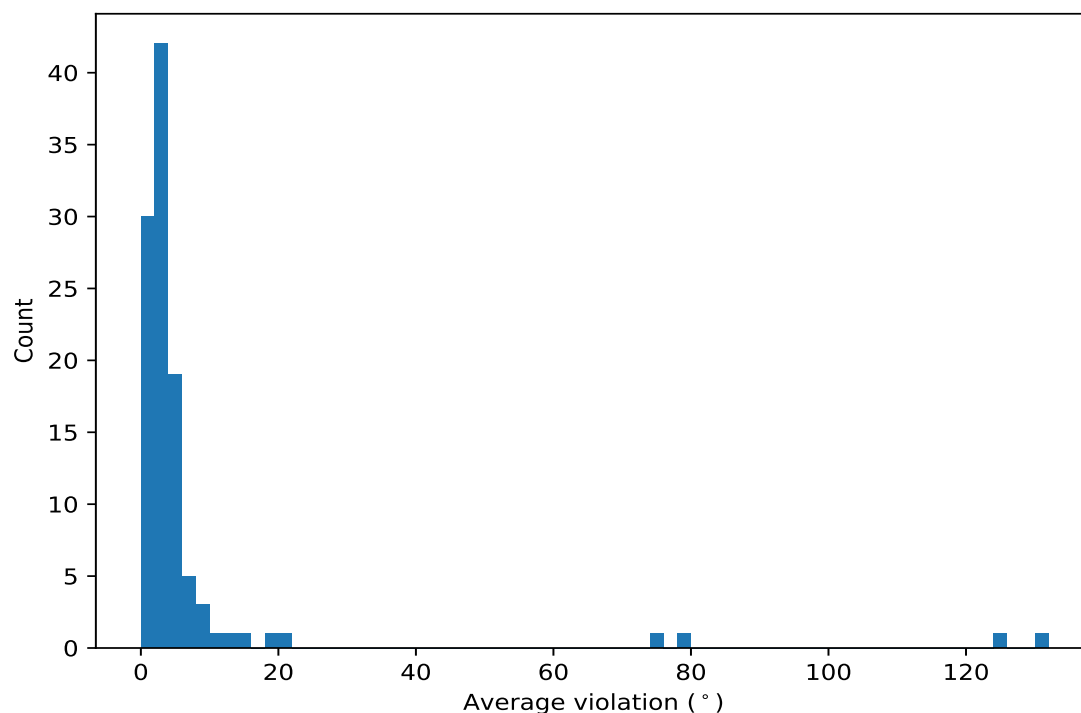
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	10	131.99	18.56	134.61
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	10	125.32	3.31	125.43
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	10	74.63	15.89	66.35
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	10	10.38	1.04	10.47
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	10	9.9	7.0	7.43
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	10	8.4	4.92	8.61
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	10	8.32	1.46	7.81
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	10	7.63	5.43	5.66
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	10	5.16	2.46	5.35
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	10	4.52	1.91	5.08
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	10	4.48	0.99	4.88
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	10	3.47	0.95	3.39
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	10	2.96	1.63	2.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	9	79.65	25.31	88.06
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	9	5.83	1.99	5.92
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	9	4.38	2.21	4.11
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	9	4.08	2.06	3.97
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	9	3.99	1.76	4.28
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	9	3.61	1.49	3.28
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	9	2.51	0.7	2.49
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	8	15.7	1.26	15.66
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	8	12.75	0.61	12.74
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	8	7.52	6.01	5.6
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	8	4.07	1.97	4.66
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	8	3.44	1.14	3.56
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	8	3.32	0.91	3.4
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	8	2.13	0.47	2.06
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	8	1.98	0.45	1.88
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	8	1.72	0.46	1.56
(1,190)	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	1:104:A:HIS:N	7	6.0	3.41	5.5
(1,198)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLY:N	7	5.11	2.83	5.38
(1,191)	1:103:A:HIS:C	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	7	4.95	3.98	3.61
(1,187)	1:101:A:PRO:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	7	4.65	2.7	6.1
(1,189)	1:102:A:GLY:C	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	7	2.91	1.1	2.43
(1,85)	1:49:A:LEU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	7	2.72	1.11	2.52
(1,52)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ASN:N	7	2.61	1.14	2.13
(1,53)	1:32:A:LEU:C	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	7	2.44	0.8	2.37
(1,96)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:GLU:N	7	2.05	0.91	1.7
(1,200)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:LEU:N	6	20.92	15.3	21.22
(1,180)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:GLU:N	6	7.56	5.5	6.6
(1,176)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:GLY:N	6	5.33	2.62	4.2
(1,185)	1:100:A:GLY:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	6	4.56	2.92	3.38
(1,204)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLU:N	6	3.76	3.43	2.41
(1,6)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:LEU:N	6	2.91	0.98	3.24
(1,4)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:GLN:N	6	2.86	1.23	3.03
(1,160)	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	1:89:A:ALA:N	6	2.23	0.74	2.06
(1,105)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:HIS:N	6	2.02	0.42	1.96
(1,201)	1:108:A:GLY:C	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	5	19.5	12.48	27.06
(1,184)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:PRO:N	5	6.05	3.47	6.24
(1,181)	1:98:A:ASP:C	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	5	5.76	2.66	4.05
(1,193)	1:104:A:HIS:C	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	5	4.27	3.27	3.46
(1,136)	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	1:77:A:GLU:N	5	3.2	1.88	2.34
(1,132)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	1:75:A:SER:N	5	2.99	0.65	3.24
(1,194)	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	1:106:A:LYS:N	5	2.9	1.48	2.0
(1,170)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:MET:N	5	2.63	1.28	2.21
(1,121)	1:68:A:THR:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	5	2.49	0.83	2.3
(1,43)	1:25:A:LYS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	5	2.35	0.92	2.33
(1,89)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	5	2.31	0.81	2.29
(1,92)	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	1:54:A:LYS:N	5	1.73	0.75	1.4
(1,5)	1:6:A:SER:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	5	1.73	0.59	1.64
(1,192)	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	1:105:A:HIS:N	4	5.57	3.29	4.72
(1,48)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:THR:N	4	3.64	2.55	2.84
(1,75)	1:44:A:ASP:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	4	3.37	0.38	3.38
(1,169)	1:92:A:GLU:C	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	4	3.06	2.24	1.97

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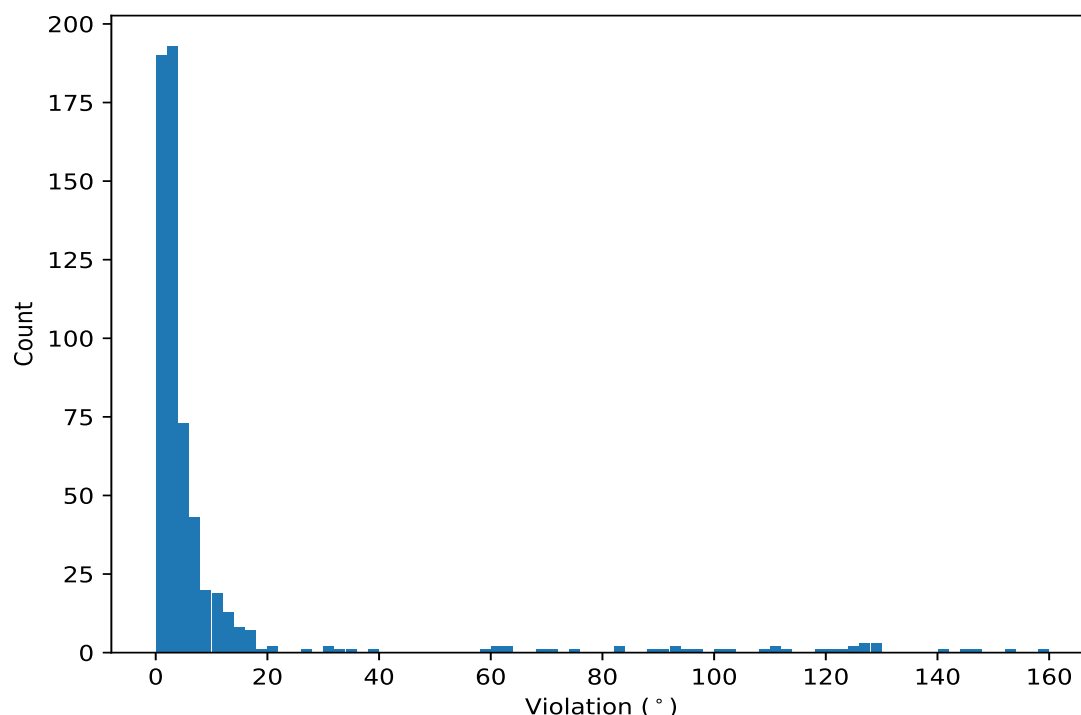
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,188)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:HIS:N	4	2.62	0.66	2.84
(1,142)	1:79:A:PHE:N	1:79:A:PHE:CA	1:79:A:PHE:C	1:80:A:ILE:N	4	2.48	0.5	2.44
(1,74)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:LEU:N	4	2.31	0.51	2.34
(1,35)	1:21:A:GLN:C	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	4	1.64	0.43	1.48
(1,109)	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	1:63:A:MET:N	4	1.6	0.32	1.46
(1,34)	1:21:A:GLN:N	1:21:A:GLN:CA	1:21:A:GLN:C	1:22:A:TYR:N	4	1.57	0.34	1.47
(1,10)	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	1:10:A:ARG:N	4	1.44	0.36	1.42
(1,90)	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1:53:A:ASN:N	4	1.41	0.43	1.17
(1,40)	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	1:25:A:LYS:N	4	1.4	0.37	1.25
(1,57)	1:34:A:GLN:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	4	1.3	0.15	1.32
(1,173)	1:94:A:MET:C	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	3	4.12	2.26	2.87
(1,177)	1:96:A:GLU:C	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	3	4.07	3.16	2.67
(1,182)	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	1:100:A:GLY:N	3	3.77	1.84	3.15
(1,162)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:SER:N	3	3.34	2.14	2.67
(1,135)	1:75:A:SER:C	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	3	3.02	1.79	2.2
(1,18)	1:13:A:GLU:N	1:13:A:GLU:CA	1:13:A:GLU:C	1:14:A:THR:N	3	2.8	1.18	3.01
(1,195)	1:105:A:HIS:C	1:106:A:LYS:N	1:106:A:LYS:CA	1:106:A:LYS:C	3	2.51	0.51	2.17
(1,157)	1:86:A:LEU:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	3	1.69	0.46	1.89
(1,159)	1:87:A:THR:C	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	3	1.68	0.17	1.56
(1,127)	1:71:A:ASP:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	3	1.5	0.23	1.38
(1,31)	1:19:A:PHE:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	3	1.45	0.17	1.42
(1,164)	1:90:A:SER:N	1:90:A:SER:CA	1:90:A:SER:C	1:91:A:HIS:N	2	5.1	3.25	5.1
(1,205)	1:110:A:GLY:C	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	2	5.08	3.94	5.08
(1,117)	1:66:A:LEU:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	2	3.42	1.48	3.42
(1,8)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:GLU:N	2	2.95	1.81	2.95
(1,32)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:GLN:N	2	2.68	0.5	2.68
(1,119)	1:67:A:ASP:C	1:68:A:THR:N	1:68:A:THR:CA	1:68:A:THR:C	2	2.33	0.53	2.33
(1,171)	1:93:A:LYS:C	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	2	2.16	1.1	2.16
(1,16)	1:12:A:ILE:N	1:12:A:ILE:CA	1:12:A:ILE:C	1:13:A:GLU:N	2	2.04	0.47	2.04
(1,209)	1:112:A:GLY:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	2	1.86	0.09	1.86
(1,129)	1:72:A:LYS:C	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	2	1.82	0.25	1.82
(1,124)	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	1:71:A:ASP:N	2	1.79	0.69	1.79
(1,51)	1:31:A:THR:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	2	1.74	0.62	1.74
(1,116)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:ASP:N	2	1.71	0.19	1.71
(1,210)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:PRO:N	2	1.7	0.32	1.7
(1,80)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:PHE:N	2	1.66	0.48	1.66
(1,28)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:PHE:N	2	1.55	0.54	1.55
(1,88)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:GLU:N	2	1.54	0.54	1.54
(1,42)	1:25:A:LYS:N	1:25:A:LYS:CA	1:25:A:LYS:C	1:26:A:LEU:N	2	1.5	0.2	1.5
(1,120)	1:68:A:THR:N	1:68:A:THR:CA	1:68:A:THR:C	1:69:A:ASN:N	2	1.43	0.11	1.43
(1,61)	1:36:A:GLU:C	1:37:A:PHE:N	1:37:A:PHE:CA	1:37:A:PHE:C	2	1.38	0.31	1.38
(1,44)	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	1:27:A:GLY:N	2	1.25	0.07	1.25
(1,111)	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	1:64:A:GLU:N	2	1.2	0.04	1.2
(1,19)	1:13:A:GLU:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	2	1.04	0.04	1.04

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 (°)
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	3	158.81
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	6	153.85
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	1	146.94
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	5	145.76
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	2	141.66
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	6	129.82
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	8	129.25
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	4	129.05
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	4	127.56
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	1	126.28
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	2	126.14
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	7	124.72
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	9	124.0
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	10	123.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	5	121.37
(1,166)	1:91:A:HIS:N	1:91:A:HIS:CA	1:91:A:HIS:C	1:92:A:GLU:N	3	119.29
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	7	113.43
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	8	111.94
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	10	111.44
(1,172)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:HIS:N	9	108.49
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	7	102.82
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	5	100.65
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	8	97.47
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	2	94.24
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	9	92.96
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	1	92.42
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	8	91.69
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	10	88.06
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	3	83.96
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	7	83.91
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	2	75.12
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	4	70.18
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	10	69.38
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	6	63.33
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	4	62.58
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	1	61.75
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	5	61.1
(1,174)	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	1:96:A:GLU:N	3	59.75
(1,200)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:LEU:N	1	39.33
(1,200)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:LEU:N	9	35.37
(1,200)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:LEU:N	6	33.2
(1,201)	1:108:A:GLY:C	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1	31.18
(1,201)	1:108:A:GLY:C	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	9	30.54
(1,201)	1:108:A:GLY:C	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	6	27.06
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	9	21.37
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	7	20.0
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	6	19.36
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1	17.62
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	10	17.11
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	6	16.54
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	5	16.54
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	2	16.37
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	9	16.24
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	2	16.07
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	9	15.92
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	7	15.72
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	4	15.24
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	7	14.78
(1,180)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:GLU:N	7	14.73
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	8	14.28
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	4	14.11
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1	14.06
(1,49)	1:30:A:ASP:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	3	13.93
(1,191)	1:103:A:HIS:C	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	2	13.51
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	10	13.51

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,180)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:GLU:N	10	13.4
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	9	13.2
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	5	12.95
(1,190)	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	1:104:A:HIS:N	2	12.92
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	10	12.88
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	3	12.84
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	7	12.63
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	2	12.37
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	8	12.34
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	9	12.25
(1,47)	1:29:A:PRO:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1	11.91
(1,46)	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1:30:A:ASP:N	6	11.77
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	3	11.76
(1,204)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLU:N	7	11.41
(1,184)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:PRO:N	4	11.41
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	6	11.4
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	2	11.1
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	5	10.84
(1,192)	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	1:105:A:HIS:N	5	10.68
(1,180)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:GLU:N	9	10.65
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	8	10.56
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	1	10.54
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	4	10.5
(1,193)	1:104:A:HIS:C	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	5	10.39
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	1	10.38
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	7	10.3
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	9	10.13
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	2	10.03
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	7	10.0
(1,181)	1:98:A:ASP:C	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	10	9.93
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	2	9.91
(1,185)	1:100:A:GLY:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	3	9.88
(1,176)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:GLY:N	8	9.65
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	3	9.52
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	3	9.52
(1,198)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLY:N	5	9.45
(1,200)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:LEU:N	5	9.24
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	4	9.18
(1,205)	1:110:A:GLY:C	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	7	9.03
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	10	8.96
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	5	8.91
(1,112)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:ASP:N	10	8.58
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	7	8.49
(1,177)	1:96:A:GLU:C	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	10	8.44
(1,164)	1:90:A:SER:N	1:90:A:SER:CA	1:90:A:SER:C	1:91:A:HIS:N	3	8.35
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	2	8.33
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	3	8.1
(1,176)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:GLY:N	10	8.04
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	8	8.02
(1,187)	1:101:A:PRO:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	4	7.95
(1,184)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:PRO:N	3	7.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	8	7.88
(1,181)	1:98:A:ASP:C	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	7	7.88
(1,198)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLY:N	3	7.85
(1,48)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:THR:N	9	7.84
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	2	7.63
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	4	7.6
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	5	7.58
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	10	7.51
(1,190)	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	1:104:A:HIS:N	4	7.49
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	3	7.33
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	8	7.31
(1,173)	1:94:A:MET:C	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	3	7.29
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	10	7.21
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	8	7.15
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	4	7.15
(1,187)	1:101:A:PRO:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	2	7.14
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	4	6.98
(1,169)	1:92:A:GLU:C	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	3	6.93
(1,190)	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	1:104:A:HIS:N	5	6.9
(1,185)	1:100:A:GLY:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	4	6.88
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1	6.82
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	4	6.76
(1,198)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLY:N	8	6.63
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	3	6.62
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	10	6.58
(1,187)	1:101:A:PRO:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	5	6.57
(1,191)	1:103:A:HIS:C	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	4	6.49
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	1	6.46
(1,200)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:LEU:N	3	6.36
(1,76)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:GLN:N	6	6.34
(1,136)	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	1:77:A:GLU:N	8	6.32
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	8	6.28
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	3	6.28
(1,182)	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	1:100:A:GLY:N	10	6.27
(1,184)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:PRO:N	8	6.24
(1,162)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:SER:N	3	6.23
(1,192)	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	1:105:A:HIS:N	10	6.16
(1,187)	1:101:A:PRO:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	8	6.1
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	10	6.09
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	5	6.04
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	2	6.0
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	5	5.98
(1,191)	1:103:A:HIS:C	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	5	5.96
(1,201)	1:108:A:GLY:C	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	5	5.95
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	2	5.92
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	6	5.9
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	6	5.88
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	7	5.73
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	5	5.66
(1,194)	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	1:106:A:LYS:N	9	5.65
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	1	5.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	3	5.62
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	5	5.59
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	3	5.59
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	5	5.57
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	6	5.55
(1,190)	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	1:104:A:HIS:N	3	5.5
(1,135)	1:75:A:SER:C	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	8	5.5
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	4	5.5
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	1	5.5
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	3	5.49
(1,158)	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	1:88:A:TRP:N	3	5.46
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	5	5.43
(1,198)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLY:N	2	5.38
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	7	5.37
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	8	5.35
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	7	5.34
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	7	5.2
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	5	5.2
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1	5.15
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	4	5.15
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	8	5.15
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	2	4.99
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	9	4.99
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	8	4.95
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	2	4.91
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	8	4.9
(1,117)	1:66:A:LEU:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	3	4.9
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	5	4.9
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	8	4.87
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	4	4.83
(1,189)	1:102:A:GLY:C	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	5	4.78
(1,85)	1:49:A:LEU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	5	4.78
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	8	4.78
(1,8)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:GLU:N	10	4.76
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	2	4.75
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	4	4.68
(1,176)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:GLY:N	9	4.68
(1,52)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ASN:N	4	4.68
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	10	4.62
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	9	4.6
(1,190)	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	1:104:A:HIS:N	10	4.57
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	9	4.53
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	9	4.46
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	7	4.44
(1,193)	1:104:A:HIS:C	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	10	4.43
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	5	4.41
(1,170)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:MET:N	3	4.4
(1,4)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:GLN:N	10	4.4
(1,136)	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	1:77:A:GLU:N	3	4.38
(1,189)	1:102:A:GLY:C	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	8	4.32
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	9	4.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	2	4.28
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1	4.23
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	10	4.21
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	1	4.14
(1,96)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:GLU:N	3	4.12
(1,18)	1:13:A:GLU:N	1:13:A:GLU:CA	1:13:A:GLU:C	1:14:A:THR:N	8	4.12
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	4	4.11
(1,4)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:GLN:N	4	4.11
(1,181)	1:98:A:ASP:C	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	9	4.05
(1,175)	1:95:A:HIS:C	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	3	4.05
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	4	4.04
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	4	4.0
(1,6)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:LEU:N	6	3.98
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	10	3.97
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	1	3.97
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	2	3.96
(1,75)	1:44:A:ASP:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	9	3.88
(1,185)	1:100:A:GLY:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	5	3.87
(1,170)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:MET:N	9	3.86
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	4	3.84
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	10	3.82
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	10	3.8
(1,132)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	1:75:A:SER:N	4	3.78
(1,43)	1:25:A:LYS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	9	3.77
(1,160)	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	1:89:A:ALA:N	9	3.76
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	3	3.74
(1,181)	1:98:A:ASP:C	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	3	3.73
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	8	3.73
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	6	3.72
(1,176)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:GLY:N	3	3.71
(1,85)	1:49:A:LEU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	7	3.7
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	3	3.64
(1,6)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:LEU:N	4	3.64
(1,176)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:GLY:N	7	3.62
(1,191)	1:103:A:HIS:C	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	3	3.61
(1,167)	1:91:A:HIS:C	1:92:A:GLU:N	1:92:A:GLU:CA	1:92:A:GLU:C	3	3.61
(1,6)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:LEU:N	1	3.61
(1,121)	1:68:A:THR:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	4	3.57
(1,53)	1:32:A:LEU:C	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	7	3.56
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	2	3.55
(1,89)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	4	3.52
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	10	3.52
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	8	3.51
(1,53)	1:32:A:LEU:C	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	3	3.51
(1,75)	1:44:A:ASP:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	3	3.5
(1,52)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ASN:N	1	3.49
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	6	3.48
(1,132)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	1:75:A:SER:N	1	3.47
(1,193)	1:104:A:HIS:C	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	7	3.46
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	3	3.4
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	7	3.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	8	3.38
(1,194)	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	1:106:A:LYS:N	6	3.29
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	4	3.28
(1,192)	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	1:105:A:HIS:N	2	3.28
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	4	3.28
(1,188)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:HIS:N	8	3.27
(1,171)	1:93:A:LYS:C	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	5	3.27
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	7	3.26
(1,75)	1:44:A:ASP:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	2	3.26
(1,48)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:THR:N	6	3.26
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	7	3.25
(1,132)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	1:75:A:SER:N	5	3.24
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	1	3.24
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	4	3.24
(1,195)	1:105:A:HIS:C	1:106:A:LYS:N	1:106:A:LYS:CA	1:106:A:LYS:C	6	3.23
(1,181)	1:98:A:ASP:C	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	5	3.23
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	7	3.23
(1,121)	1:68:A:THR:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	9	3.22
(1,142)	1:79:A:PHE:N	1:79:A:PHE:CA	1:79:A:PHE:C	1:80:A:ILE:N	10	3.19
(1,32)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:GLN:N	4	3.18
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	8	3.16
(1,182)	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	1:100:A:GLY:N	2	3.15
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	10	3.14
(1,52)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ASN:N	6	3.13
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	7	3.12
(1,4)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:GLN:N	8	3.08
(1,92)	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	1:54:A:LYS:N	6	3.06
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	6	3.05
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	9	3.04
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	7	3.02
(1,18)	1:13:A:GLU:N	1:13:A:GLU:CA	1:13:A:GLU:C	1:14:A:THR:N	7	3.01
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	1	2.99
(1,4)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:GLN:N	5	2.98
(1,190)	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	1:104:A:HIS:N	7	2.96
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1	2.94
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	2	2.93
(1,189)	1:102:A:GLY:C	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	9	2.91
(1,188)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:HIS:N	5	2.9
(1,85)	1:49:A:LEU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	6	2.9
(1,185)	1:100:A:GLY:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	6	2.88
(1,6)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:LEU:N	7	2.88
(1,173)	1:94:A:MET:C	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	7	2.87
(1,107)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ILE:N	4	2.87
(1,74)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:LEU:N	5	2.87
(1,119)	1:67:A:ASP:C	1:68:A:THR:N	1:68:A:THR:CA	1:68:A:THR:C	4	2.86
(1,183)	1:99:A:GLU:C	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	10	2.85
(1,43)	1:25:A:LYS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	8	2.84
(1,198)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLY:N	4	2.83
(1,75)	1:44:A:ASP:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	7	2.83
(1,89)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	7	2.82
(1,201)	1:108:A:GLY:C	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	3	2.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,188)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:HIS:N	4	2.78
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	4	2.77
(1,74)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:LEU:N	8	2.76
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	5	2.75
(1,78)	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	1:47:A:ASN:N	5	2.72
(1,184)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:PRO:N	5	2.71
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	9	2.7
(1,177)	1:96:A:GLU:C	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	2	2.67
(1,162)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:SER:N	7	2.67
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	10	2.67
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	2	2.62
(1,142)	1:79:A:PHE:N	1:79:A:PHE:CA	1:79:A:PHE:C	1:80:A:ILE:N	6	2.62
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	2	2.62
(1,5)	1:6:A:SER:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	5	2.62
(1,204)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLU:N	3	2.6
(1,204)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLU:N	5	2.6
(1,53)	1:32:A:LEU:C	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	8	2.6
(1,180)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:GLU:N	3	2.55
(1,105)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:HIS:N	4	2.55
(1,105)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:HIS:N	8	2.55
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	9	2.55
(1,85)	1:49:A:LEU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	10	2.52
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	9	2.52
(1,180)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:GLU:N	5	2.51
(1,16)	1:12:A:ILE:N	1:12:A:ILE:CA	1:12:A:ILE:C	1:13:A:GLU:N	6	2.51
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	10	2.49
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	2	2.48
(1,124)	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	1:71:A:ASP:N	8	2.48
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	5	2.48
(1,189)	1:102:A:GLY:C	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	10	2.43
(1,48)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:THR:N	8	2.42
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	8	2.41
(1,207)	1:111:A:GLU:C	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	7	2.39
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	6	2.39
(1,53)	1:32:A:LEU:C	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	5	2.37
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	10	2.36
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	7	2.36
(1,185)	1:100:A:GLY:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	8	2.35
(1,132)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	1:75:A:SER:N	2	2.35
(1,51)	1:31:A:THR:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	9	2.35
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	5	2.34
(1,136)	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	1:77:A:GLU:N	4	2.34
(1,43)	1:25:A:LYS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	5	2.33
(1,160)	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	1:89:A:ALA:N	1	2.32
(1,35)	1:21:A:GLN:C	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	2	2.31
(1,121)	1:68:A:THR:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1	2.3
(1,176)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:GLY:N	4	2.29
(1,89)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1	2.29
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	6	2.27
(1,189)	1:102:A:GLY:C	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	7	2.27
(1,142)	1:79:A:PHE:N	1:79:A:PHE:CA	1:79:A:PHE:C	1:80:A:ILE:N	2	2.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,198)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLY:N	10	2.25
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	6	2.25
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	2	2.23
(1,204)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLU:N	2	2.22
(1,160)	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	1:89:A:ALA:N	3	2.22
(1,96)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:GLU:N	9	2.22
(1,170)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:MET:N	1	2.21
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	1	2.21
(1,9)	1:8:A:LEU:C	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	10	2.21
(1,173)	1:94:A:MET:C	1:95:A:HIS:N	1:95:A:HIS:CA	1:95:A:HIS:C	9	2.2
(1,135)	1:75:A:SER:C	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	7	2.2
(1,191)	1:103:A:HIS:C	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	9	2.19
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	5	2.18
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	3	2.18
(1,32)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:GLN:N	1	2.18
(1,6)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:LEU:N	2	2.18
(1,195)	1:105:A:HIS:C	1:106:A:LYS:N	1:106:A:LYS:CA	1:106:A:LYS:C	5	2.17
(1,85)	1:49:A:LEU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	9	2.17
(1,192)	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	1:105:A:HIS:N	7	2.16
(1,140)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:PHE:N	3	2.16
(1,121)	1:68:A:THR:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	2	2.16
(1,90)	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1:53:A:ASN:N	2	2.16
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	2	2.16
(1,5)	1:6:A:SER:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	8	2.16
(1,109)	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	1:63:A:MET:N	4	2.15
(1,80)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:PHE:N	8	2.15
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	8	2.15
(1,195)	1:105:A:HIS:C	1:106:A:LYS:N	1:106:A:LYS:CA	1:106:A:LYS:C	9	2.14
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1	2.14
(1,157)	1:86:A:LEU:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	3	2.13
(1,53)	1:32:A:LEU:C	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	10	2.13
(1,52)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ASN:N	7	2.13
(1,34)	1:21:A:GLN:N	1:21:A:GLN:CA	1:21:A:GLN:C	1:22:A:TYR:N	1	2.13
(1,137)	1:76:A:PHE:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	8	2.12
(1,54)	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	1:34:A:GLN:N	3	2.11
(1,132)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	1:75:A:SER:N	10	2.1
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	7	2.1
(1,50)	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1:32:A:LEU:N	1	2.1
(1,28)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:PHE:N	6	2.09
(1,88)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:GLU:N	2	2.08
(1,193)	1:104:A:HIS:C	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	6	2.07
(1,129)	1:72:A:LYS:C	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	8	2.07
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	5	2.07
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	10	2.06
(1,96)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:GLU:N	1	2.05
(1,210)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:PRO:N	9	2.03
(1,40)	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	1:25:A:LYS:N	8	2.03
(1,187)	1:101:A:PRO:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	9	2.02
(1,200)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:LEU:N	8	2.01
(1,92)	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	1:54:A:LYS:N	5	2.01
(1,194)	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	1:106:A:LYS:N	5	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:11:A:ASN:N	1:11:A:ASN:CA	1:11:A:ASN:C	1:12:A:ILE:N	7	2.0
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	1	1.99
(1,105)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:HIS:N	3	1.99
(1,169)	1:92:A:GLU:C	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1	1.98
(1,169)	1:92:A:GLU:C	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	2	1.96
(1,209)	1:112:A:GLY:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	2	1.95
(1,197)	1:106:A:LYS:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	9	1.95
(1,184)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:PRO:N	6	1.95
(1,52)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ASN:N	10	1.95
(1,204)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLU:N	4	1.94
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	5	1.94
(1,117)	1:66:A:LEU:C	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	8	1.94
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	10	1.93
(1,189)	1:102:A:GLY:C	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	2	1.92
(1,178)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:ASP:N	6	1.92
(1,159)	1:87:A:THR:C	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	6	1.92
(1,105)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:HIS:N	2	1.92
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	3	1.91
(1,74)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:LEU:N	4	1.91
(1,26)	1:17:A:ASN:N	1:17:A:ASN:CA	1:17:A:ASN:C	1:18:A:THR:N	6	1.91
(1,182)	1:99:A:GLU:N	1:99:A:GLU:CA	1:99:A:GLU:C	1:100:A:GLY:N	5	1.9
(1,160)	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	1:89:A:ALA:N	4	1.9
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	1	1.9
(1,116)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:ASP:N	6	1.9
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	4	1.9
(1,72)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:LYS:N	3	1.9
(1,163)	1:89:A:ALA:C	1:90:A:SER:N	1:90:A:SER:CA	1:90:A:SER:C	9	1.89
(1,157)	1:86:A:LEU:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	7	1.89
(1,10)	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	1:10:A:ARG:N	9	1.88
(1,194)	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	1:106:A:LYS:N	4	1.87
(1,141)	1:78:A:GLU:C	1:79:A:PHE:N	1:79:A:PHE:CA	1:79:A:PHE:C	7	1.86
(1,52)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ASN:N	9	1.86
(1,24)	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	1:17:A:ASN:N	5	1.86
(1,164)	1:90:A:SER:N	1:90:A:SER:CA	1:90:A:SER:C	1:91:A:HIS:N	9	1.85
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	6	1.85
(1,142)	1:79:A:PHE:N	1:79:A:PHE:CA	1:79:A:PHE:C	1:80:A:ILE:N	1	1.84
(1,30)	1:19:A:PHE:N	1:19:A:PHE:CA	1:19:A:PHE:C	1:20:A:HIS:N	4	1.84
(1,191)	1:103:A:HIS:C	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	6	1.83
(1,127)	1:71:A:ASP:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	8	1.82
(1,66)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:LEU:N	6	1.82
(1,204)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLU:N	8	1.8
(1,130)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:LEU:N	5	1.8
(1,119)	1:67:A:ASP:C	1:68:A:THR:N	1:68:A:THR:CA	1:68:A:THR:C	9	1.8
(1,77)	1:45:A:LEU:C	1:46:A:GLN:N	1:46:A:GLN:CA	1:46:A:GLN:C	6	1.79
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	1	1.78
(1,131)	1:73:A:GLN:C	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	1	1.77
(1,209)	1:112:A:GLY:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	10	1.76
(1,189)	1:102:A:GLY:C	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	4	1.76
(1,43)	1:25:A:LYS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	1	1.76
(1,203)	1:109:A:LEU:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	3	1.75
(1,38)	1:23:A:SER:N	1:23:A:SER:CA	1:23:A:SER:C	1:24:A:VAL:N	8	1.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	6	1.74
(1,160)	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	1:89:A:ALA:N	8	1.72
(1,10)	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	1:10:A:ARG:N	5	1.72
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:GLY:N	8	1.71
(1,194)	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	1:106:A:LYS:N	10	1.71
(1,105)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:HIS:N	1	1.7
(1,96)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:GLU:N	6	1.7
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	6	1.7
(1,42)	1:25:A:LYS:N	1:25:A:LYS:CA	1:25:A:LYS:C	1:26:A:LEU:N	5	1.7
(1,74)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:LEU:N	10	1.69
(1,61)	1:36:A:GLU:C	1:37:A:PHE:N	1:37:A:PHE:CA	1:37:A:PHE:C	3	1.69
(1,35)	1:21:A:GLN:C	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	6	1.69
(1,96)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:GLU:N	10	1.68
(1,84)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:LYS:N	3	1.67
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	4	1.67
(1,31)	1:19:A:PHE:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	4	1.67
(1,190)	1:103:A:HIS:N	1:103:A:HIS:CA	1:103:A:HIS:C	1:104:A:HIS:N	8	1.66
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	3	1.66
(1,89)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	10	1.65
(1,136)	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	1:77:A:GLU:N	6	1.64
(1,5)	1:6:A:SER:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	3	1.64
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	5	1.61
(1,93)	1:53:A:ASN:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	8	1.59
(1,55)	1:33:A:ASN:C	1:34:A:GLN:N	1:34:A:GLN:CA	1:34:A:GLN:C	9	1.58
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	7	1.57
(1,170)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:MET:N	6	1.57
(1,16)	1:12:A:ILE:N	1:12:A:ILE:CA	1:12:A:ILE:C	1:13:A:GLU:N	10	1.57
(1,159)	1:87:A:THR:C	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	2	1.56
(1,129)	1:72:A:LYS:C	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	7	1.56
(1,85)	1:49:A:LEU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	2	1.56
(1,196)	1:106:A:LYS:N	1:106:A:LYS:CA	1:106:A:LYS:C	1:107:A:PRO:N	8	1.55
(1,180)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:GLU:N	2	1.55
(1,159)	1:87:A:THR:C	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	9	1.55
(1,34)	1:21:A:GLN:N	1:21:A:GLN:CA	1:21:A:GLN:C	1:22:A:TYR:N	6	1.55
(1,120)	1:68:A:THR:N	1:68:A:THR:CA	1:68:A:THR:C	1:69:A:ASN:N	6	1.54
(1,103)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:GLU:N	8	1.54
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	9	1.52
(1,116)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:ASP:N	8	1.52
(1,188)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:HIS:N	3	1.51
(1,122)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ALA:N	6	1.51
(1,185)	1:100:A:GLY:C	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	2	1.5
(1,109)	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	1:63:A:MET:N	6	1.5
(1,96)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:GLU:N	8	1.5
(1,4)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:GLN:N	6	1.5
(1,53)	1:32:A:LEU:C	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	9	1.48
(1,160)	1:88:A:TRP:N	1:88:A:TRP:CA	1:88:A:TRP:C	1:89:A:ALA:N	6	1.46
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	4	1.46
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	10	1.46
(1,82)	1:48:A:PHE:N	1:48:A:PHE:CA	1:48:A:PHE:C	1:49:A:LEU:N	1	1.45
(1,57)	1:34:A:GLN:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	4	1.45
(1,187)	1:101:A:PRO:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1	1.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,109)	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	1:63:A:MET:N	5	1.43
(1,73)	1:43:A:LYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	9	1.43
(1,53)	1:32:A:LEU:C	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	2	1.43
(1,57)	1:34:A:GLN:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	6	1.42
(1,31)	1:19:A:PHE:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	9	1.42
(1,92)	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	1:54:A:LYS:N	4	1.4
(1,85)	1:49:A:LEU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	4	1.4
(1,60)	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	1:37:A:PHE:N	9	1.4
(1,198)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLY:N	9	1.39
(1,179)	1:97:A:GLY:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	6	1.39
(1,169)	1:92:A:GLU:C	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	6	1.39
(1,105)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:HIS:N	10	1.39
(1,34)	1:21:A:GLN:N	1:21:A:GLN:CA	1:21:A:GLN:C	1:22:A:TYR:N	4	1.39
(1,210)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:PRO:N	2	1.38
(1,127)	1:71:A:ASP:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	7	1.38
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	5	1.37
(1,135)	1:75:A:SER:C	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	1	1.36
(1,187)	1:101:A:PRO:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	7	1.35
(1,136)	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	1:77:A:GLU:N	2	1.34
(1,40)	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	1:25:A:LYS:N	1	1.34
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	7	1.33
(1,25)	1:16:A:ILE:C	1:17:A:ASN:N	1:17:A:ASN:CA	1:17:A:ASN:C	1	1.33
(1,120)	1:68:A:THR:N	1:68:A:THR:CA	1:68:A:THR:C	1:69:A:ASN:N	2	1.32
(1,109)	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	1:63:A:MET:N	8	1.32
(1,44)	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	1:27:A:GLY:N	7	1.32
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	1	1.31
(1,127)	1:71:A:ASP:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	6	1.3
(1,70)	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	1:42:A:ARG:N	3	1.29
(1,42)	1:25:A:LYS:N	1:25:A:LYS:CA	1:25:A:LYS:C	1:26:A:LEU:N	3	1.29
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	3	1.28
(1,35)	1:21:A:GLN:C	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	9	1.28
(1,89)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	8	1.26
(1,35)	1:21:A:GLN:C	1:22:A:TYR:N	1:22:A:TYR:CA	1:22:A:TYR:C	8	1.26
(1,31)	1:19:A:PHE:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	6	1.26
(1,18)	1:13:A:GLU:N	1:13:A:GLU:CA	1:13:A:GLU:C	1:14:A:THR:N	9	1.26
(1,114)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:LEU:N	3	1.24
(1,111)	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	1:64:A:GLU:N	10	1.24
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	9	1.23
(1,208)	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1:113:A:THR:N	6	1.22
(1,121)	1:68:A:THR:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	5	1.22
(1,113)	1:64:A:GLU:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	4	1.22
(1,34)	1:21:A:GLN:N	1:21:A:GLN:CA	1:21:A:GLN:C	1:22:A:TYR:N	7	1.22
(1,57)	1:34:A:GLN:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	7	1.21
(1,90)	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1:53:A:ASN:N	8	1.2
(1,44)	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	1:27:A:GLY:N	9	1.19
(1,186)	1:101:A:PRO:N	1:101:A:PRO:CA	1:101:A:PRO:C	1:102:A:GLY:N	6	1.18
(1,80)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:PHE:N	1	1.18
(1,40)	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	1:25:A:LYS:N	10	1.17
(1,111)	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	1:64:A:GLU:N	9	1.16
(1,90)	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1:53:A:ASN:N	1	1.15
(1,6)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:LEU:N	9	1.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,205)	1:110:A:GLY:C	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	6	1.14
(1,202)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:GLY:N	2	1.14
(1,90)	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1:53:A:ASN:N	7	1.14
(1,8)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	1:9:A:GLU:N	3	1.14
(1,5)	1:6:A:SER:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	9	1.14
(1,162)	1:89:A:ALA:N	1:89:A:ALA:CA	1:89:A:ALA:C	1:90:A:SER:N	5	1.13
(1,152)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:ARG:N	3	1.13
(1,10)	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	1:10:A:ARG:N	4	1.13
(1,170)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:MET:N	7	1.12
(1,92)	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	1:54:A:LYS:N	9	1.12
(1,51)	1:31:A:THR:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	6	1.12
(1,177)	1:96:A:GLU:C	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	8	1.1
(1,125)	1:70:A:ALA:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	9	1.1
(1,124)	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	1:71:A:ASP:N	2	1.1
(1,57)	1:34:A:GLN:C	1:35:A:GLY:N	1:35:A:GLY:CA	1:35:A:GLY:C	2	1.1
(1,1)	1:4:A:LYS:C	1:5:A:MET:N	1:5:A:MET:CA	1:5:A:MET:C	6	1.1
(1,40)	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	1:25:A:LYS:N	6	1.08
(1,19)	1:13:A:GLU:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	7	1.08
(1,4)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:GLN:N	9	1.08
(1,191)	1:103:A:HIS:C	1:104:A:HIS:N	1:104:A:HIS:CA	1:104:A:HIS:C	10	1.07
(1,96)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:GLU:N	4	1.07
(1,61)	1:36:A:GLU:C	1:37:A:PHE:N	1:37:A:PHE:CA	1:37:A:PHE:C	1	1.07
(1,43)	1:25:A:LYS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	7	1.07
(1,5)	1:6:A:SER:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	4	1.07
(1,171)	1:93:A:LYS:C	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	6	1.06
(1,157)	1:86:A:LEU:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	4	1.06
(1,92)	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	1:54:A:LYS:N	3	1.05
(1,199)	1:107:A:PRO:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	2	1.04
(1,145)	1:80:A:ILE:C	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	8	1.04
(1,45)	1:28:A:HIS:C	1:29:A:PRO:N	1:29:A:PRO:CA	1:29:A:PRO:C	9	1.04
(1,10)	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	1:10:A:ARG:N	8	1.04
(1,48)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:THR:N	4	1.03
(1,193)	1:104:A:HIS:C	1:105:A:HIS:N	1:105:A:HIS:CA	1:105:A:HIS:C	3	1.02
(1,88)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:GLU:N	6	1.01
(1,86)	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	1:51:A:LYS:N	3	1.01
(1,52)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ASN:N	2	1.01
(1,28)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:PHE:N	10	1.01
(1,19)	1:13:A:GLU:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	3	1.0