



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:43 PM UTC

PDB ID : 2N93 / pdb_00002n93
BMRB ID : 25400
Title : Solution structure of lcFABP
Authors : Tseng, K.; Lyu, P.
Deposited on : 2015-11-05

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

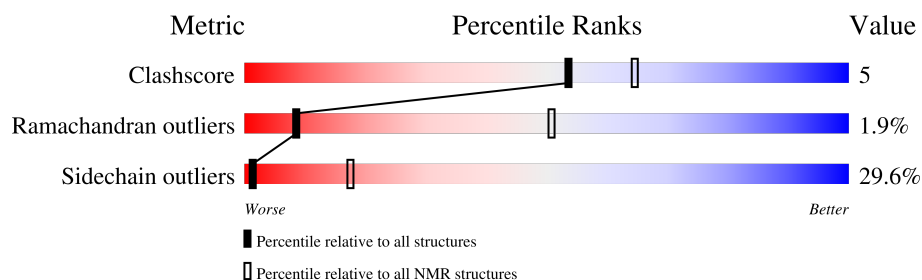
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	130	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:130 (129)	0.70	8

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2033 atoms, of which 1022 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fatty acid-binding protein.

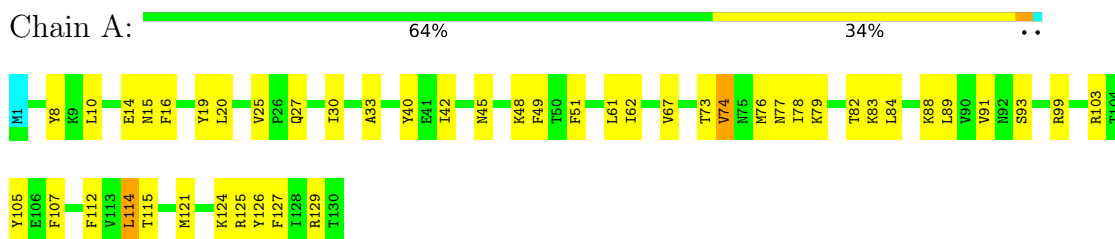
Mol	Chain	Residues	Atoms						Trace
1	A	130	Total	C	H	N	O	S	0
			2033	640	1022	166	198	7	

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: Fatty acid-binding protein

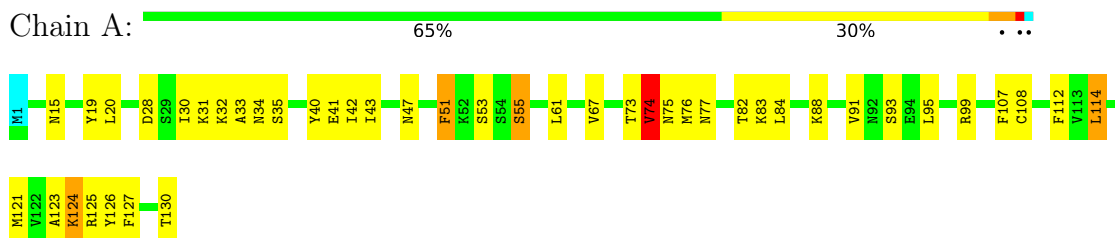


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

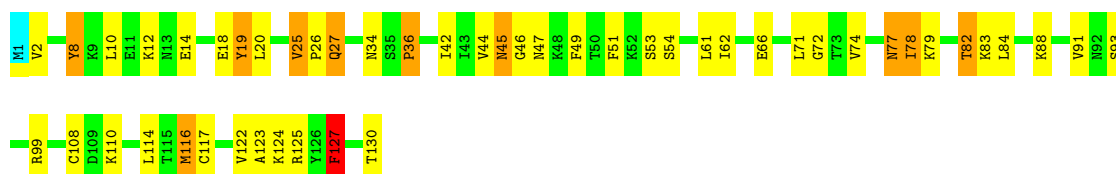
- Molecule 1: Fatty acid-binding protein



4.2.2 Score per residue for model 2

- Molecule 1: Fatty acid-binding protein

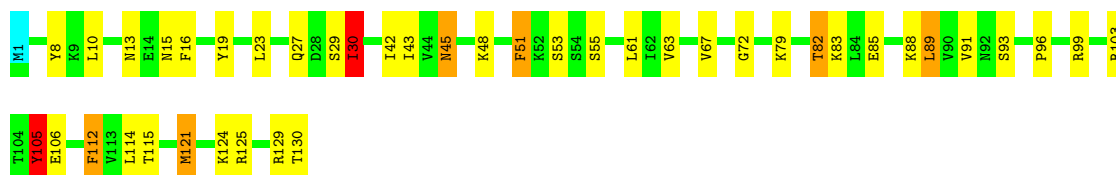




4.2.3 Score per residue for model 3

- Molecule 1: Fatty acid-binding protein

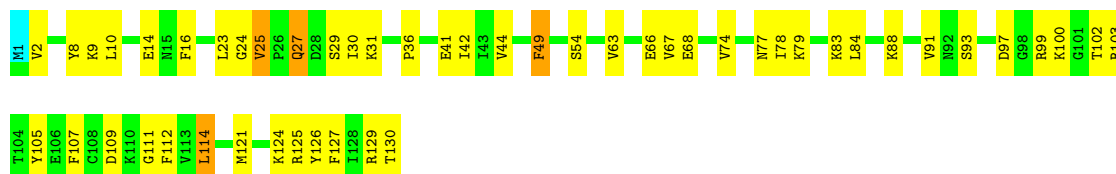
Chain A: 67% 26% 5% ..



4.2.4 Score per residue for model 4

- Molecule 1: Fatty acid-binding protein

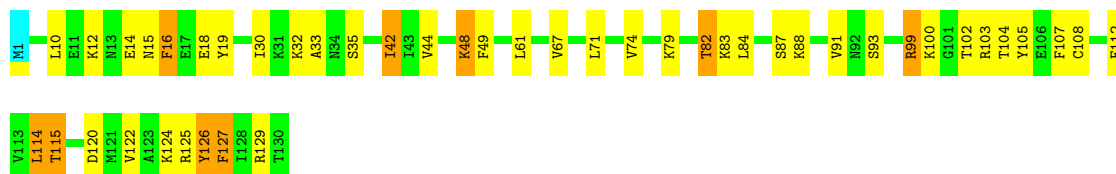
Chain A: 61% 35% ..



4.2.5 Score per residue for model 5

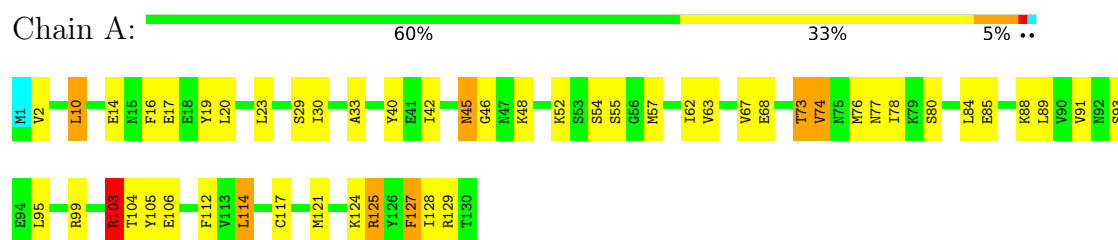
- Molecule 1: Fatty acid-binding protein

Chain A: 65% 28% 7% ..



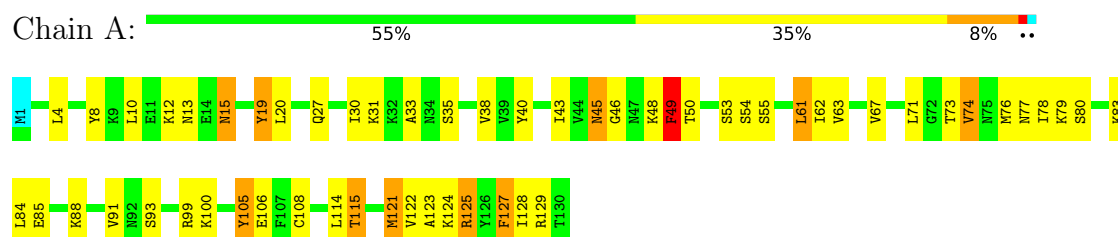
4.2.6 Score per residue for model 6

- Molecule 1: Fatty acid-binding protein



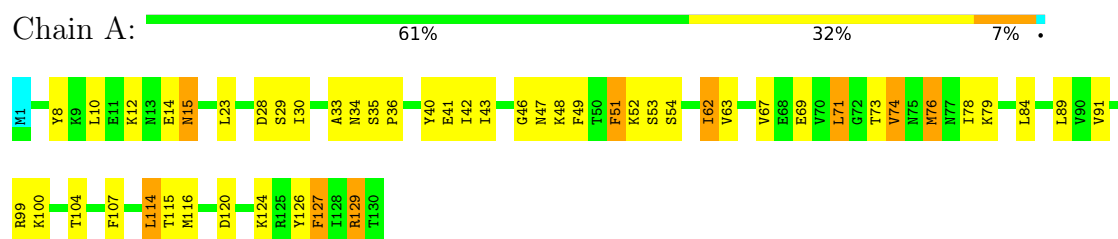
4.2.7 Score per residue for model 7

- Molecule 1: Fatty acid-binding protein



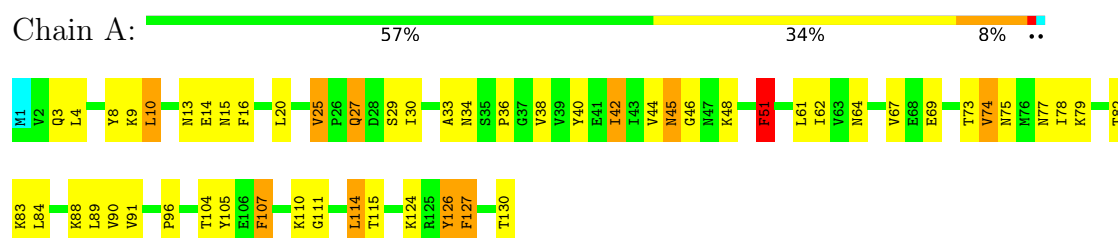
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Fatty acid-binding protein



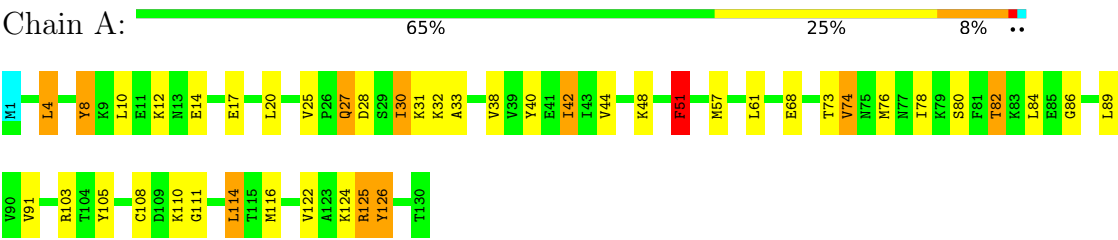
4.2.9 Score per residue for model 9

- Molecule 1: Fatty acid-binding protein



4.2.10 Score per residue for model 10

● Molecule 1: Fatty acid-binding protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

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 solution	1.1
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1501
Number of shifts mapped to atoms	1501
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	0.82±0.02	0±0/1017 (0.0± 0.0%)	1.56±0.04	9±3/1366 (0.6± 0.2%)
All	All	0.82	0/10170 (0.0%)	1.57	88/13660 (0.6%)

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	2.4±1.1
All	All	0	24

There are no bond-length outliers.

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	49	PHE	CA-CB-CG	9.03	122.83	113.80	7	5
1	A	126	TYR	N-CA-C	7.65	120.55	107.93	10	5
1	A	73	THR	CA-C-N	7.51	130.78	121.85	6	2
1	A	73	THR	C-N-CA	7.51	130.78	121.85	6	2
1	A	107	PHE	CA-CB-CG	7.36	121.16	113.80	8	4
1	A	51	PHE	CA-CB-CG	7.19	120.99	113.80	1	4
1	A	27	GLN	OE1-CD-NE2	-7.13	115.47	122.60	2	2
1	A	44	VAL	N-CA-CB	7.13	118.30	110.53	2	2
1	A	45	ASN	CA-CB-CG	6.78	119.38	112.60	6	4
1	A	25	VAL	CA-C-N	6.76	127.29	119.99	2	3
1	A	25	VAL	C-N-CA	6.76	127.29	119.99	2	3
1	A	16	PHE	CA-CB-CG	6.71	120.51	113.80	9	2
1	A	127	PHE	CA-CB-CG	6.60	120.40	113.80	8	5
1	A	15	ASN	CA-CB-CG	6.39	118.99	112.60	9	4
1	A	28	ASP	CA-CB-CG	6.33	118.93	112.60	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	ASN	OD1-CG-ND2	-6.29	116.31	122.60	9	1
1	A	129	ARG	N-CA-C	6.00	118.75	110.35	4	1
1	A	115	THR	CB-CA-C	5.89	119.52	109.80	5	1
1	A	30	ILE	CA-CB-CG2	5.78	120.32	110.50	3	1
1	A	29	SER	CA-C-N	5.75	128.33	120.46	6	3
1	A	29	SER	C-N-CA	5.75	128.33	120.46	6	3
1	A	124	LYS	N-CA-C	5.65	118.30	108.76	1	1
1	A	121	MET	N-CA-C	5.61	115.95	108.38	3	2
1	A	19	TYR	N-CA-CB	5.44	117.85	109.91	7	1
1	A	19	TYR	CA-C-N	5.42	128.00	120.63	2	1
1	A	19	TYR	C-N-CA	5.42	128.00	120.63	2	1
1	A	111	GLY	N-CA-C	5.39	117.45	110.45	4	2
1	A	76	MET	CA-C-N	5.38	130.43	123.00	8	1
1	A	76	MET	C-N-CA	5.38	130.43	123.00	8	1
1	A	123	ALA	N-CA-C	5.35	116.76	107.93	1	1
1	A	74	VAL	CA-CB-CG2	5.30	119.40	110.40	1	1
1	A	77	ASN	OD1-CG-ND2	-5.29	117.31	122.60	2	1
1	A	15	ASN	CA-C-N	5.27	127.60	120.38	1	2
1	A	15	ASN	C-N-CA	5.27	127.60	120.38	1	2
1	A	115	THR	CA-C-N	5.19	130.42	122.95	7	1
1	A	115	THR	C-N-CA	5.19	130.42	122.95	7	1
1	A	32	LYS	CA-C-N	5.14	127.43	120.44	1	1
1	A	32	LYS	C-N-CA	5.14	127.43	120.44	1	1
1	A	34	ASN	CA-CB-CG	5.11	117.71	112.60	2	1
1	A	78	ILE	CA-CB-CG1	5.10	119.07	110.40	2	1
1	A	95	LEU	CB-CA-C	5.09	115.52	110.33	1	1
1	A	44	VAL	CA-CB-CG1	5.08	119.04	110.40	2	1
1	A	3	GLN	OE1-CD-NE2	-5.05	117.55	122.60	9	1
1	A	96	PRO	CA-C-N	5.04	127.74	120.38	9	1
1	A	96	PRO	C-N-CA	5.04	127.74	120.38	9	1
1	A	64	ASN	N-CA-C	5.02	118.53	111.90	9	1
1	A	125	ARG	CA-C-O	-5.02	115.59	121.46	10	1

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	A	126	TYR	Sidechain	4
1	A	103	ARG	Sidechain	4
1	A	19	TYR	Sidechain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	8	TYR	Sidechain	2
1	A	105	TYR	Sidechain	2
1	A	127	PHE	Sidechain	1
1	A	16	PHE	Sidechain	1
1	A	99	ARG	Sidechain	1
1	A	49	PHE	Sidechain	1
1	A	15	ASN	Peptide	1
1	A	129	ARG	Sidechain	1
1	A	34	ASN	Peptide	1
1	A	107	PHE	Sidechain	1
1	A	111	GLY	Peptide	1

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	1003	1011	1011	10±4
All	All	10030	10110	10110	105

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:PHE:CZ	1:A:89:LEU:HD13	0.75	2.17	10	3
1:A:33:ALA:HB1	1:A:74:VAL:HG22	0.72	1.60	6	3
1:A:20:LEU:HD12	1:A:30:ILE:HD11	0.72	1.61	10	1
1:A:105:TYR:CE1	1:A:114:LEU:HD13	0.71	2.21	6	2
1:A:61:LEU:HD13	1:A:82:THR:HG21	0.68	1.64	3	5
1:A:114:LEU:HD11	1:A:127:PHE:CZ	0.66	2.25	5	2
1:A:71:LEU:HD23	1:A:74:VAL:CG1	0.64	2.22	8	1
1:A:105:TYR:CZ	1:A:114:LEU:HD13	0.61	2.30	3	1
1:A:42:ILE:HG21	1:A:112:PHE:CZ	0.61	2.31	5	1
1:A:10:LEU:HD23	1:A:127:PHE:CD2	0.56	2.36	2	1
1:A:51:PHE:CE1	1:A:89:LEU:HD13	0.56	2.36	10	2
1:A:20:LEU:HD13	1:A:30:ILE:HD11	0.55	1.77	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:PHE:HB2	1:A:63:VAL:HG22	0.55	1.77	7	1
1:A:33:ALA:HB1	1:A:74:VAL:HG12	0.54	1.79	7	3
1:A:33:ALA:CB	1:A:74:VAL:HG22	0.54	2.32	6	2
1:A:20:LEU:CD1	1:A:30:ILE:HD11	0.54	2.32	10	1
1:A:103:ARG:CD	1:A:114:LEU:HD11	0.52	2.34	3	1
1:A:10:LEU:HD23	1:A:38:VAL:HB	0.52	1.79	7	2
1:A:114:LEU:HD22	1:A:127:PHE:CZ	0.52	2.40	7	1
1:A:42:ILE:HD13	1:A:51:PHE:CD2	0.52	2.39	10	1
1:A:42:ILE:HG21	1:A:112:PHE:CE2	0.50	2.42	5	1
1:A:114:LEU:HB3	1:A:125:ARG:CZ	0.50	2.37	6	1
1:A:23:LEU:HD22	1:A:95:LEU:HG	0.50	1.84	6	1
1:A:61:LEU:CD1	1:A:82:THR:HG21	0.49	2.37	3	1
1:A:10:LEU:HD13	1:A:127:PHE:CD1	0.49	2.43	5	2
1:A:10:LEU:HD13	1:A:127:PHE:CE1	0.49	2.42	7	1
1:A:10:LEU:HD12	1:A:38:VAL:HB	0.48	1.83	9	1
1:A:103:ARG:NE	1:A:114:LEU:HD11	0.48	2.23	6	1
1:A:71:LEU:HD23	1:A:74:VAL:HG11	0.48	1.84	8	1
1:A:25:VAL:HG11	1:A:74:VAL:HG12	0.48	1.84	9	1
1:A:61:LEU:HD12	1:A:61:LEU:C	0.48	2.34	5	3
1:A:16:PHE:HA	1:A:19:TYR:CE1	0.47	2.44	6	2
1:A:27:GLN:HA	1:A:30:ILE:CG2	0.47	2.40	9	1
1:A:40:TYR:CD1	1:A:127:PHE:CE2	0.47	3.03	9	1
1:A:61:LEU:CD2	1:A:67:VAL:HG21	0.47	2.40	7	1
1:A:42:ILE:HD11	1:A:44:VAL:HG13	0.46	1.85	9	2
1:A:27:GLN:HA	1:A:30:ILE:HG22	0.46	1.88	4	3
1:A:114:LEU:HD21	1:A:127:PHE:CE1	0.46	2.45	9	1
1:A:40:TYR:CD2	1:A:127:PHE:CZ	0.46	3.04	1	3
1:A:20:LEU:HD11	1:A:26:PRO:C	0.45	2.37	2	1
1:A:10:LEU:HD13	1:A:10:LEU:C	0.45	2.37	6	1
1:A:25:VAL:CG1	1:A:74:VAL:HG23	0.45	2.42	2	1
1:A:44:VAL:HG12	1:A:49:PHE:CD2	0.45	2.47	4	1
1:A:33:ALA:HB1	1:A:74:VAL:CG2	0.44	2.39	1	2
1:A:16:PHE:CE1	1:A:30:ILE:HG23	0.44	2.47	3	1
1:A:71:LEU:HD22	1:A:76:MET:O	0.44	2.12	8	1
1:A:4:LEU:HD22	1:A:4:LEU:C	0.44	2.37	10	1
1:A:25:VAL:HG11	1:A:74:VAL:HG23	0.44	1.89	10	2
1:A:42:ILE:C	1:A:42:ILE:HD13	0.44	2.38	9	1
1:A:105:TYR:HB3	1:A:112:PHE:CE2	0.44	2.47	5	2
1:A:105:TYR:HE1	1:A:114:LEU:HD13	0.44	1.71	6	1
1:A:116:MET:HB3	1:A:123:ALA:HB3	0.43	1.90	2	1
1:A:105:TYR:CE1	1:A:114:LEU:CD1	0.43	3.00	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:VAL:HG23	1:A:80:SER:HB2	0.43	1.91	7	1
1:A:13:ASN:HA	1:A:125:ARG:HB3	0.43	1.89	7	1
1:A:10:LEU:HD11	1:A:36:PRO:CB	0.43	2.44	2	1
1:A:103:ARG:HD3	1:A:114:LEU:HD11	0.42	1.91	3	1
1:A:10:LEU:HD23	1:A:127:PHE:CE1	0.42	2.49	6	1
1:A:42:ILE:HD13	1:A:112:PHE:CD2	0.42	2.49	6	1
1:A:105:TYR:CG	1:A:114:LEU:HD12	0.42	2.50	10	1
1:A:13:ASN:HA	1:A:125:ARG:CB	0.42	2.44	7	1
1:A:105:TYR:CE1	1:A:114:LEU:HD12	0.42	2.49	7	1
1:A:105:TYR:CE1	1:A:114:LEU:HB3	0.42	2.49	9	1
1:A:114:LEU:CD2	1:A:127:PHE:CZ	0.42	3.02	1	1
1:A:33:ALA:HB1	1:A:74:VAL:CG1	0.42	2.44	8	1
1:A:42:ILE:HD11	1:A:44:VAL:CG1	0.42	2.43	9	1
1:A:19:TYR:CE1	1:A:20:LEU:HG	0.41	2.50	1	1
1:A:15:ASN:CB	1:A:123:ALA:HA	0.41	2.45	7	1
1:A:17:GLU:OE2	1:A:31:LYS:HE3	0.41	2.16	10	1
1:A:40:TYR:CG	1:A:127:PHE:CE2	0.41	3.08	6	2
1:A:71:LEU:HD23	1:A:74:VAL:HG13	0.41	1.89	8	1
1:A:125:ARG:HD2	1:A:125:ARG:C	0.41	2.40	6	1
1:A:104:THR:CG2	1:A:115:THR:HG22	0.41	2.46	5	1
1:A:61:LEU:HD22	1:A:67:VAL:HG21	0.41	1.92	7	1
1:A:114:LEU:HD21	1:A:127:PHE:CE2	0.41	2.51	8	1
1:A:91:VAL:CG2	1:A:105:TYR:CZ	0.40	3.04	7	1
1:A:128:ILE:HG22	1:A:129:ARG:N	0.40	2.31	6	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	128/130 (98%)	106±4 (82±3%)	20±3 (16±2%)	2±1 (2±1%)	8	51
All	All	1280/1300 (98%)	1055 (82%)	201 (16%)	24 (2%)	8	51

All 13 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	46	GLY	5
1	A	36	PRO	4
1	A	55	SER	2
1	A	72	GLY	2
1	A	48	LYS	2
1	A	62	ILE	2
1	A	47	ASN	1
1	A	112	PHE	1
1	A	24	GLY	1
1	A	107	PHE	1
1	A	109	ASP	1
1	A	45	ASN	1
1	A	86	GLY	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/113 (99%)	79±3 (70±3%)	33±3 (30±3%)	1	17
All	All	1120/1130 (99%)	789 (70%)	331 (30%)	1	17

All 86 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	124	LYS	10
1	A	84	LEU	9
1	A	91	VAL	9
1	A	42	ILE	8
1	A	88	LYS	8
1	A	99	ARG	8
1	A	114	LEU	8
1	A	125	ARG	8
1	A	67	VAL	7
1	A	83	LYS	7
1	A	93	SER	7
1	A	8	TYR	7
1	A	14	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	78	ILE	7
1	A	79	LYS	7
1	A	30	ILE	6
1	A	74	VAL	6
1	A	77	ASN	6
1	A	48	LYS	6
1	A	51	PHE	5
1	A	53	SER	5
1	A	73	THR	5
1	A	108	CYS	5
1	A	121	MET	5
1	A	130	THR	5
1	A	12	LYS	5
1	A	27	GLN	5
1	A	45	ASN	5
1	A	54	SER	5
1	A	82	THR	5
1	A	10	LEU	5
1	A	35	SER	4
1	A	43	ILE	4
1	A	76	MET	4
1	A	62	ILE	4
1	A	71	LEU	4
1	A	122	VAL	4
1	A	63	VAL	4
1	A	115	THR	4
1	A	129	ARG	4
1	A	100	LYS	4
1	A	31	LYS	3
1	A	41	GLU	3
1	A	55	SER	3
1	A	2	VAL	3
1	A	110	LYS	3
1	A	116	MET	3
1	A	23	LEU	3
1	A	85	GLU	3
1	A	106	GLU	3
1	A	68	GLU	3
1	A	104	THR	3
1	A	4	LEU	3
1	A	34	ASN	2
1	A	47	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	75	ASN	2
1	A	112	PHE	2
1	A	18	GLU	2
1	A	66	GLU	2
1	A	117	CYS	2
1	A	29	SER	2
1	A	89	LEU	2
1	A	9	LYS	2
1	A	102	THR	2
1	A	15	ASN	2
1	A	32	LYS	2
1	A	120	ASP	2
1	A	20	LEU	2
1	A	52	LYS	2
1	A	57	MET	2
1	A	80	SER	2
1	A	40	TYR	2
1	A	28	ASP	2
1	A	69	GLU	2
1	A	127	PHE	1
1	A	13	ASN	1
1	A	96	PRO	1
1	A	105	TYR	1
1	A	97	ASP	1
1	A	87	SER	1
1	A	17	GLU	1
1	A	103	ARG	1
1	A	50	THR	1
1	A	61	LEU	1
1	A	128	ILE	1
1	A	90	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1501
Number of shifts mapped to atoms	1501
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
$^{13}\text{C}_\alpha$	130	-0.31 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	-0.07 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	130	0.08 ± 0.12	None needed (< 0.5 ppm)
^{15}N	124	-0.97 ± 0.47	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 86%, i.e. 1495 atoms were assigned a chemical shift out of a possible 1735. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	646/650 (99%)	264/266 (99%)	258/258 (100%)	124/126 (98%)
Sidechain	835/970 (86%)	572/629 (91%)	251/305 (82%)	12/36 (33%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	14/115 (12%)	14/55 (25%)	0/60 (0%)	0/0 (—%)
Overall	1495/1735 (86%)	850/950 (89%)	509/623 (82%)	136/162 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1501 atoms were assigned a chemical shift out of a possible 1750. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	649/655 (99%)	265/268 (99%)	260/260 (100%)	124/127 (98%)
Sidechain	838/980 (86%)	574/636 (90%)	252/308 (82%)	12/36 (33%)
Aromatic	14/115 (12%)	14/55 (25%)	0/60 (0%)	0/0 (—%)
Overall	1501/1750 (86%)	853/959 (89%)	512/628 (82%)	136/163 (83%)

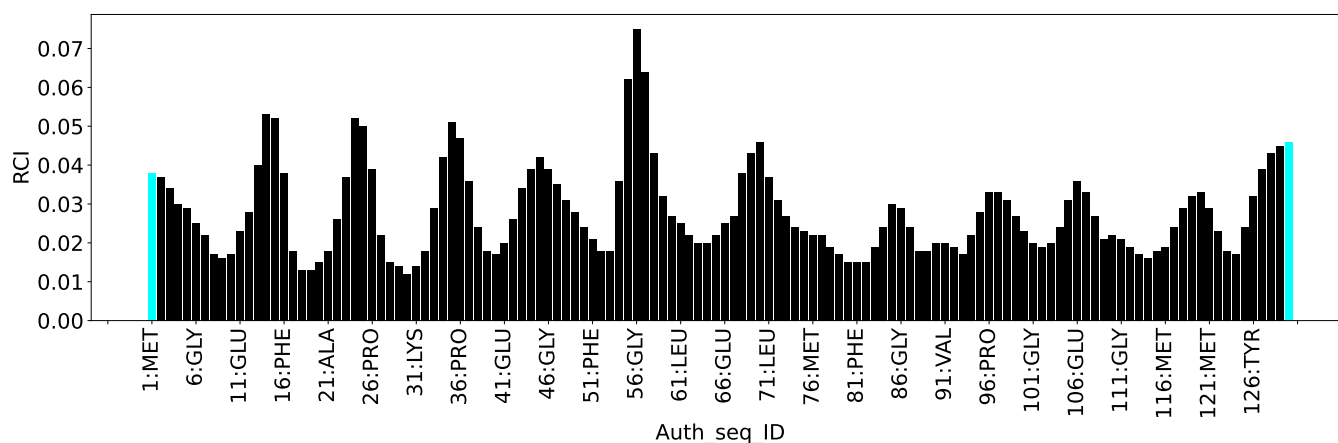
7.1.4 Statistically unusual chemical shifts [i](#)

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	2137
Intra-residue ($ i-j =0$)	522
Sequential ($ i-j =1$)	588
Medium range ($ i-j >1$ and $ i-j <5$)	284
Long range ($ i-j \geq 5$)	679
Inter-chain	0
Hydrogen bond restraints	64
Disulfide bond restraints	0
Total dihedral-angle restraints	232
Number of unmapped restraints	0
Number of restraints per residue	18.2
Number of long range restraints per residue ¹	5.6

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)	41.6	0.2
0.2-0.5 (Medium)	112.5	0.5
>0.5 (Large)	117.0	9.49

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)	36.5	9.99
10.0-20.0 (Medium)	18.6	19.95
>20.0 (Large)	13.1	59.14

9 Distance violation analysis ⓘ

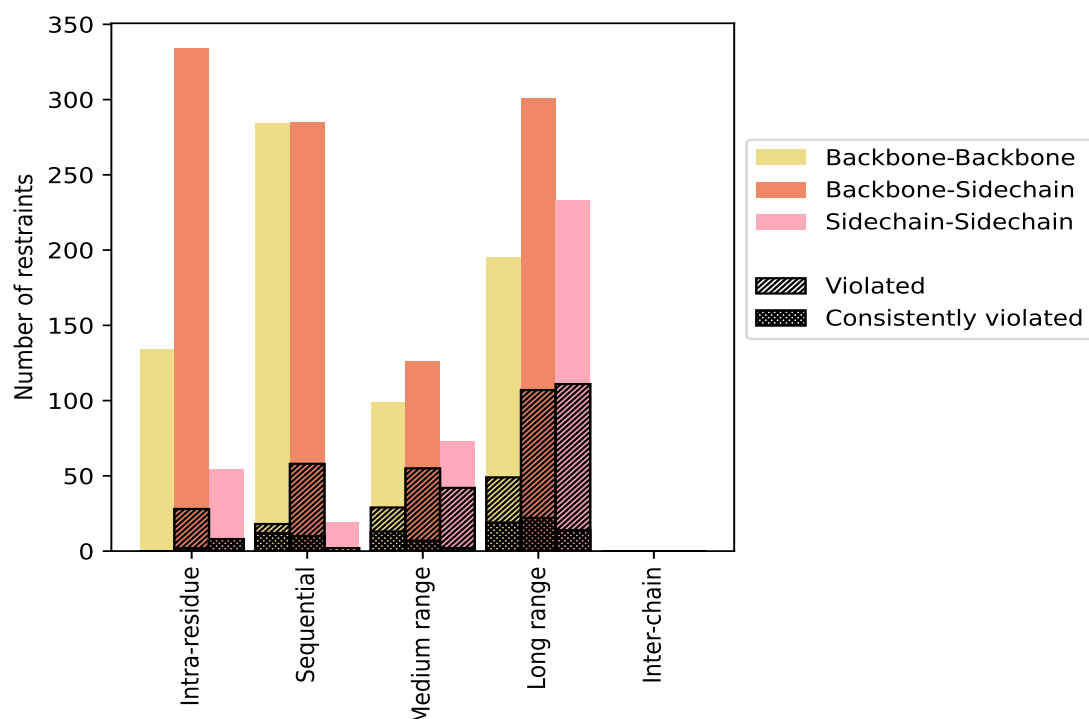
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	522	24.4	36	6.9	1.7	10	1.9	0.5
Backbone-Backbone	134	6.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	334	15.6	28	8.4	1.3	2	0.6	0.1
Sidechain-Sidechain	54	2.5	8	14.8	0.4	8	14.8	0.4
Sequential (i-j =1)	588	27.5	78	13.3	3.6	22	3.7	1.0
Backbone-Backbone	284	13.3	18	6.3	0.8	12	4.2	0.6
Backbone-Sidechain	285	13.3	58	20.4	2.7	10	3.5	0.5
Sidechain-Sidechain	19	0.9	2	10.5	0.1	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	284	13.3	115	40.5	5.4	21	7.4	1.0
Backbone-Backbone	99	4.6	29	29.3	1.4	13	13.1	0.6
Backbone-Sidechain	112	5.2	44	39.3	2.1	6	5.4	0.3
Sidechain-Sidechain	73	3.4	42	57.5	2.0	2	2.7	0.1
Long range (i-j ≥5)	679	31.8	252	37.1	11.8	52	7.7	2.4
Backbone-Backbone	195	9.1	49	25.1	2.3	19	9.7	0.9
Backbone-Sidechain	251	11.7	92	36.7	4.3	19	7.6	0.9
Sidechain-Sidechain	233	10.9	111	47.6	5.2	14	6.0	0.7
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	64	3.0	26	40.6	1.2	4	6.2	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2137	100.0	507	23.7	23.7	109	5.1	5.1
Backbone-Backbone	712	33.3	96	13.5	4.5	44	6.2	2.1
Backbone-Sidechain	1046	48.9	248	23.7	11.6	41	3.9	1.9
Sidechain-Sidechain	379	17.7	163	43.0	7.6	24	6.3	1.1

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 disulfide bonds are counted in their appropriate category on the x-axis

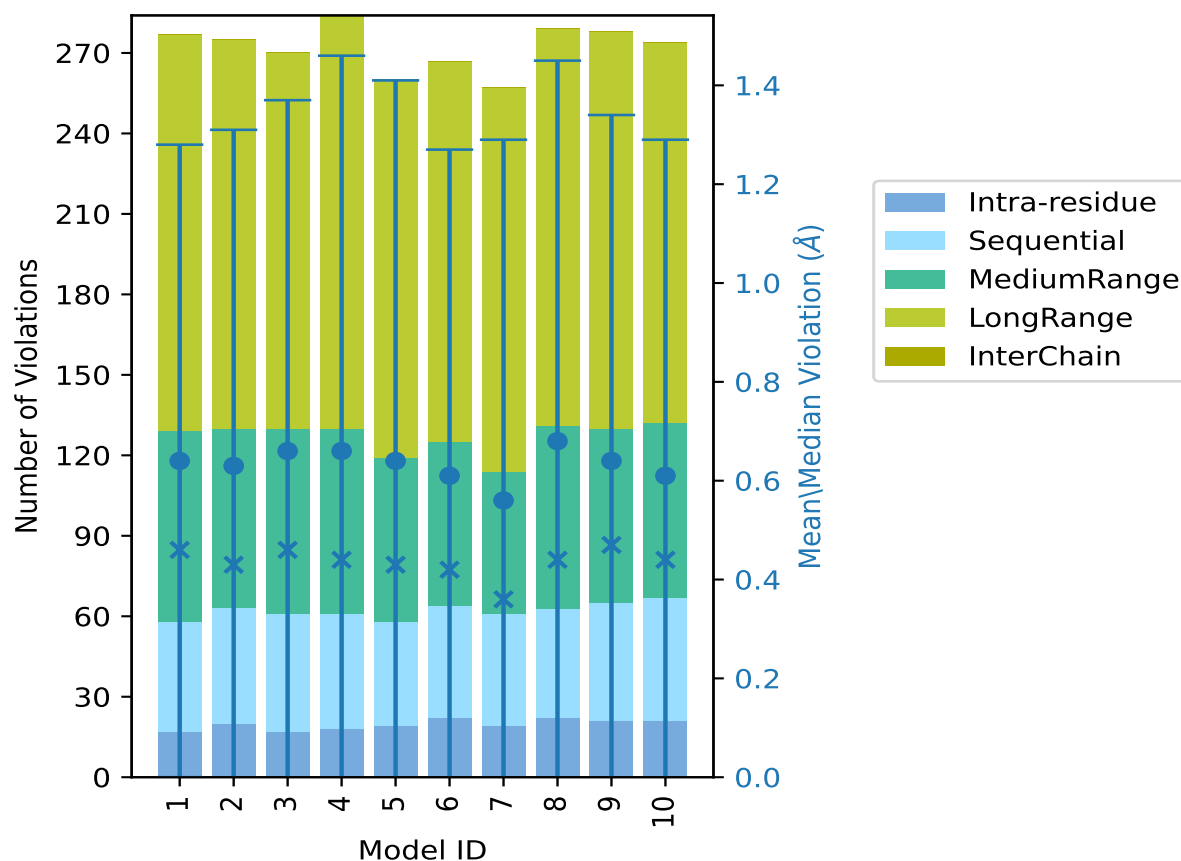
9.2 Distance violation statistics for each model [i](#)

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	17	41	71	148	0	277	0.64	7.22	0.64	0.46
2	20	43	67	145	0	275	0.63	7.52	0.68	0.43
3	17	44	69	140	0	270	0.66	7.41	0.71	0.46
4	18	43	69	154	0	284	0.66	9.49	0.8	0.44
5	19	39	61	141	0	260	0.64	8.7	0.77	0.43
6	22	42	61	142	0	267	0.61	7.43	0.66	0.42
7	19	42	53	143	0	257	0.56	8.66	0.73	0.36
8	22	41	68	148	0	279	0.68	7.92	0.77	0.44
9	21	44	65	148	0	278	0.64	7.78	0.7	0.47
10	21	46	65	142	0	274	0.61	7.71	0.68	0.44

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1592(IR:486, SQ:510, MR:169, LR:427, IC:0) 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	%
8	15	23	43	0	89	1	10.0
5	8	15	29	0	57	2	20.0
3	9	8	26	0	46	3	30.0

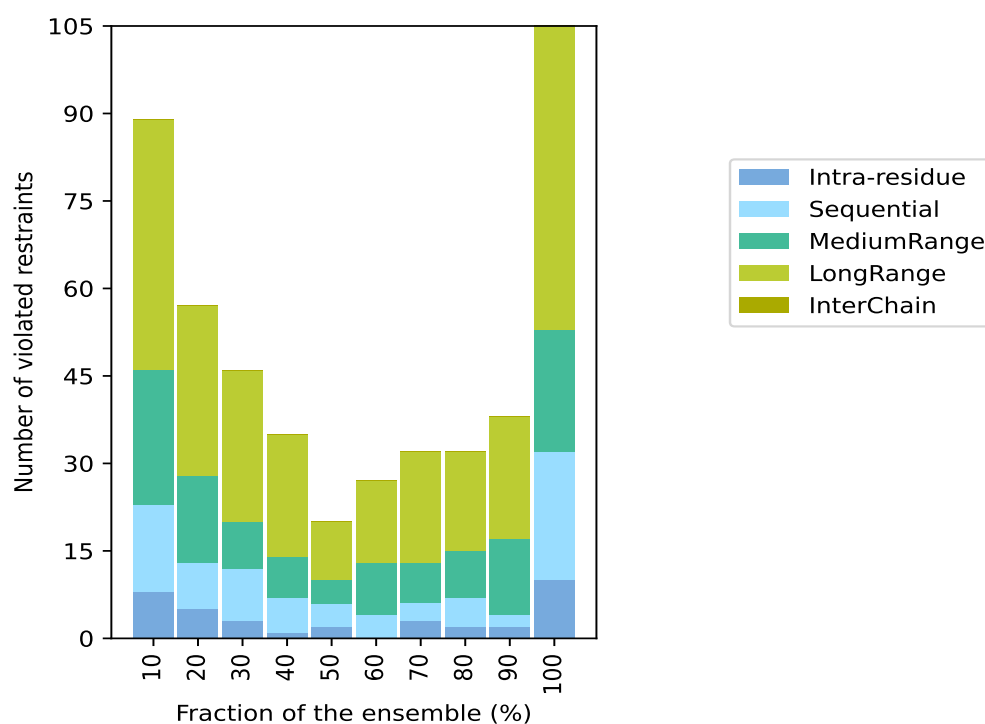
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	6	7	21	0	35	4	40.0
2	4	4	10	0	20	5	50.0
0	4	9	14	0	27	6	60.0
3	3	7	19	0	32	7	70.0
2	5	8	17	0	32	8	80.0
2	2	13	21	0	38	9	90.0
10	22	21	52	0	105	10	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](#)

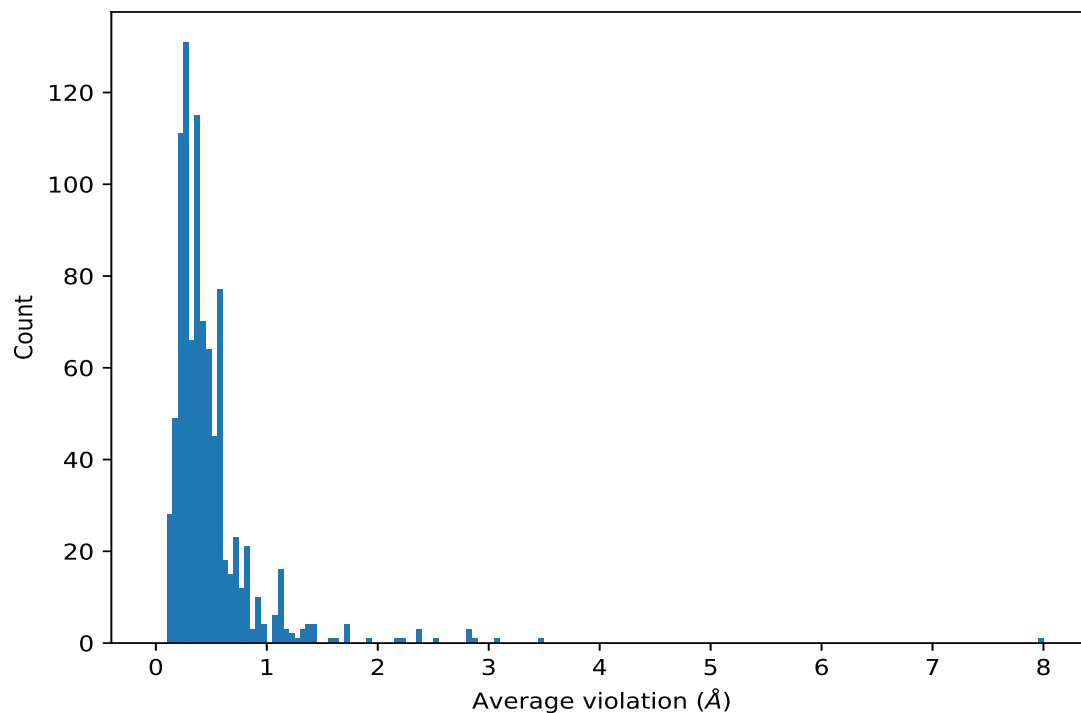


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	10	7.98	0.69	7.74
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	10	3.49	0.94	3.72
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	10	3.09	0.88	3.15
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	10	2.85	0.79	2.9
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	10	2.82	0.31	2.95
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	10	2.81	0.38	2.9
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	10	2.81	0.38	2.9
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	10	2.51	0.4	2.57
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	10	2.21	0.18	2.18
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	10	1.95	0.43	2.14
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	10	1.74	0.47	1.9
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	10	1.74	0.47	1.9
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	10	1.72	0.28	1.7
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	10	1.72	0.28	1.7
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	10	1.61	0.17	1.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	10	1.45	0.68	1.48
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	10	1.45	0.68	1.48
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	10	1.45	0.3	1.53
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	10	1.44	0.4	1.38
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	10	1.4	0.19	1.42
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	10	1.37	0.24	1.4
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	10	1.37	0.24	1.4
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	10	1.37	0.24	1.4
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	10	1.27	0.08	1.3
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	10	1.22	0.28	1.23
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	10	1.2	0.22	1.18
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	10	1.2	0.22	1.18
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	10	1.2	0.22	1.18
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	10	1.14	0.18	1.18
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	10	1.14	0.06	1.14
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	10	1.14	0.06	1.14
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	10	1.11	0.35	1.07
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	10	1.07	0.21	1.11
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	10	1.07	0.21	1.11
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	10	1.07	0.21	1.11
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	10	1.06	0.11	1.06
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	10	1.05	0.31	1.05
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	10	0.97	0.17	0.96
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	10	0.97	0.17	0.96
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	10	0.95	0.25	0.94
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	10	0.94	0.11	0.93
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	10	0.91	0.23	0.94
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	10	0.9	0.36	0.91
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	10	0.87	0.29	0.76
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	10	0.85	0.24	0.84
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	10	0.83	0.27	0.81
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	10	0.83	0.23	0.9
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	10	0.83	0.23	0.9
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	10	0.83	0.23	0.9
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	10	0.82	0.28	0.77
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	10	0.82	0.23	0.8
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	10	0.82	0.23	0.8
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	10	0.8	0.17	0.78
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	10	0.8	0.17	0.78
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	10	0.8	0.17	0.78
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	10	0.8	0.25	0.85
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	10	0.8	0.11	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	10	0.79	0.13	0.84
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	10	0.79	0.13	0.84
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	10	0.79	0.13	0.84
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	10	0.75	0.34	0.68
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	10	0.75	0.34	0.68
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	10	0.75	0.34	0.68
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	10	0.74	0.21	0.76
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	10	0.73	0.09	0.72
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	10	0.71	0.24	0.66
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	10	0.7	0.29	0.58
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	10	0.7	0.29	0.58
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	10	0.7	0.29	0.58
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	10	0.7	0.22	0.68
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	10	0.69	0.25	0.67
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	10	0.68	0.15	0.72
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	10	0.68	0.1	0.68
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	10	0.64	0.22	0.62
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	10	0.64	0.2	0.55
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	10	0.63	0.22	0.68
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	10	0.58	0.18	0.56
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	10	0.58	0.09	0.6
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	10	0.58	0.09	0.6
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	10	0.57	0.22	0.57
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	10	0.57	0.22	0.57
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	10	0.57	0.22	0.57
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	10	0.57	0.22	0.57
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	10	0.57	0.22	0.57
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	10	0.57	0.22	0.57
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	10	0.57	0.17	0.57
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	10	0.57	0.17	0.57
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	10	0.56	0.17	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	10	0.56	0.17	0.62
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	10	0.56	0.17	0.62
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	10	0.56	0.07	0.55
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	10	0.55	0.17	0.57
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	10	0.55	0.17	0.57
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	10	0.55	0.17	0.57
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	10	0.54	0.09	0.52
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	10	0.52	0.17	0.51
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	10	0.51	0.18	0.52
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	10	0.51	0.18	0.52
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	10	0.51	0.18	0.52
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	10	0.51	0.18	0.52
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	10	0.51	0.18	0.52
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	10	0.51	0.18	0.52
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	10	0.51	0.18	0.52
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	10	0.51	0.18	0.52
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	10	0.51	0.18	0.52
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	10	0.51	0.18	0.52
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	10	0.51	0.18	0.52
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	10	0.51	0.18	0.52
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	10	0.51	0.28	0.48
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	10	0.51	0.14	0.56
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	10	0.51	0.14	0.56
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	10	0.51	0.14	0.56
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	10	0.51	0.22	0.55
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	10	0.51	0.21	0.52
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	10	0.49	0.11	0.52
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	10	0.49	0.12	0.49
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	10	0.49	0.12	0.49
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	10	0.49	0.12	0.49
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	10	0.49	0.12	0.44
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	10	0.49	0.12	0.44
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	10	0.47	0.17	0.49
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	10	0.47	0.17	0.49
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	10	0.47	0.17	0.49
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	10	0.46	0.21	0.44
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	10	0.46	0.17	0.43
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	10	0.46	0.17	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	10	0.46	0.17	0.43
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	10	0.46	0.05	0.47
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	10	0.45	0.19	0.46
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	10	0.42	0.16	0.39
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	10	0.42	0.19	0.4
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	10	0.42	0.19	0.4
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	10	0.41	0.29	0.21
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	10	0.41	0.03	0.4
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	10	0.41	0.04	0.42
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	10	0.41	0.14	0.45
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	10	0.41	0.14	0.45
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	10	0.41	0.14	0.45
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	10	0.41	0.14	0.45
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	10	0.41	0.14	0.45
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	10	0.41	0.14	0.45
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	10	0.41	0.14	0.45
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	10	0.41	0.14	0.45
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	10	0.39	0.04	0.4
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	10	0.39	0.11	0.38
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	10	0.39	0.11	0.38
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	10	0.38	0.07	0.38
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	10	0.38	0.1	0.41
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	10	0.38	0.1	0.36
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	10	0.38	0.09	0.42
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	10	0.38	0.18	0.36
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	10	0.36	0.04	0.36
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	10	0.35	0.12	0.39
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	10	0.35	0.12	0.39
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	10	0.35	0.12	0.39
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	10	0.35	0.12	0.39
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	10	0.35	0.12	0.39
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	10	0.35	0.12	0.39
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	10	0.34	0.08	0.3
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	10	0.34	0.08	0.3
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	10	0.34	0.08	0.3
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	10	0.34	0.08	0.3
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	10	0.34	0.08	0.3
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	10	0.34	0.08	0.3
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	10	0.34	0.03	0.34
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	10	0.33	0.15	0.32
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	10	0.32	0.15	0.3
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	10	0.31	0.08	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	10	0.27	0.07	0.28
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	10	0.26	0.08	0.22
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	10	0.24	0.01	0.24
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	10	0.24	0.01	0.24
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	10	0.24	0.01	0.24
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	10	0.24	0.01	0.24
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	10	0.24	0.01	0.24
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	10	0.24	0.01	0.24
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	10	0.24	0.01	0.24
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	10	0.24	0.01	0.24
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	10	0.24	0.01	0.23
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	10	0.24	0.01	0.23
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	10	0.24	0.01	0.23
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	10	0.24	0.01	0.23
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	10	0.23	0.05	0.24
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	10	0.23	0.05	0.24
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	10	0.23	0.01	0.23
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	10	0.23	0.01	0.23
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	10	0.23	0.01	0.23
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	10	0.23	0.01	0.23
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	9	2.4	0.52	2.55
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	9	2.4	0.52	2.55
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	9	2.4	0.52	2.55
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	9	2.16	0.74	2.52
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	9	1.55	0.32	1.69
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	9	1.22	0.5	1.36
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	9	1.15	0.49	1.05
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	9	0.98	0.47	1.04
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	9	0.85	0.35	0.85
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	9	0.85	0.35	0.85
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	9	0.85	0.35	0.85
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	9	0.82	0.27	0.77
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	9	0.82	0.27	0.77
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	9	0.73	0.3	0.73
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	9	0.73	0.3	0.73
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	9	0.73	0.3	0.73
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	9	0.71	0.24	0.69
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	9	0.65	0.33	0.76
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	9	0.65	0.33	0.76
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	9	0.6	0.21	0.61
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	9	0.6	0.21	0.61
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	9	0.6	0.21	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	9	0.57	0.16	0.57
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	9	0.57	0.16	0.57
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	9	0.57	0.16	0.57
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	9	0.56	0.09	0.54
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	9	0.56	0.09	0.54
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	9	0.56	0.28	0.61
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	9	0.56	0.28	0.61
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	9	0.54	0.26	0.56
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	9	0.54	0.26	0.56
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	9	0.54	0.26	0.56
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	9	0.54	0.26	0.56
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	9	0.54	0.3	0.43
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	9	0.54	0.3	0.43
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	9	0.54	0.3	0.43
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	9	0.54	0.13	0.52
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	9	0.53	0.17	0.46
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	9	0.53	0.17	0.46
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	9	0.52	0.16	0.54
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	9	0.51	0.15	0.42
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	9	0.49	0.25	0.37
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	9	0.49	0.25	0.37
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	9	0.49	0.25	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	9	0.49	0.25	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	9	0.49	0.25	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	9	0.49	0.25	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	9	0.49	0.25	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	9	0.49	0.25	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	9	0.49	0.25	0.37
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	9	0.47	0.24	0.44
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	9	0.47	0.24	0.44
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	9	0.44	0.15	0.41
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	9	0.44	0.15	0.41
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	9	0.44	0.15	0.41
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	9	0.43	0.25	0.4
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	9	0.43	0.25	0.4
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	9	0.43	0.13	0.43
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	9	0.43	0.13	0.43
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	9	0.43	0.13	0.43
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	9	0.41	0.16	0.42
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	9	0.39	0.1	0.44
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	9	0.39	0.1	0.44
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	9	0.39	0.1	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	9	0.36	0.1	0.4
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	9	0.36	0.09	0.35
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	9	0.36	0.09	0.35
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	9	0.36	0.16	0.33
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	9	0.28	0.13	0.29
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	9	0.27	0.14	0.23
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	9	0.26	0.1	0.25
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	9	0.25	0.11	0.18
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	9	0.25	0.11	0.18
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	9	0.23	0.12	0.2
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	9	0.23	0.12	0.2
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	9	0.23	0.12	0.2
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	9	0.18	0.07	0.16
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	8	1.14	0.86	0.88
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	8	1.14	0.86	0.88
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	8	1.14	0.86	0.88
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	8	1.05	0.39	0.98
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	8	0.93	0.2	0.96
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	8	0.86	0.22	0.86
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	8	0.83	0.36	0.96
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	8	0.73	0.3	0.65
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	8	0.72	0.17	0.7
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	8	0.72	0.17	0.7
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	8	0.72	0.17	0.7
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	8	0.7	0.17	0.7
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	8	0.61	0.28	0.58
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	8	0.59	0.25	0.56
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	8	0.59	0.25	0.56
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	8	0.59	0.25	0.56
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	8	0.48	0.38	0.23
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	8	0.48	0.38	0.23
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	8	0.48	0.38	0.23
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	8	0.46	0.15	0.44
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	8	0.46	0.15	0.44
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	8	0.46	0.15	0.44
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	8	0.44	0.27	0.34
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	8	0.44	0.27	0.34
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	8	0.44	0.27	0.34
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	8	0.43	0.17	0.44
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	8	0.43	0.17	0.44
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	8	0.43	0.17	0.37
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	8	0.43	0.14	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	8	0.43	0.14	0.45
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	8	0.43	0.14	0.45
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	8	0.43	0.14	0.45
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	8	0.41	0.15	0.41
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	8	0.39	0.1	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	8	0.39	0.1	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	8	0.39	0.1	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	8	0.39	0.1	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	8	0.39	0.1	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	8	0.39	0.1	0.36
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	8	0.38	0.22	0.31
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	8	0.38	0.22	0.31
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	8	0.31	0.09	0.31
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	8	0.31	0.09	0.31
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	8	0.28	0.14	0.24
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	8	0.27	0.08	0.24
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	8	0.27	0.08	0.24
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	8	0.26	0.07	0.28
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	8	0.25	0.09	0.22
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	8	0.25	0.1	0.2
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	8	0.25	0.09	0.24
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	8	0.25	0.09	0.24
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	8	0.25	0.09	0.24
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	8	0.25	0.09	0.24
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	8	0.25	0.09	0.24
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	8	0.25	0.09	0.24
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	8	0.25	0.09	0.24
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	8	0.25	0.09	0.24
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	8	0.25	0.09	0.24
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	8	0.25	0.09	0.24
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	8	0.25	0.09	0.24
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	8	0.25	0.09	0.24
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	8	0.25	0.09	0.24
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	8	0.25	0.09	0.24
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	8	0.25	0.09	0.24
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	8	0.25	0.09	0.24
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	8	0.21	0.07	0.21
(1,1967)	1:124:A:LYS:HB2	1:14:A:GLU:HB3	7	0.9	0.37	0.88
(1,1788)	1:47:A:ASN:H	1:45:A:ASN:HB3	7	0.86	0.49	1.2
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG11	7	0.79	0.13	0.82
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG12	7	0.79	0.13	0.82
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG13	7	0.79	0.13	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,491)	1:41:A:GLU:H	1:51:A:PHE:HA	7	0.72	0.22	0.75
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG2	7	0.63	0.16	0.59
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG3	7	0.63	0.16	0.59
(1,1957)	1:114:A:LEU:HD21	1:10:A:LEU:HA	7	0.62	0.48	0.46
(1,1957)	1:114:A:LEU:HD22	1:10:A:LEU:HA	7	0.62	0.48	0.46
(1,1957)	1:114:A:LEU:HD23	1:10:A:LEU:HA	7	0.62	0.48	0.46
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG11	7	0.58	0.24	0.5
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG12	7	0.58	0.24	0.5
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG13	7	0.58	0.24	0.5
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG11	7	0.58	0.24	0.5
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG12	7	0.58	0.24	0.5
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG13	7	0.58	0.24	0.5
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG11	7	0.58	0.24	0.5
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG12	7	0.58	0.24	0.5
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG13	7	0.58	0.24	0.5
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA2	7	0.56	0.16	0.52
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA3	7	0.56	0.16	0.52
(1,1978)	1:74:A:VAL:HG21	1:29:A:SER:HB3	7	0.56	0.58	0.31
(1,1978)	1:74:A:VAL:HG22	1:29:A:SER:HB3	7	0.56	0.58	0.31
(1,1978)	1:74:A:VAL:HG23	1:29:A:SER:HB3	7	0.56	0.58	0.31
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD11	7	0.56	0.29	0.6
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD12	7	0.56	0.29	0.6
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD13	7	0.56	0.29	0.6
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD11	7	0.55	0.19	0.5
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD12	7	0.55	0.19	0.5
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD13	7	0.55	0.19	0.5
(3,10)	1:10:A:LEU:H	1:40:A:TYR:O	7	0.53	0.27	0.53
(1,2019)	1:63:A:VAL:HG21	1:89:A:LEU:HB2	7	0.48	0.24	0.43
(1,2019)	1:63:A:VAL:HG22	1:89:A:LEU:HB2	7	0.48	0.24	0.43
(1,2019)	1:63:A:VAL:HG23	1:89:A:LEU:HB2	7	0.48	0.24	0.43
(1,572)	1:84:A:LEU:H	1:89:A:LEU:HG	7	0.48	0.25	0.49
(1,1885)	1:22:A:ALA:HB1	1:18:A:GLU:HB2	7	0.43	0.15	0.39
(1,1885)	1:22:A:ALA:HB2	1:18:A:GLU:HB2	7	0.43	0.15	0.39
(1,1885)	1:22:A:ALA:HB3	1:18:A:GLU:HB2	7	0.43	0.15	0.39
(1,1991)	1:82:A:THR:HB	1:61:A:LEU:HB2	7	0.4	0.13	0.44
(1,1935)	1:94:A:GLU:HG2	1:96:A:PRO:HB2	7	0.39	0.16	0.44
(1,1935)	1:94:A:GLU:HG3	1:96:A:PRO:HB2	7	0.39	0.16	0.44
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD2	7	0.39	0.14	0.44
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD3	7	0.39	0.14	0.44
(1,1799)	1:47:A:ASN:HD21	1:2:A:VAL:HB	7	0.36	0.16	0.38
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG2	7	0.35	0.23	0.28
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG3	7	0.35	0.23	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,51)	1:106:A:GLU:N	1:113:A:VAL:O	7	0.34	0.15	0.25
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB2	7	0.32	0.19	0.24
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB3	7	0.32	0.19	0.24
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG11	7	0.32	0.19	0.27
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG12	7	0.32	0.19	0.27
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG13	7	0.32	0.19	0.27
(1,614)	1:121:A:MET:H	1:118:A:ALA:HA	7	0.31	0.11	0.35
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB1	7	0.3	0.2	0.23
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB2	7	0.3	0.2	0.23
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB3	7	0.3	0.2	0.23
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB1	7	0.3	0.2	0.23
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB2	7	0.3	0.2	0.23
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB3	7	0.3	0.2	0.23
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB1	7	0.3	0.2	0.23
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB2	7	0.3	0.2	0.23
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB3	7	0.3	0.2	0.23
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE2	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE3	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE2	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE3	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE2	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE3	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE2	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE3	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE2	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE3	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE2	7	0.28	0.14	0.26
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE3	7	0.28	0.14	0.26
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD21	7	0.26	0.09	0.25
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD22	7	0.26	0.09	0.25
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD23	7	0.26	0.09	0.25
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG2	7	0.25	0.08	0.26
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG3	7	0.25	0.08	0.26
(1,409)	1:124:A:LYS:H	1:14:A:GLU:H	7	0.25	0.09	0.21
(1,627)	1:14:A:GLU:H	1:124:A:LYS:H	7	0.25	0.09	0.21
(1,725)	1:29:A:SER:H	1:32:A:LYS:HG2	7	0.25	0.08	0.21
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB2	7	0.22	0.1	0.15
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB3	7	0.22	0.1	0.15
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB2	7	0.21	0.05	0.19
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB3	7	0.21	0.05	0.19
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB2	7	0.21	0.05	0.19
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB3	7	0.21	0.05	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,33)	1:48:A:LYS:N	1:45:A:ASN:O	7	0.16	0.04	0.16
(1,1886)	1:22:A:ALA:HB1	1:18:A:GLU:HG3	6	1.13	0.22	1.18
(1,1886)	1:22:A:ALA:HB2	1:18:A:GLU:HG3	6	1.13	0.22	1.18
(1,1886)	1:22:A:ALA:HB3	1:18:A:GLU:HG3	6	1.13	0.22	1.18
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB1	6	1.13	0.22	1.18
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB2	6	1.13	0.22	1.18
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB3	6	1.13	0.22	1.18
(1,2023)	1:78:A:ILE:HG13	1:93:A:SER:HB3	6	0.92	0.42	1.0
(1,1784)	1:27:A:GLN:HE21	1:29:A:SER:H	6	0.63	0.17	0.64
(1,1791)	1:45:A:ASN:HD21	1:48:A:LYS:HG2	6	0.61	0.38	0.7
(1,1286)	1:88:A:LYS:H	1:84:A:LEU:HG	6	0.54	0.25	0.52
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB2	6	0.49	0.29	0.44
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB3	6	0.49	0.29	0.44
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB2	6	0.49	0.29	0.44
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB3	6	0.49	0.29	0.44
(1,139)	1:33:A:ALA:H	1:73:A:THR:HB	6	0.48	0.17	0.5
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB2	6	0.48	0.27	0.39
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB3	6	0.48	0.27	0.39
(3,64)	1:129:A:ARG:H	1:109:A:ASP:O	6	0.44	0.22	0.44
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB2	6	0.43	0.16	0.45
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB3	6	0.43	0.16	0.45
(1,275)	1:77:A:ASN:HB2	1:70:A:VAL:HA	6	0.4	0.17	0.37
(1,275)	1:77:A:ASN:HB3	1:70:A:VAL:HA	6	0.4	0.17	0.37
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG11	6	0.38	0.14	0.42
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG12	6	0.38	0.14	0.42
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG13	6	0.38	0.14	0.42
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG21	6	0.38	0.14	0.42
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG22	6	0.38	0.14	0.42
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG23	6	0.38	0.14	0.42
(1,430)	1:24:A:GLY:H	1:20:A:LEU:HA	6	0.36	0.13	0.39
(1,394)	1:126:A:TYR:HB2	1:113:A:VAL:HA	6	0.32	0.15	0.26
(1,113)	1:59:A:SER:H	1:53:A:SER:H	6	0.31	0.15	0.27
(1,124)	1:53:A:SER:H	1:59:A:SER:H	6	0.31	0.15	0.27
(1,2051)	1:12:A:LYS:HE2	1:126:A:TYR:HD1	6	0.3	0.1	0.29
(1,2051)	1:12:A:LYS:HE3	1:126:A:TYR:HD1	6	0.3	0.1	0.29
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG11	6	0.28	0.08	0.29
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG12	6	0.28	0.08	0.29
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG13	6	0.28	0.08	0.29
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD11	6	0.26	0.12	0.23
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD12	6	0.26	0.12	0.23
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD13	6	0.26	0.12	0.23
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB1	6	0.24	0.18	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB2	6	0.24	0.18	0.13
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB3	6	0.24	0.18	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB1	6	0.24	0.18	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB2	6	0.24	0.18	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB3	6	0.24	0.18	0.13
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB2	6	0.23	0.11	0.22
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB3	6	0.23	0.11	0.22
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB2	6	0.23	0.05	0.23
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB3	6	0.23	0.05	0.23
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG11	6	0.22	0.07	0.2
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG12	6	0.22	0.07	0.2
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG13	6	0.22	0.07	0.2
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG11	6	0.22	0.07	0.2
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG12	6	0.22	0.07	0.2
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG13	6	0.22	0.07	0.2
(1,1356)	1:99:A:ARG:H	1:95:A:LEU:HG	6	0.22	0.06	0.22
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB2	6	0.16	0.02	0.15
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB3	6	0.16	0.02	0.15
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB2	6	0.16	0.02	0.15
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB3	6	0.16	0.02	0.15
(1,1973)	1:121:A:MET:HB2	1:18:A:GLU:HG3	5	0.99	0.59	0.88
(1,1761)	1:75:A:ASN:H	1:76:A:MET:HB3	5	0.94	0.39	1.11
(1,654)	1:89:A:LEU:HA	1:84:A:LEU:HG	5	0.83	0.23	0.79
(1,1907)	1:34:A:ASN:HB2	1:30:A:ILE:HG13	5	0.67	0.18	0.67
(1,1914)	1:30:A:ILE:HG13	1:34:A:ASN:HB2	5	0.67	0.18	0.67
(1,1921)	1:48:A:LYS:HD2	1:45:A:ASN:HB3	5	0.66	0.5	0.55
(1,1921)	1:48:A:LYS:HD3	1:45:A:ASN:HB3	5	0.66	0.5	0.55
(1,1813)	1:3:A:GLN:HE22	1:45:A:ASN:HA	5	0.61	0.25	0.63
(1,257)	1:112:A:PHE:H	1:128:A:ILE:HA	5	0.57	0.39	0.48
(1,78)	1:35:A:SER:H	1:33:A:ALA:H	5	0.52	0.18	0.48
(1,390)	1:106:A:GLU:HA	1:88:A:LYS:HB3	5	0.52	0.1	0.51
(3,18)	1:124:A:LYS:H	1:14:A:GLU:O	5	0.36	0.13	0.4
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD11	5	0.33	0.22	0.27
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD12	5	0.33	0.22	0.27
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD13	5	0.33	0.22	0.27
(1,1627)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	5	0.31	0.07	0.28
(1,1627)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	5	0.31	0.07	0.28
(1,1628)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	5	0.31	0.07	0.28
(1,1628)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	5	0.31	0.07	0.28
(1,197)	1:89:A:LEU:H	1:106:A:GLU:HA	5	0.3	0.11	0.26
(1,123)	1:60:A:THR:H	1:59:A:SER:HB2	5	0.3	0.13	0.24
(1,123)	1:60:A:THR:H	1:59:A:SER:HB3	5	0.3	0.13	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE2	5	0.28	0.1	0.27
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE3	5	0.28	0.1	0.27
(1,192)	1:104:A:THR:H	1:104:A:THR:HB	5	0.23	0.07	0.23
(1,766)	1:124:A:LYS:HA	1:115:A:THR:H	5	0.21	0.09	0.16
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB2	5	0.18	0.07	0.14
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB3	5	0.18	0.07	0.14
(1,649)	1:44:A:VAL:HB	1:49:A:PHE:HA	5	0.15	0.05	0.14
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD21	4	1.32	0.14	1.32
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD22	4	1.32	0.14	1.32
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD23	4	1.32	0.14	1.32
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD11	4	0.72	0.27	0.82
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD12	4	0.72	0.27	0.82
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD13	4	0.72	0.27	0.82
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD11	4	0.72	0.27	0.82
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD12	4	0.72	0.27	0.82
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD13	4	0.72	0.27	0.82
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD11	4	0.72	0.27	0.82
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD12	4	0.72	0.27	0.82
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD13	4	0.72	0.27	0.82
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD11	4	0.64	0.07	0.62
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD12	4	0.64	0.07	0.62
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD13	4	0.64	0.07	0.62
(1,1943)	1:45:A:ASN:HB3	1:2:A:VAL:HA	4	0.64	0.32	0.58
(1,1458)	1:115:A:THR:H	1:114:A:LEU:HG	4	0.64	0.23	0.72
(1,387)	1:10:A:LEU:HG	1:38:A:VAL:HB	4	0.57	0.07	0.57
(1,1330)	1:82:A:THR:H	1:91:A:VAL:HB	4	0.57	0.11	0.54
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG12	4	0.57	0.47	0.35
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG13	4	0.57	0.47	0.35
(1,1901)	1:32:A:LYS:HE2	1:29:A:SER:HB2	4	0.56	0.39	0.45
(1,1901)	1:32:A:LYS:HE3	1:29:A:SER:HB2	4	0.56	0.39	0.45
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD21	4	0.48	0.22	0.52
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD22	4	0.48	0.22	0.52
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD23	4	0.48	0.22	0.52
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD21	4	0.48	0.22	0.52
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD22	4	0.48	0.22	0.52
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD23	4	0.48	0.22	0.52
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD21	4	0.48	0.22	0.52
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD22	4	0.48	0.22	0.52
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD23	4	0.48	0.22	0.52
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE2	4	0.47	0.27	0.4
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE3	4	0.47	0.27	0.4
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD2	4	0.44	0.17	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD3	4	0.44	0.17	0.37
(1,12)	1:130:A:THR:H	1:8:A:TYR:HA	4	0.38	0.18	0.35
(1,1923)	1:67:A:VAL:HG21	1:65:A:GLU:HB2	4	0.37	0.22	0.32
(1,1923)	1:67:A:VAL:HG22	1:65:A:GLU:HB2	4	0.37	0.22	0.32
(1,1923)	1:67:A:VAL:HG23	1:65:A:GLU:HB2	4	0.37	0.22	0.32
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD21	4	0.37	0.13	0.32
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD22	4	0.37	0.13	0.32
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD23	4	0.37	0.13	0.32
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD21	4	0.37	0.13	0.32
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD22	4	0.37	0.13	0.32
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD23	4	0.37	0.13	0.32
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG2	4	0.37	0.13	0.32
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG3	4	0.37	0.13	0.32
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG2	4	0.37	0.13	0.32
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG3	4	0.37	0.13	0.32
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG2	4	0.37	0.13	0.32
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG3	4	0.37	0.13	0.32
(1,2032)	1:105:A:TYR:HB2	1:112:A:PHE:HA	4	0.37	0.12	0.38
(1,2032)	1:105:A:TYR:HB3	1:112:A:PHE:HA	4	0.37	0.12	0.38
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB2	4	0.35	0.17	0.37
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB3	4	0.35	0.17	0.37
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB1	4	0.34	0.2	0.26
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB2	4	0.34	0.2	0.26
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB3	4	0.34	0.2	0.26
(1,347)	1:43:A:ILE:H	1:50:A:THR:HB	4	0.34	0.19	0.26
(3,34)	1:48:A:LYS:H	1:45:A:ASN:O	4	0.28	0.07	0.3
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG11	4	0.28	0.17	0.22
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG12	4	0.28	0.17	0.22
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG13	4	0.28	0.17	0.22
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG21	4	0.28	0.17	0.22
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG22	4	0.28	0.17	0.22
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG23	4	0.28	0.17	0.22
(1,2052)	1:14:A:GLU:HB2	1:126:A:TYR:HD1	4	0.28	0.09	0.24
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB2	4	0.28	0.1	0.28
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB3	4	0.28	0.1	0.28
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD11	4	0.28	0.11	0.26
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD12	4	0.28	0.11	0.26
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD13	4	0.28	0.11	0.26
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG11	4	0.26	0.05	0.25
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG12	4	0.26	0.05	0.25
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG13	4	0.26	0.05	0.25
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG21	4	0.26	0.05	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG22	4	0.26	0.05	0.25
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG23	4	0.26	0.05	0.25
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG11	4	0.26	0.05	0.25
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG12	4	0.26	0.05	0.25
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG13	4	0.26	0.05	0.25
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG21	4	0.26	0.05	0.25
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG22	4	0.26	0.05	0.25
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG23	4	0.26	0.05	0.25
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD11	4	0.25	0.07	0.25
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD12	4	0.25	0.07	0.25
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD13	4	0.25	0.07	0.25
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD21	4	0.25	0.07	0.25
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD22	4	0.25	0.07	0.25
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD23	4	0.25	0.07	0.25
(1,1638)	1:130:A:THR:H	1:7:A:THR:H	4	0.25	0.06	0.26
(1,1639)	1:7:A:THR:H	1:130:A:THR:H	4	0.25	0.06	0.26
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD21	4	0.23	0.09	0.2
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD22	4	0.23	0.09	0.2
(1,1755)	1:60:A:THR:H	1:61:A:LEU:HG	4	0.23	0.09	0.21
(1,1566)	1:43:A:ILE:HB	1:7:A:THR:HB	4	0.2	0.07	0.2
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB2	4	0.2	0.07	0.19
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB3	4	0.2	0.07	0.19
(1,1822)	1:34:A:ASN:HD21	1:71:A:LEU:HB2	4	0.19	0.06	0.17
(3,11)	1:12:A:LYS:N	1:126:A:TYR:O	4	0.18	0.05	0.18
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG11	4	0.14	0.03	0.12
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG12	4	0.14	0.03	0.12
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG13	4	0.14	0.03	0.12
(1,743)	1:121:A:MET:HB3	1:18:A:GLU:HG3	3	1.13	0.41	1.31
(1,1902)	1:32:A:LYS:HE2	1:29:A:SER:HB3	3	0.91	0.13	0.86
(1,1902)	1:32:A:LYS:HE3	1:29:A:SER:HB3	3	0.91	0.13	0.86
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD11	3	0.79	0.13	0.78
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD12	3	0.79	0.13	0.78
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD13	3	0.79	0.13	0.78
(1,754)	1:79:A:LYS:HG3	1:68:A:GLU:HA	3	0.72	0.16	0.71
(1,1770)	1:13:A:ASN:HD21	1:10:A:LEU:HG	3	0.7	0.2	0.56
(1,1906)	1:27:A:GLN:HA	1:30:A:ILE:HG13	3	0.64	0.18	0.58
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD21	3	0.58	0.15	0.56
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD22	3	0.58	0.15	0.56
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD23	3	0.58	0.15	0.56
(1,1970)	1:124:A:LYS:HG3	1:14:A:GLU:HB3	3	0.52	0.14	0.54
(1,217)	1:116:A:MET:H	1:115:A:THR:HG21	3	0.49	0.09	0.53
(1,217)	1:116:A:MET:H	1:115:A:THR:HG22	3	0.49	0.09	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,217)	1:116:A:MET:H	1:115:A:THR:HG23	3	0.49	0.09	0.53
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG11	3	0.49	0.16	0.57
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG12	3	0.49	0.16	0.57
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG13	3	0.49	0.16	0.57
(1,2047)	1:113:A:VAL:HG21	1:124:A:LYS:HB2	3	0.44	0.31	0.27
(1,2047)	1:113:A:VAL:HG22	1:124:A:LYS:HB2	3	0.44	0.31	0.27
(1,2047)	1:113:A:VAL:HG23	1:124:A:LYS:HB2	3	0.44	0.31	0.27
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG11	3	0.42	0.06	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG12	3	0.42	0.06	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG13	3	0.42	0.06	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG21	3	0.42	0.06	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG22	3	0.42	0.06	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG23	3	0.42	0.06	0.46
(1,276)	1:25:A:VAL:HG11	1:74:A:VAL:HB	3	0.42	0.06	0.46
(1,276)	1:25:A:VAL:HG12	1:74:A:VAL:HB	3	0.42	0.06	0.46
(1,276)	1:25:A:VAL:HG13	1:74:A:VAL:HB	3	0.42	0.06	0.46
(1,276)	1:25:A:VAL:HG21	1:74:A:VAL:HB	3	0.42	0.06	0.46
(1,276)	1:25:A:VAL:HG22	1:74:A:VAL:HB	3	0.42	0.06	0.46
(1,276)	1:25:A:VAL:HG23	1:74:A:VAL:HB	3	0.42	0.06	0.46
(1,907)	1:25:A:VAL:H	1:23:A:LEU:HG	3	0.39	0.1	0.38
(1,2056)	1:14:A:GLU:HB3	1:126:A:TYR:HE1	3	0.37	0.17	0.44
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG21	3	0.36	0.05	0.33
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG22	3	0.36	0.05	0.33
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG23	3	0.36	0.05	0.33
(1,594)	1:93:A:SER:H	1:101:A:GLY:H	3	0.36	0.12	0.33
(1,392)	1:79:A:LYS:HE2	1:94:A:GLU:HG2	3	0.33	0.1	0.26
(1,392)	1:79:A:LYS:HE2	1:94:A:GLU:HG3	3	0.33	0.1	0.26
(1,392)	1:79:A:LYS:HE3	1:94:A:GLU:HG2	3	0.33	0.1	0.26
(1,392)	1:79:A:LYS:HE3	1:94:A:GLU:HG3	3	0.33	0.1	0.26
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB1	3	0.32	0.14	0.23
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB2	3	0.32	0.14	0.23
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB3	3	0.32	0.14	0.23
(1,193)	1:104:A:THR:H	1:104:A:THR:HG21	3	0.32	0.12	0.29
(1,193)	1:104:A:THR:H	1:104:A:THR:HG22	3	0.32	0.12	0.29
(1,193)	1:104:A:THR:H	1:104:A:THR:HG23	3	0.32	0.12	0.29
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG21	3	0.31	0.02	0.31
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG22	3	0.31	0.02	0.31
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG23	3	0.31	0.02	0.31
(1,1793)	1:87:A:SER:H	1:85:A:GLU:HG2	3	0.31	0.2	0.25
(1,1793)	1:87:A:SER:H	1:85:A:GLU:HG3	3	0.31	0.2	0.25
(1,383)	1:36:A:PRO:HG2	1:12:A:LYS:HA	3	0.3	0.13	0.31
(1,383)	1:36:A:PRO:HG3	1:12:A:LYS:HA	3	0.3	0.13	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1757)	1:64:A:ASN:HD22	1:63:A:VAL:HB	3	0.29	0.09	0.33
(1,1053)	1:48:A:LYS:H	1:45:A:ASN:HA	3	0.25	0.07	0.2
(1,55)	1:24:A:GLY:H	1:23:A:LEU:HB2	3	0.24	0.1	0.19
(1,55)	1:24:A:GLY:H	1:23:A:LEU:HB3	3	0.24	0.1	0.19
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD21	3	0.24	0.08	0.22
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD22	3	0.24	0.08	0.22
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD23	3	0.24	0.08	0.22
(1,2059)	1:11:A:GLU:HA	1:127:A:PHE:HA	3	0.24	0.07	0.24
(1,1322)	1:105:A:TYR:H	1:89:A:LEU:HG	3	0.23	0.09	0.23
(1,1459)	1:125:A:ARG:H	1:114:A:LEU:HG	3	0.23	0.06	0.27
(3,49)	1:101:A:GLY:N	1:93:A:SER:O	3	0.21	0.07	0.21
(1,2028)	1:91:A:VAL:HA	1:103:A:ARG:HB2	3	0.2	0.09	0.18
(1,214)	1:125:A:ARG:H	1:114:A:LEU:H	3	0.2	0.05	0.23
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG11	3	0.2	0.05	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG12	3	0.2	0.05	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG13	3	0.2	0.05	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG21	3	0.2	0.05	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG22	3	0.2	0.05	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG23	3	0.2	0.05	0.19
(1,2033)	1:126:A:TYR:HA	1:113:A:VAL:HB	3	0.19	0.06	0.17
(1,1786)	1:31:A:LYS:H	1:27:A:GLN:HB2	3	0.19	0.03	0.2
(1,448)	1:31:A:LYS:H	1:30:A:ILE:HG12	3	0.17	0.05	0.14
(1,448)	1:31:A:LYS:H	1:30:A:ILE:HG13	3	0.17	0.05	0.14
(1,1494)	1:124:A:LYS:H	1:124:A:LYS:HE2	3	0.16	0.04	0.19
(1,1494)	1:124:A:LYS:H	1:124:A:LYS:HE3	3	0.16	0.04	0.19
(1,59)	1:27:A:GLN:H	1:26:A:PRO:HB2	3	0.16	0.01	0.15
(1,59)	1:27:A:GLN:H	1:26:A:PRO:HB3	3	0.16	0.01	0.15
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG11	3	0.16	0.04	0.15
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG12	3	0.16	0.04	0.15
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG13	3	0.16	0.04	0.15
(1,129)	1:51:A:PHE:H	1:62:A:ILE:HA	3	0.15	0.06	0.11
(1,187)	1:104:A:THR:H	1:103:A:ARG:HB2	3	0.13	0.02	0.11
(1,187)	1:104:A:THR:H	1:103:A:ARG:HB3	3	0.13	0.02	0.11
(1,188)	1:104:A:THR:H	1:103:A:ARG:HB2	3	0.13	0.02	0.11
(1,188)	1:104:A:THR:H	1:103:A:ARG:HB3	3	0.13	0.02	0.11
(1,542)	1:79:A:LYS:H	1:79:A:LYS:HD2	3	0.13	0.0	0.13
(1,542)	1:79:A:LYS:H	1:79:A:LYS:HD3	3	0.13	0.0	0.13
(1,852)	1:15:A:ASN:H	1:16:A:PHE:HB2	3	0.12	0.0	0.12
(1,852)	1:15:A:ASN:H	1:16:A:PHE:HB3	3	0.12	0.0	0.12
(1,1630)	1:113:A:VAL:HG11	1:126:A:TYR:HE1	3	0.12	0.02	0.11
(1,1630)	1:113:A:VAL:HG12	1:126:A:TYR:HE1	3	0.12	0.02	0.11
(1,1630)	1:113:A:VAL:HG13	1:126:A:TYR:HE1	3	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2057)	1:113:A:VAL:HG11	1:126:A:TYR:HE1	3	0.12	0.02	0.11
(1,2057)	1:113:A:VAL:HG12	1:126:A:TYR:HE1	3	0.12	0.02	0.11
(1,2057)	1:113:A:VAL:HG13	1:126:A:TYR:HE1	3	0.12	0.02	0.11
(1,2042)	1:93:A:SER:HB3	1:116:A:MET:HG3	2	1.12	0.12	1.12
(1,1905)	1:27:A:GLN:HA	1:30:A:ILE:HG12	2	0.81	0.13	0.81
(1,1972)	1:27:A:GLN:HA	1:17:A:GLU:HA	2	0.72	0.06	0.72
(1,451)	1:35:A:SER:H	1:31:A:LYS:HA	2	0.57	0.04	0.57
(1,1956)	1:130:A:THR:HB	1:9:A:LYS:HB2	2	0.54	0.02	0.54
(1,1956)	1:130:A:THR:HB	1:9:A:LYS:HB3	2	0.54	0.02	0.54
(1,2064)	1:9:A:LYS:HB2	1:130:A:THR:HB	2	0.54	0.02	0.54
(1,2064)	1:9:A:LYS:HB3	1:130:A:THR:HB	2	0.54	0.02	0.54
(3,20)	1:19:A:TYR:H	1:15:A:ASN:O	2	0.53	0.09	0.53
(1,1974)	1:121:A:MET:HB2	1:19:A:TYR:HA	2	0.5	0.3	0.5
(1,2045)	1:19:A:TYR:HA	1:121:A:MET:HB2	2	0.5	0.3	0.5
(1,2041)	1:93:A:SER:HB2	1:116:A:MET:HG3	2	0.5	0.21	0.5
(1,1948)	1:44:A:VAL:HB	1:4:A:LEU:HB3	2	0.48	0.01	0.48
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG21	2	0.48	0.09	0.48
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG22	2	0.48	0.09	0.48
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG23	2	0.48	0.09	0.48
(1,1779)	1:15:A:ASN:HD22	1:18:A:GLU:HB3	2	0.44	0.21	0.44
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG11	2	0.43	0.04	0.43
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG12	2	0.43	0.04	0.43
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG13	2	0.43	0.04	0.43
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD11	2	0.42	0.08	0.42
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD12	2	0.42	0.08	0.42
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD13	2	0.42	0.08	0.42
(1,186)	1:102:A:THR:H	1:102:A:THR:HG21	2	0.4	0.06	0.4
(1,186)	1:102:A:THR:H	1:102:A:THR:HG22	2	0.4	0.06	0.4
(1,186)	1:102:A:THR:H	1:102:A:THR:HG23	2	0.4	0.06	0.4
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG11	2	0.38	0.05	0.38
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG12	2	0.38	0.05	0.38
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG13	2	0.38	0.05	0.38
(1,377)	1:74:A:VAL:HG11	1:71:A:LEU:HB2	2	0.38	0.17	0.38
(1,377)	1:74:A:VAL:HG12	1:71:A:LEU:HB2	2	0.38	0.17	0.38
(1,377)	1:74:A:VAL:HG13	1:71:A:LEU:HB2	2	0.38	0.17	0.38
(1,2004)	1:93:A:SER:HB2	1:78:A:ILE:HG12	2	0.37	0.25	0.37
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD21	2	0.36	0.24	0.36
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD22	2	0.36	0.24	0.36
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD23	2	0.36	0.24	0.36
(1,183)	1:99:A:ARG:H	1:99:A:ARG:HD2	2	0.36	0.12	0.36
(1,183)	1:99:A:ARG:H	1:99:A:ARG:HD3	2	0.36	0.12	0.36
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG21	2	0.35	0.13	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG22	2	0.35	0.13	0.35
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG23	2	0.35	0.13	0.35
(1,1737)	1:43:A:ILE:HG12	1:41:A:GLU:HB2	2	0.33	0.19	0.33
(1,1737)	1:43:A:ILE:HG12	1:41:A:GLU:HB3	2	0.33	0.19	0.33
(1,1737)	1:43:A:ILE:HG13	1:41:A:GLU:HB2	2	0.33	0.19	0.33
(1,1737)	1:43:A:ILE:HG13	1:41:A:GLU:HB3	2	0.33	0.19	0.33
(1,1531)	1:130:A:THR:HB	1:7:A:THR:HB	2	0.32	0.2	0.32
(1,643)	1:126:A:TYR:HB2	1:12:A:LYS:HB2	2	0.3	0.1	0.3
(1,643)	1:126:A:TYR:HB2	1:12:A:LYS:HB3	2	0.3	0.1	0.3
(1,643)	1:126:A:TYR:HB3	1:12:A:LYS:HB2	2	0.3	0.1	0.3
(1,643)	1:126:A:TYR:HB3	1:12:A:LYS:HB3	2	0.3	0.1	0.3
(1,644)	1:126:A:TYR:HB2	1:12:A:LYS:HB2	2	0.3	0.1	0.3
(1,644)	1:126:A:TYR:HB2	1:12:A:LYS:HB3	2	0.3	0.1	0.3
(1,644)	1:126:A:TYR:HB3	1:12:A:LYS:HB2	2	0.3	0.1	0.3
(1,644)	1:126:A:TYR:HB3	1:12:A:LYS:HB3	2	0.3	0.1	0.3
(1,157)	1:85:A:GLU:H	1:86:A:GLY:H	2	0.3	0.05	0.3
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG21	2	0.3	0.05	0.3
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG22	2	0.3	0.05	0.3
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG23	2	0.3	0.05	0.3
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG11	2	0.28	0.0	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG12	2	0.28	0.0	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG13	2	0.28	0.0	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG21	2	0.28	0.0	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG22	2	0.28	0.0	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG23	2	0.28	0.0	0.28
(1,5)	1:5:A:ALA:H	1:4:A:LEU:HB2	2	0.26	0.02	0.26
(1,5)	1:5:A:ALA:H	1:4:A:LEU:HB3	2	0.26	0.02	0.26
(1,441)	1:29:A:SER:H	1:27:A:GLN:HA	2	0.26	0.06	0.26
(1,554)	1:84:A:LEU:H	1:83:A:LYS:HG2	2	0.26	0.01	0.26
(1,554)	1:84:A:LEU:H	1:83:A:LYS:HG3	2	0.26	0.01	0.26
(1,764)	1:12:A:LYS:HE2	1:126:A:TYR:HE1	2	0.24	0.1	0.24
(1,764)	1:12:A:LYS:HE3	1:126:A:TYR:HE1	2	0.24	0.1	0.24
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD11	2	0.24	0.03	0.24
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD12	2	0.24	0.03	0.24
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD13	2	0.24	0.03	0.24
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD11	2	0.24	0.03	0.24
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD12	2	0.24	0.03	0.24
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD13	2	0.24	0.03	0.24
(1,268)	1:31:A:LYS:HB2	1:28:A:ASP:HA	2	0.24	0.11	0.24
(1,268)	1:31:A:LYS:HB3	1:28:A:ASP:HA	2	0.24	0.11	0.24
(1,269)	1:28:A:ASP:HA	1:31:A:LYS:HB2	2	0.24	0.11	0.24
(1,269)	1:28:A:ASP:HA	1:31:A:LYS:HB3	2	0.24	0.11	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,386)	1:31:A:LYS:HB2	1:28:A:ASP:HA	2	0.24	0.11	0.24
(1,386)	1:31:A:LYS:HB3	1:28:A:ASP:HA	2	0.24	0.11	0.24
(1,140)	1:73:A:THR:H	1:73:A:THR:HB	2	0.24	0.0	0.24
(1,1632)	1:9:A:LYS:HA	1:127:A:PHE:HD1	2	0.22	0.02	0.22
(1,1632)	1:9:A:LYS:HA	1:127:A:PHE:HD2	2	0.22	0.02	0.22
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD11	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD12	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD13	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD21	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD22	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD23	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD11	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD12	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD13	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD21	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD22	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD23	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD11	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD12	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD13	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD21	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD22	2	0.22	0.04	0.22
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD23	2	0.22	0.04	0.22
(1,356)	1:63:A:VAL:H	1:62:A:ILE:HA	2	0.21	0.06	0.21
(1,348)	1:116:A:MET:HA	1:103:A:ARG:HG2	2	0.2	0.06	0.2
(1,348)	1:116:A:MET:HA	1:103:A:ARG:HG3	2	0.2	0.06	0.2
(1,1823)	1:34:A:ASN:HD22	1:71:A:LEU:HB2	2	0.2	0.03	0.2
(1,583)	1:101:A:GLY:H	1:93:A:SER:HB2	2	0.2	0.03	0.2
(1,583)	1:101:A:GLY:H	1:93:A:SER:HB3	2	0.2	0.03	0.2
(1,265)	1:130:A:THR:H	1:130:A:THR:HG21	2	0.18	0.05	0.18
(1,265)	1:130:A:THR:H	1:130:A:THR:HG22	2	0.18	0.05	0.18
(1,265)	1:130:A:THR:H	1:130:A:THR:HG23	2	0.18	0.05	0.18
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD11	2	0.18	0.06	0.18
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD12	2	0.18	0.06	0.18
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD13	2	0.18	0.06	0.18
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD21	2	0.18	0.06	0.18
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD22	2	0.18	0.06	0.18
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD23	2	0.18	0.06	0.18
(1,1703)	1:104:A:THR:H	1:115:A:THR:HB	2	0.18	0.04	0.18
(1,25)	1:128:A:ILE:H	1:11:A:GLU:HG2	2	0.18	0.06	0.18
(1,25)	1:128:A:ILE:H	1:11:A:GLU:HG3	2	0.18	0.06	0.18
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD11	2	0.17	0.04	0.17

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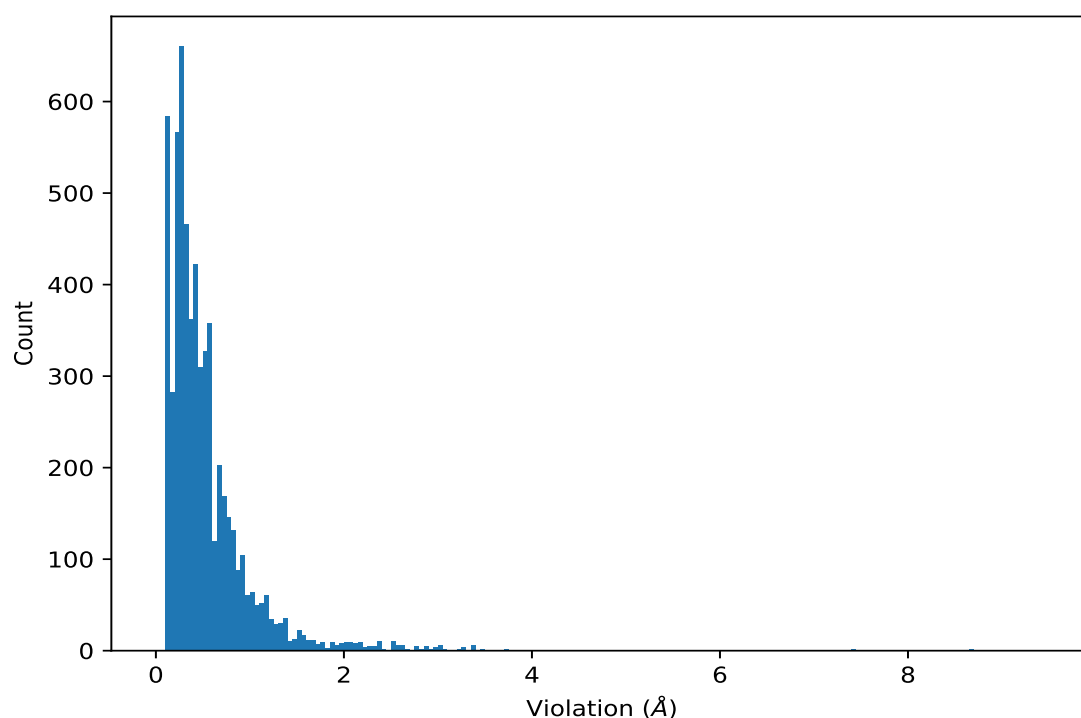
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD12	2	0.17	0.04	0.17
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD13	2	0.17	0.04	0.17
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD21	2	0.17	0.04	0.17
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD22	2	0.17	0.04	0.17
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD23	2	0.17	0.04	0.17
(1,1645)	1:14:A:GLU:H	1:124:A:LYS:HB2	2	0.17	0.05	0.17
(1,1645)	1:14:A:GLU:H	1:124:A:LYS:HB3	2	0.17	0.05	0.17
(1,1646)	1:14:A:GLU:H	1:124:A:LYS:HB2	2	0.17	0.05	0.17
(1,1646)	1:14:A:GLU:H	1:124:A:LYS:HB3	2	0.17	0.05	0.17
(1,1706)	1:77:A:ASN:H	1:96:A:PRO:HG2	2	0.16	0.03	0.16
(1,1706)	1:77:A:ASN:H	1:96:A:PRO:HG3	2	0.16	0.03	0.16
(1,1036)	1:50:A:THR:H	1:43:A:ILE:HB	2	0.16	0.05	0.16
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD21	2	0.16	0.04	0.16
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD22	2	0.16	0.04	0.16
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD23	2	0.16	0.04	0.16
(1,135)	1:66:A:GLU:H	1:65:A:GLU:HB2	2	0.14	0.03	0.14
(1,135)	1:66:A:GLU:H	1:65:A:GLU:HB3	2	0.14	0.03	0.14
(1,1168)	1:66:A:GLU:H	1:65:A:GLU:HB2	2	0.14	0.03	0.14
(1,1168)	1:66:A:GLU:H	1:65:A:GLU:HB3	2	0.14	0.03	0.14
(3,61)	1:116:A:MET:N	1:123:A:ALA:O	2	0.14	0.01	0.14
(1,553)	1:83:A:LYS:H	1:83:A:LYS:HG2	2	0.12	0.01	0.12
(1,553)	1:83:A:LYS:H	1:83:A:LYS:HG3	2	0.12	0.01	0.12
(1,722)	1:5:A:ALA:H	1:3:A:GLN:HG2	2	0.12	0.01	0.12
(1,722)	1:5:A:ALA:H	1:3:A:GLN:HG3	2	0.12	0.01	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)
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	4	9.49
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	5	8.7
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	7	8.66
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	8	7.92
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	9	7.78
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	10	7.71
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	2	7.52
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	6	7.43
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	3	7.41
(1,1982)	1:37:A:GLY:HA3	1:31:A:LYS:HG2	1	7.22
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	8	4.88
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	4	4.57
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	3	4.44
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	7	4.16
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	9	4.05
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	5	4.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	4	3.78
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	8	3.72
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	10	3.71
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	3	3.64
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	7	3.48
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	2	3.47
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	2	3.38
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	4	3.37
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	4	3.37
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	8	3.35
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	8	3.35
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	8	3.35
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	5	3.29
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	4	3.27
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	5	3.26
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	5	3.26
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	10	3.24
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	1	3.23
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	3	3.14
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	6	3.09
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	3	3.06
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	1	3.05
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	1	3.05
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	9	3.04
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	8	3.03
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	8	3.02
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	8	3.02
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	10	2.98
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	10	2.98
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	10	2.97
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	9	2.96
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	3	2.94
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	9	2.93
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	8	2.89
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	8	2.88
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	5	2.87
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	10	2.87
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	7	2.87
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	7	2.81
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	7	2.81
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	6	2.79
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	3	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	3	2.79
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	3	2.79
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	2	2.75
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	10	2.69
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	6	2.68
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	4	2.63
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	4	2.63
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	9	2.62
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	2	2.6
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	2	2.6
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	2	2.6
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	4	2.59
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	4	2.59
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	4	2.59
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	8	2.58
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	9	2.57
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	4	2.56
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	9	2.55
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	9	2.55
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	9	2.55
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	2	2.52
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	6	2.52
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	6	2.52
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	9	2.52
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	9	2.52
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	6	2.51
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	5	2.5
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	5	2.43
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	1	2.41
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	8	2.38
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	8	2.38
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	8	2.37
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	1	2.37
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	1	2.37
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	1	2.37
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	5	2.36
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	6	2.36
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	4	2.36
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	4	2.36
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	2	2.34
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	2	2.34
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	2	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	8	2.32
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	4	2.32
(1,388)	1:49:A:PHE:HB3	1:63:A:VAL:HB	2	2.3
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	3	2.28
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	3	2.28
(1,393)	1:77:A:ASN:HB2	1:96:A:PRO:HG3	2	2.25
(1,393)	1:77:A:ASN:HB3	1:96:A:PRO:HG3	2	2.25
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	6	2.21
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	2	2.2
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	2	2.2
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	1	2.2
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	3	2.19
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	7	2.19
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	1	2.18
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	7	2.18
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	10	2.16
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	5	2.16
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	5	2.15
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	5	2.15
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	5	2.15
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	3	2.13
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	3	2.13
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	8	2.12
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	8	2.12
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	4	2.12
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	7	2.12
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	1	2.11
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	9	2.1
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	2	2.08
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	2	2.08
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	9	2.07
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	9	2.07
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	2	2.06
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	9	2.06
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	3	2.06
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	3	2.06
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	9	2.06
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	4	2.05
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	4	2.05
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	9	2.03
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	9	2.03
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	5	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	5	2.02
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	8	2.01
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	8	2.01
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	8	2.01
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	1	1.99
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	5	1.97
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	1	1.97
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	5	1.97
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	5	1.97
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	5	1.97
(1,2027)	1:77:A:ASN:HA	1:96:A:PRO:HG3	3	1.96
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	10	1.96
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	10	1.93
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	10	1.93
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	10	1.93
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	5	1.91
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	5	1.91
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	7	1.91
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	8	1.9
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	8	1.9
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	5	1.87
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	4	1.87
(1,1960)	1:125:A:ARG:HB2	1:10:A:LEU:HB3	1	1.87
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	2	1.87
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	5	1.85
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	5	1.85
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	8	1.85
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	10	1.82
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	7	1.8
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	7	1.8
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	1	1.79
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	4	1.79
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	3	1.78
(1,1973)	1:121:A:MET:HB2	1:18:A:GLU:HG3	1	1.77
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	6	1.77
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	6	1.76
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	6	1.76
(1,1904)	1:34:A:ASN:HB3	1:30:A:ILE:HB	2	1.76
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	2	1.76
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	8	1.73
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	4	1.71
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	4	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	4	1.71
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	3	1.71
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	10	1.71
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	1	1.71
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	1	1.7
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	1	1.7
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	1	1.7
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	6	1.7
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	2	1.7
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	6	1.7
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	6	1.7
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	6	1.7
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	10	1.69
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	8	1.69
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	10	1.66
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	6	1.64
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	10	1.62
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	10	1.62
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	6	1.62
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	1	1.62
(1,1978)	1:74:A:VAL:HG21	1:29:A:SER:HB3	9	1.61
(1,1978)	1:74:A:VAL:HG22	1:29:A:SER:HB3	9	1.61
(1,1978)	1:74:A:VAL:HG23	1:29:A:SER:HB3	9	1.61
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	5	1.61
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	7	1.61
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	6	1.6
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	6	1.59
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	6	1.59
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	9	1.59
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	6	1.59
(1,1921)	1:48:A:LYS:HD2	1:45:A:ASN:HB3	7	1.58
(1,1921)	1:48:A:LYS:HD3	1:45:A:ASN:HB3	7	1.58
(1,2023)	1:78:A:ILE:HG13	1:93:A:SER:HB3	8	1.57
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	9	1.57
(1,1973)	1:121:A:MET:HB2	1:18:A:GLU:HG3	9	1.57
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	8	1.57
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	10	1.57
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	6	1.56
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	4	1.55
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	4	1.55
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	5	1.55
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	5	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	5	1.55
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	4	1.54
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	4	1.54
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	5	1.54
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	1	1.52
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	1	1.52
(1,743)	1:121:A:MET:HB3	1:18:A:GLU:HG3	1	1.52
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	8	1.52
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	8	1.52
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	8	1.52
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	8	1.52
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	3	1.51
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	3	1.51
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	3	1.51
(1,1957)	1:114:A:LEU:HD21	1:10:A:LEU:HA	6	1.51
(1,1957)	1:114:A:LEU:HD22	1:10:A:LEU:HA	6	1.51
(1,1957)	1:114:A:LEU:HD23	1:10:A:LEU:HA	6	1.51
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	3	1.51
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD21	7	1.5
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD22	7	1.5
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD23	7	1.5
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	5	1.5
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	2	1.5
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	8	1.49
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	6	1.49
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	7	1.49
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	3	1.49
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	10	1.48
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	10	1.48
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	10	1.48
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	1	1.47
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	4	1.47
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	9	1.46
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG11	6	1.46
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG12	6	1.46
(1,379)	1:48:A:LYS:HG3	1:2:A:VAL:HG13	6	1.46
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	7	1.45
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	5	1.45
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	8	1.44
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	10	1.43
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	9	1.43
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	3	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	2	1.41
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	2	1.41
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	2	1.41
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	2	1.41
(1,1979)	1:75:A:ASN:HB3	1:29:A:SER:HB3	1	1.4
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	2	1.4
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	10	1.39
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	10	1.39
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	9	1.39
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	9	1.39
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	9	1.39
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD21	1	1.39
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD22	1	1.39
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD23	1	1.39
(1,791)	1:129:A:ARG:H	1:7:A:THR:HA	7	1.39
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	5	1.39
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	10	1.39
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	6	1.39
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	2	1.39
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG12	1	1.38
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG13	1	1.38
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	8	1.37
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB1	1	1.37
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB2	1	1.37
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB3	1	1.37
(1,1886)	1:22:A:ALA:HB1	1:18:A:GLU:HG3	1	1.37
(1,1886)	1:22:A:ALA:HB2	1:18:A:GLU:HG3	1	1.37
(1,1886)	1:22:A:ALA:HB3	1:18:A:GLU:HG3	1	1.37
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	4	1.37
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB1	9	1.36
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB2	9	1.36
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB3	9	1.36
(1,1886)	1:22:A:ALA:HB1	1:18:A:GLU:HG3	9	1.36
(1,1886)	1:22:A:ALA:HB2	1:18:A:GLU:HG3	9	1.36
(1,1886)	1:22:A:ALA:HB3	1:18:A:GLU:HG3	9	1.36
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	2	1.36
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	8	1.36
(1,1788)	1:47:A:ASN:H	1:45:A:ASN:HB3	4	1.35
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	3	1.35
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	4	1.35
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	8	1.33
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	5	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	10	1.33
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	10	1.33
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	10	1.33
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	10	1.33
(3,27)	1:23:A:LEU:N	1:19:A:TYR:O	2	1.32
(1,1967)	1:124:A:LYS:HB2	1:14:A:GLU:HB3	8	1.32
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	5	1.32
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	3	1.32
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	3	1.32
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	3	1.32
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	6	1.32
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB2	3	1.31
(1,2062)	1:111:A:GLY:HA3	1:129:A:ARG:HB3	3	1.31
(1,743)	1:121:A:MET:HB3	1:18:A:GLU:HG3	9	1.31
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	3	1.31
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	7	1.31
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	7	1.31
(1,1978)	1:74:A:VAL:HG21	1:29:A:SER:HB3	1	1.3
(1,1978)	1:74:A:VAL:HG22	1:29:A:SER:HB3	1	1.3
(1,1978)	1:74:A:VAL:HG23	1:29:A:SER:HB3	1	1.3
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	10	1.3
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	10	1.3
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	10	1.3
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	2	1.3
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	7	1.3
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	10	1.3
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	10	1.3
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	10	1.3
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	7	1.29
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	7	1.29
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	7	1.29
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	1	1.29
(1,746)	1:75:A:ASN:HB2	1:29:A:SER:HB3	1	1.29
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	3	1.28
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	1	1.27
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	5	1.27
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	5	1.27
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	5	1.27
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	8	1.27
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	8	1.26
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	8	1.26
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	8	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1967)	1:124:A:LYS:HB2	1:14:A:GLU:HB3	7	1.26
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	6	1.26
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD21	10	1.26
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD22	10	1.26
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD23	10	1.26
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	3	1.26
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	5	1.26
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	1	1.25
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	1	1.25
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	1	1.25
(1,1788)	1:47:A:ASN:H	1:45:A:ASN:HB3	2	1.25
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	1	1.25
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	1	1.25
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	1	1.25
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	1	1.25
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	9	1.24
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	8	1.23
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	8	1.23
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	8	1.23
(1,2042)	1:93:A:SER:HB3	1:116:A:MET:HG3	1	1.23
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	6	1.23
(1,1788)	1:47:A:ASN:H	1:45:A:ASN:HB3	9	1.23
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	10	1.23
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB1	10	1.22
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB2	10	1.22
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB3	10	1.22
(1,1886)	1:22:A:ALA:HB1	1:18:A:GLU:HG3	10	1.22
(1,1886)	1:22:A:ALA:HB2	1:18:A:GLU:HG3	10	1.22
(1,1886)	1:22:A:ALA:HB3	1:18:A:GLU:HG3	10	1.22
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	1	1.22
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	4	1.22
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	4	1.22
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	4	1.22
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	3	1.22
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	10	1.21
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	1	1.21
(1,1967)	1:124:A:LYS:HB2	1:14:A:GLU:HB3	9	1.21
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	8	1.21
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	8	1.21
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	7	1.21
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	1	1.21
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	1	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	1	1.21
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	2	1.21
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	2	1.21
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	1	1.21
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	3	1.21
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	3	1.21
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	3	1.21
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	10	1.2
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	10	1.2
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	6	1.2
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	3	1.2
(1,1788)	1:47:A:ASN:H	1:45:A:ASN:HB3	3	1.2
(1,1761)	1:75:A:ASN:H	1:76:A:MET:HB3	2	1.2
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	4	1.2
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	4	1.2
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	4	1.2
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	9	1.2
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	9	1.2
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	4	1.2
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	1	1.2
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	1	1.19
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	1	1.19
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	3	1.19
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	8	1.19
(1,654)	1:89:A:LEU:HA	1:84:A:LEU:HG	8	1.19
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	5	1.19
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	4	1.19
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	4	1.19
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	2	1.19
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	2	1.19
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	2	1.19
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	5	1.19
(1,1968)	1:124:A:LYS:HB3	1:14:A:GLU:HB3	2	1.18
(1,1957)	1:114:A:LEU:HD21	1:10:A:LEU:HA	3	1.18
(1,1957)	1:114:A:LEU:HD22	1:10:A:LEU:HA	3	1.18
(1,1957)	1:114:A:LEU:HD23	1:10:A:LEU:HA	3	1.18
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	1	1.18
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	3	1.18
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	3	1.18
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	4	1.18
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	4	1.18
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	5	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	5	1.18
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	5	1.18
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	7	1.18
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	7	1.18
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	7	1.18
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	1	1.18
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	9	1.18
(1,1901)	1:32:A:LYS:HE2	1:29:A:SER:HB2	8	1.17
(1,1901)	1:32:A:LYS:HE3	1:29:A:SER:HB2	8	1.17
(1,1888)	1:23:A:LEU:HD11	1:20:A:LEU:HB3	2	1.17
(1,1888)	1:23:A:LEU:HD12	1:20:A:LEU:HB3	2	1.17
(1,1888)	1:23:A:LEU:HD13	1:20:A:LEU:HB3	2	1.17
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	6	1.17
(1,1761)	1:75:A:ASN:H	1:76:A:MET:HB3	6	1.17
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	2	1.17
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	4	1.17
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	3	1.16
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	6	1.16
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	7	1.16
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	5	1.16
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	5	1.16
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	10	1.16
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	10	1.16
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	8	1.16
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	8	1.16
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	8	1.16
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB1	4	1.15
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB2	4	1.15
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB3	4	1.15
(1,1886)	1:22:A:ALA:HB1	1:18:A:GLU:HG3	4	1.15
(1,1886)	1:22:A:ALA:HB2	1:18:A:GLU:HG3	4	1.15
(1,1886)	1:22:A:ALA:HB3	1:18:A:GLU:HG3	4	1.15
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	8	1.15
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	8	1.15
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	5	1.15
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	5	1.15
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	9	1.15
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	3	1.15
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	9	1.14
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	6	1.14
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	6	1.14
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	6	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	5	1.14
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	10	1.14
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	3	1.14
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	9	1.14
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	3	1.14
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	9	1.14
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	9	1.14
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	8	1.14
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD21	5	1.13
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD22	5	1.13
(1,1805)	1:128:A:ILE:H	1:10:A:LEU:HD23	5	1.13
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	1	1.13
(1,256)	1:128:A:ILE:H	1:127:A:PHE:H	2	1.13
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD11	2	1.12
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD12	2	1.12
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD13	2	1.12
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	6	1.12
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	6	1.12
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	8	1.12
(3,10)	1:10:A:LEU:H	1:40:A:TYR:O	5	1.11
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	9	1.11
(1,1943)	1:45:A:ASN:HB3	1:2:A:VAL:HA	4	1.11
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	8	1.11
(1,1761)	1:75:A:ASN:H	1:76:A:MET:HB3	9	1.11
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	4	1.11
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	1	1.11
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	10	1.11
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	3	1.1
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	3	1.1
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	3	1.1
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	4	1.1
(1,257)	1:112:A:PHE:H	1:128:A:ILE:HA	4	1.1
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	1	1.1
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	1	1.1
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	8	1.1
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	8	1.1
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	2	1.09
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	2	1.09
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	2	1.09
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	9	1.09
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	9	1.09
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	4	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	4	1.09
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	4	1.09
(1,1902)	1:32:A:LYS:HE2	1:29:A:SER:HB3	1	1.09
(1,1902)	1:32:A:LYS:HE3	1:29:A:SER:HB3	1	1.09
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	2	1.09
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	2	1.09
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	7	1.09
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	6	1.08
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	6	1.08
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	6	1.08
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	3	1.08
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	3	1.08
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	5	1.07
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	5	1.07
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	5	1.07
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	1	1.07
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	1	1.07
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	1	1.07
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	4	1.07
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	4	1.07
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	4	1.07
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	10	1.07
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	4	1.07
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	4	1.07
(1,2023)	1:78:A:ILE:HG13	1:93:A:SER:HB3	1	1.06
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	4	1.06
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	8	1.06
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	8	1.06
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	8	1.06
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	2	1.06
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	4	1.06
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	6	1.06
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	4	1.05
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	4	1.05
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	7	1.05
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	7	1.05
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	5	1.05
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	5	1.05
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	5	1.05
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	9	1.05
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	5	1.05
(1,491)	1:41:A:GLU:H	1:51:A:PHE:HA	9	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	3	1.05
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	3	1.05
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	6	1.04
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	8	1.04
(1,2023)	1:78:A:ILE:HG13	1:93:A:SER:HB3	5	1.04
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	10	1.04
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	10	1.04
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	3	1.04
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	3	1.04
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	3	1.04
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	5	1.04
(1,1761)	1:75:A:ASN:H	1:76:A:MET:HB3	7	1.04
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	6	1.04
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	5	1.04
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	7	1.04
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	9	1.04
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	4	1.03
(1,1791)	1:45:A:ASN:HD21	1:48:A:LYS:HG2	3	1.03
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	7	1.03
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	3	1.03
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	3	1.03
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	3	1.03
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	3	1.03
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	1	1.03
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	1	1.03
(1,350)	1:124:A:LYS:H	1:15:A:ASN:HA	4	1.03
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA2	7	1.03
(1,97)	1:45:A:ASN:H	1:46:A:GLY:HA3	7	1.03
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	1	1.03
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	1	1.03
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	2	1.02
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	1	1.02
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	5	1.02
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	5	1.02
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	5	1.02
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	6	1.02
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	6	1.02
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	6	1.02
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	6	1.02
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	4	1.02
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	2	1.02
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	2	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	1	1.02
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	5	1.02
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	4	1.01
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	1	1.01
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	8	1.01
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	4	1.01
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	4	1.01
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB2	1	1.01
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB3	1	1.01
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB2	1	1.01
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB3	1	1.01
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	6	1.01
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	6	1.01
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	6	1.01
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	1	1.01
(1,2042)	1:93:A:SER:HB3	1:116:A:MET:HG3	7	1.0
(1,745)	1:20:A:LEU:HB3	1:25:A:VAL:HG11	2	1.0
(1,745)	1:20:A:LEU:HB3	1:25:A:VAL:HG12	2	1.0
(1,745)	1:20:A:LEU:HB3	1:25:A:VAL:HG13	2	1.0
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	2	1.0
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	2	1.0
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG2	4	1.0
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG3	4	1.0
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	3	1.0
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	3	0.99
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	8	0.99
(1,1969)	1:124:A:LYS:HE2	1:14:A:GLU:HB3	6	0.99
(1,1969)	1:124:A:LYS:HE3	1:14:A:GLU:HB3	6	0.99
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	1	0.99
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	1	0.99
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	1	0.99
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	10	0.99
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	10	0.99
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	3	0.98
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	2	0.98
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	3	0.98
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	3	0.98
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	3	0.98
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	5	0.98
(1,1770)	1:13:A:ASN:HD21	1:10:A:LEU:HG	8	0.98
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	8	0.98
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	10	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	10	0.98
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	10	0.98
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	9	0.98
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	9	0.98
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	9	0.98
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	6	0.98
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	1	0.98
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	9	0.98
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	9	0.98
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	9	0.98
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	9	0.98
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	10	0.98
(1,2023)	1:78:A:ILE:HG13	1:93:A:SER:HB3	3	0.97
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	5	0.97
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	5	0.97
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	5	0.97
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	5	0.97
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	5	0.97
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	5	0.97
(1,1914)	1:30:A:ILE:HG13	1:34:A:ASN:HB2	8	0.97
(1,1907)	1:34:A:ASN:HB2	1:30:A:ILE:HG13	8	0.97
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	6	0.97
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	6	0.97
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	6	0.97
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	5	0.97
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	8	0.97
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	9	0.97
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	4	0.97
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	6	0.97
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	4	0.97
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	10	0.97
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	6	0.97
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB1	7	0.96
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB2	7	0.96
(1,2046)	1:14:A:GLU:HB3	1:123:A:ALA:HB3	7	0.96
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	4	0.96
(1,1791)	1:45:A:ASN:HD21	1:48:A:LYS:HG2	9	0.96
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	6	0.96
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	1	0.96
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	6	0.96
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	1	0.96
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	1	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	1	0.96
(3,28)	1:23:A:LEU:H	1:19:A:TYR:O	2	0.95
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD11	3	0.95
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD12	3	0.95
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD13	3	0.95
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	3	0.95
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	8	0.95
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB2	3	0.95
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB3	3	0.95
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD11	8	0.95
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD12	8	0.95
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD13	8	0.95
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD11	8	0.95
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD12	8	0.95
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD13	8	0.95
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD11	8	0.95
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD12	8	0.95
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD13	8	0.95
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	2	0.95
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	8	0.95
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	10	0.95
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG11	8	0.94
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG12	8	0.94
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG13	8	0.94
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	1	0.94
(1,1905)	1:27:A:GLN:HA	1:30:A:ILE:HG12	10	0.94
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	7	0.94
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG11	1	0.94
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG12	1	0.94
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG13	1	0.94
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG11	1	0.94
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG12	1	0.94
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG13	1	0.94
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG11	1	0.94
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG12	1	0.94
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG13	1	0.94
(1,654)	1:89:A:LEU:HA	1:84:A:LEU:HG	9	0.94
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	5	0.94
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	5	0.94
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	5	0.94
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	7	0.94
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	7	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	7	0.94
(1,257)	1:112:A:PHE:H	1:128:A:ILE:HA	3	0.94
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	4	0.94
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	8	0.94
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	6	0.93
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	1	0.93
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	1	0.93
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	5	0.93
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	2	0.93
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	5	0.93
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	6	0.93
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	4	0.93
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	4	0.93
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	4	0.93
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	2	0.92
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	2	0.92
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	2	0.92
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	4	0.92
(1,754)	1:79:A:LYS:HG3	1:68:A:GLU:HA	6	0.92
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	2	0.92
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	2	0.92
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	2	0.92
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	2	0.92
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	2	0.92
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	2	0.92
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	2	0.92
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	2	0.92
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	2	0.92
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	3	0.92
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	7	0.92
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	5	0.92
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	1	0.91
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	1	0.91
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	1	0.91
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	8	0.91
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	8	0.91
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	8	0.91
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	10	0.91
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD11	7	0.91
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD12	7	0.91
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD13	7	0.91
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD11	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD12	7	0.91
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD13	7	0.91
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD11	7	0.91
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD12	7	0.91
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD13	7	0.91
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	6	0.91
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	6	0.91
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	6	0.91
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE2	6	0.91
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE3	6	0.91
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	5	0.91
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	4	0.9
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	4	0.9
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	4	0.9
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	6	0.9
(1,1791)	1:45:A:ASN:HD21	1:48:A:LYS:HG2	10	0.9
(1,1784)	1:27:A:GLN:HE21	1:29:A:SER:H	5	0.9
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	10	0.9
(1,1286)	1:88:A:LYS:H	1:84:A:LEU:HG	1	0.9
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	8	0.9
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	5	0.9
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	2	0.89
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	3	0.89
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	2	0.89
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	2	0.89
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG11	1	0.89
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG12	1	0.89
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG13	1	0.89
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG11	3	0.89
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG12	3	0.89
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG13	3	0.89
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	2	0.89
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	2	0.89
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	2	0.89
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	9	0.89
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	9	0.89
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	9	0.89
(1,1813)	1:3:A:GLN:HE22	1:45:A:ASN:HA	5	0.89
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	3	0.89
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	3	0.89
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	3	0.89
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	3	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	3	0.89
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	3	0.89
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA2	4	0.89
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA3	4	0.89
(1,572)	1:84:A:LEU:H	1:89:A:LEU:HG	4	0.89
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	2	0.89
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	2	0.89
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	3	0.89
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	6	0.89
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	3	0.89
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	4	0.89
(1,2047)	1:113:A:VAL:HG21	1:124:A:LYS:HB2	2	0.88
(1,2047)	1:113:A:VAL:HG22	1:124:A:LYS:HB2	2	0.88
(1,2047)	1:113:A:VAL:HG23	1:124:A:LYS:HB2	2	0.88
(1,1973)	1:121:A:MET:HB2	1:18:A:GLU:HG3	4	0.88
(1,1967)	1:124:A:LYS:HB2	1:14:A:GLU:HB3	5	0.88
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	1	0.88
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	1	0.88
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	1	0.88
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	4	0.88
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	4	0.88
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	4	0.88
(1,1906)	1:27:A:GLN:HA	1:30:A:ILE:HG13	2	0.88
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	7	0.88
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	8	0.88
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	8	0.88
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	8	0.88
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	3	0.88
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	10	0.88
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	7	0.88
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	2	0.88
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	2	0.88
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	9	0.88
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	9	0.88
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	5	0.87
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	4	0.87
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	4	0.87
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	4	0.87
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	4	0.87
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	4	0.87
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	4	0.87
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	5	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	5	0.87
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	5	0.87
(1,491)	1:41:A:GLU:H	1:51:A:PHE:HA	10	0.87
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	8	0.87
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	8	0.87
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	8	0.87
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	6	0.87
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	9	0.87
(3,64)	1:129:A:ARG:H	1:109:A:ASP:O	10	0.86
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	5	0.86
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	3	0.86
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	3	0.86
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	3	0.86
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	6	0.86
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	6	0.86
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	6	0.86
(1,1902)	1:32:A:LYS:HE2	1:29:A:SER:HB3	8	0.86
(1,1902)	1:32:A:LYS:HE3	1:29:A:SER:HB3	8	0.86
(1,1813)	1:3:A:GLN:HE22	1:45:A:ASN:HA	8	0.86
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	2	0.86
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	2	0.86
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	2	0.86
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	2	0.86
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	4	0.86
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	6	0.86
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	2	0.85
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	2	0.85
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	2	0.85
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	1	0.85
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	1	0.85
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	1	0.85
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	7	0.85
(1,1458)	1:115:A:THR:H	1:114:A:LEU:HG	8	0.85
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	6	0.85
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD11	9	0.85
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD12	9	0.85
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD13	9	0.85
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	6	0.85
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	6	0.85
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	6	0.85
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	7	0.85
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	9	0.85
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	9	0.85
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	2	0.85
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	10	0.85
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	3	0.85
(1,56)	1:22:A:ALA:H	1:23:A:LEU:HG	6	0.85
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	5	0.84
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	3	0.84
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	3	0.84
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	3	0.84
(1,1967)	1:124:A:LYS:HB2	1:14:A:GLU:HB3	1	0.84
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB1	6	0.84
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB2	6	0.84
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB3	6	0.84
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB1	8	0.84
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB2	8	0.84
(1,1892)	1:18:A:GLU:HG3	1:22:A:ALA:HB3	8	0.84
(1,1886)	1:22:A:ALA:HB1	1:18:A:GLU:HG3	6	0.84
(1,1886)	1:22:A:ALA:HB2	1:18:A:GLU:HG3	6	0.84
(1,1886)	1:22:A:ALA:HB3	1:18:A:GLU:HG3	6	0.84
(1,1886)	1:22:A:ALA:HB1	1:18:A:GLU:HG3	8	0.84
(1,1886)	1:22:A:ALA:HB2	1:18:A:GLU:HG3	8	0.84
(1,1886)	1:22:A:ALA:HB3	1:18:A:GLU:HG3	8	0.84
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	5	0.84
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	5	0.84
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	5	0.84
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	10	0.84
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	9	0.84
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	9	0.84
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	9	0.84
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	3	0.84
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG11	6	0.84
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG12	6	0.84
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG13	6	0.84
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG11	6	0.84
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG12	6	0.84
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG13	6	0.84
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG11	6	0.84
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG12	6	0.84
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG13	6	0.84
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD11	2	0.84
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD12	2	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD13	2	0.84
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	4	0.84
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	4	0.84
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	4	0.84
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	7	0.84
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	7	0.84
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	7	0.84
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	1	0.84
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	4	0.84
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	3	0.84
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	4	0.84
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	10	0.83
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	9	0.83
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	8	0.83
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	8	0.83
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	8	0.83
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	10	0.83
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	9	0.83
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	1	0.83
(3,23)	1:21:A:ALA:N	1:17:A:GLU:O	2	0.82
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	8	0.82
(1,2019)	1:63:A:VAL:HG21	1:89:A:LEU:HB2	4	0.82
(1,2019)	1:63:A:VAL:HG22	1:89:A:LEU:HB2	4	0.82
(1,2019)	1:63:A:VAL:HG23	1:89:A:LEU:HB2	4	0.82
(1,1993)	1:82:A:THR:HB	1:61:A:LEU:HB3	2	0.82
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	4	0.82
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	4	0.82
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	4	0.82
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG11	5	0.82
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG12	5	0.82
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG13	5	0.82
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	6	0.82
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	6	0.82
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	6	0.82
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	7	0.82
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	8	0.82
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	8	0.82
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	8	0.82
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	8	0.82
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	8	0.82
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	8	0.82
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	5	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	3	0.82
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	6	0.82
(1,209)	1:112:A:PHE:H	1:113:A:VAL:HA	4	0.82
(1,78)	1:35:A:SER:H	1:33:A:ALA:H	3	0.82
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG21	4	0.82
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG22	4	0.82
(1,62)	1:32:A:LYS:H	1:30:A:ILE:HG23	4	0.82
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	3	0.81
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	3	0.81
(1,2045)	1:19:A:TYR:HA	1:121:A:MET:HB2	2	0.81
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	7	0.81
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	4	0.81
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	8	0.81
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	8	0.81
(1,1974)	1:121:A:MET:HB2	1:19:A:TYR:HA	2	0.81
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	2	0.81
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	2	0.81
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	2	0.81
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	2	0.81
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	9	0.81
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	9	0.81
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	9	0.81
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	3	0.81
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	3	0.81
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	3	0.81
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	7	0.81
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	10	0.81
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	10	0.81
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	8	0.8
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	10	0.8
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	4	0.8
(1,2019)	1:63:A:VAL:HG21	1:89:A:LEU:HB2	8	0.79
(1,2019)	1:63:A:VAL:HG22	1:89:A:LEU:HB2	8	0.79
(1,2019)	1:63:A:VAL:HG23	1:89:A:LEU:HB2	8	0.79
(1,1902)	1:32:A:LYS:HE2	1:29:A:SER:HB3	3	0.79
(1,1902)	1:32:A:LYS:HE3	1:29:A:SER:HB3	3	0.79
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	3	0.79
(1,654)	1:89:A:LEU:HA	1:84:A:LEU:HG	1	0.79
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	7	0.79
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	9	0.79
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	7	0.78
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD11	10	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD12	10	0.78
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD13	10	0.78
(1,1972)	1:27:A:GLN:HA	1:17:A:GLU:HA	9	0.78
(1,1966)	1:123:A:ALA:HA	1:14:A:GLU:HB3	7	0.78
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	8	0.78
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	8	0.78
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	9	0.78
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	6	0.78
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	6	0.78
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	6	0.78
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	1	0.78
(1,491)	1:41:A:GLU:H	1:51:A:PHE:HA	5	0.78
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	10	0.78
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	10	0.78
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	10	0.78
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	10	0.78
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	10	0.78
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	10	0.78
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	10	0.78
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	10	0.78
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	10	0.78
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	2	0.78
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	2	0.78
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	9	0.78
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	8	0.78
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	8	0.78
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	8	0.78
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	8	0.78
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	8	0.78
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	8	0.78
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	8	0.78
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	8	0.78
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	8	0.78
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	8	0.78
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	8	0.78
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	8	0.78
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	7	0.78
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	3	0.78
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	7	0.78
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	6	0.77
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	5	0.77
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	3	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD21	5	0.77
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD22	5	0.77
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD23	5	0.77
(1,1885)	1:22:A:ALA:HB1	1:18:A:GLU:HB2	5	0.77
(1,1885)	1:22:A:ALA:HB2	1:18:A:GLU:HB2	5	0.77
(1,1885)	1:22:A:ALA:HB3	1:18:A:GLU:HB2	5	0.77
(1,1803)	1:47:A:ASN:HD21	1:2:A:VAL:HG21	4	0.77
(1,1803)	1:47:A:ASN:HD21	1:2:A:VAL:HG22	4	0.77
(1,1803)	1:47:A:ASN:HD21	1:2:A:VAL:HG23	4	0.77
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	3	0.77
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	2	0.77
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	10	0.77
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	10	0.77
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	2	0.77
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	1	0.77
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	5	0.77
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	1	0.76
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	1	0.76
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG11	10	0.76
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG12	10	0.76
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG13	10	0.76
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	1	0.76
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	1	0.76
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	1	0.76
(1,1784)	1:27:A:GLN:HE21	1:29:A:SER:H	7	0.76
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG2	4	0.76
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG3	4	0.76
(1,1442)	1:108:A:CYS:H	1:112:A:PHE:HB2	3	0.76
(1,1442)	1:108:A:CYS:H	1:112:A:PHE:HB3	3	0.76
(1,1441)	1:108:A:CYS:H	1:112:A:PHE:HB2	3	0.76
(1,1441)	1:108:A:CYS:H	1:112:A:PHE:HB3	3	0.76
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD11	6	0.76
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD12	6	0.76
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD13	6	0.76
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	6	0.76
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	2	0.76
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	3	0.76
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	1	0.76
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	6	0.76
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	6	0.76
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	9	0.76
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	9	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	9	0.76
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	1	0.76
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	1	0.76
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	1	0.76
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	3	0.76
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	3	0.76
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	8	0.75
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	8	0.75
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	8	0.75
(1,1914)	1:30:A:ILE:HG13	1:34:A:ASN:HB2	3	0.75
(1,1907)	1:34:A:ASN:HB2	1:30:A:ILE:HG13	3	0.75
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	3	0.75
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	10	0.75
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	10	0.75
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	10	0.75
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	2	0.75
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	2	0.75
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	2	0.75
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	2	0.75
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	2	0.75
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	2	0.75
(1,1330)	1:82:A:THR:H	1:91:A:VAL:HB	10	0.75
(1,1286)	1:88:A:LYS:H	1:84:A:LEU:HG	10	0.75
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	3	0.75
(1,491)	1:41:A:GLU:H	1:51:A:PHE:HA	3	0.75
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD21	1	0.75
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD22	1	0.75
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD23	1	0.75
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD21	1	0.75
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD22	1	0.75
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD23	1	0.75
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD21	1	0.75
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD22	1	0.75
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD23	1	0.75
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	1	0.75
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	1	0.75
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	1	0.75
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	5	0.75
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	5	0.75
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	5	0.75
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	5	0.75
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	5	0.75
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	5	0.75
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	5	0.75
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	5	0.75
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	5	0.75
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	5	0.75
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	5	0.75
(1,74)	1:34:A:ASN:H	1:32:A:LYS:H	8	0.75
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	6	0.75
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	4	0.74
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	10	0.74
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	4	0.74
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	4	0.74
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	4	0.74
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	4	0.74
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	4	0.74
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	4	0.74
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	4	0.74
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	4	0.74
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	4	0.74
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	4	0.74
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	4	0.74
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	4	0.74
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	4	0.74
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	4	0.74
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	4	0.74
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	4	0.74
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	4	0.74
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	4	0.74
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG11	4	0.74
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG12	4	0.74
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG13	4	0.74
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG11	4	0.74
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG12	4	0.74
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG13	4	0.74
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG11	4	0.74
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG12	4	0.74
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG13	4	0.74
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	4	0.74
(1,491)	1:41:A:GLU:H	1:51:A:PHE:HA	7	0.74
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	2	0.74
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	7	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD11	10	0.74
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD12	10	0.74
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD13	10	0.74
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD11	10	0.74
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD12	10	0.74
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD13	10	0.74
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD11	10	0.74
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD12	10	0.74
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD13	10	0.74
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	8	0.74
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	8	0.74
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	6	0.74
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	2	0.74
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	4	0.74
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	4	0.74
(1,21)	1:10:A:LEU:H	1:10:A:LEU:HG	9	0.74
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	5	0.73
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	9	0.73
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	10	0.73
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	10	0.73
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	10	0.73
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	3	0.73
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	3	0.73
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	3	0.73
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	5	0.73
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	5	0.73
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	5	0.73
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD2	9	0.73
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD3	9	0.73
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	7	0.73
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	7	0.73
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	7	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	3	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	3	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	3	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	3	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	3	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	3	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	3	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	3	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	3	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	3	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	3	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	3	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	3	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	3	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	3	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	3	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	3	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	3	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	8	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	8	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	8	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	8	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	8	0.73
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	8	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	8	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	8	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	8	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	8	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	8	0.73
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	8	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	8	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	8	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	8	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	8	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	8	0.73
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	8	0.73
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	9	0.73
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	9	0.73
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	9	0.73
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	1	0.73
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	1	0.73
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	1	0.73
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB2	9	0.73
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB3	9	0.73
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	2	0.73
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	5	0.72
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	5	0.72
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	5	0.72
(1,1943)	1:45:A:ASN:HB3	1:2:A:VAL:HA	2	0.72
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	3	0.72
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	3	0.72
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	3	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1921)	1:48:A:LYS:HD2	1:45:A:ASN:HB3	9	0.72
(1,1921)	1:48:A:LYS:HD3	1:45:A:ASN:HB3	9	0.72
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	1	0.72
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	6	0.72
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	9	0.72
(1,1652)	1:65:A:GLU:HA	1:83:A:LYS:HA	9	0.72
(1,1458)	1:115:A:THR:H	1:114:A:LEU:HG	9	0.72
(1,1458)	1:115:A:THR:H	1:114:A:LEU:HG	10	0.72
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB2	8	0.72
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB3	8	0.72
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	9	0.72
(1,654)	1:89:A:LEU:HA	1:84:A:LEU:HG	10	0.72
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	3	0.72
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	3	0.72
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	3	0.72
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	9	0.72
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	9	0.72
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	9	0.72
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	3	0.72
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	3	0.72
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	5	0.72
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	1	0.72
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	3	0.72
(1,2041)	1:93:A:SER:HB2	1:116:A:MET:HG3	1	0.71
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	8	0.71
(1,1923)	1:67:A:VAL:HG21	1:65:A:GLU:HB2	10	0.71
(1,1923)	1:67:A:VAL:HG22	1:65:A:GLU:HB2	10	0.71
(1,1923)	1:67:A:VAL:HG23	1:65:A:GLU:HB2	10	0.71
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	4	0.71
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	8	0.71
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	8	0.71
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	8	0.71
(1,754)	1:79:A:LYS:HG3	1:68:A:GLU:HA	2	0.71
(1,742)	1:114:A:LEU:HG	1:13:A:ASN:HD22	7	0.71
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	9	0.71
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB1	6	0.71
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB2	6	0.71
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB3	6	0.71
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB1	6	0.71
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB2	6	0.71
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB3	6	0.71
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB1	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB2	6	0.71
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB3	6	0.71
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	8	0.71
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD11	8	0.71
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD12	8	0.71
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD13	8	0.71
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	4	0.71
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	5	0.71
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	1	0.71
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	1	0.71
(1,1925)	1:71:A:LEU:HD11	1:74:A:VAL:HB	8	0.7
(1,1925)	1:71:A:LEU:HD12	1:74:A:VAL:HB	8	0.7
(1,1925)	1:71:A:LEU:HD13	1:74:A:VAL:HB	8	0.7
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	6	0.7
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	5	0.7
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	8	0.7
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	8	0.7
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	8	0.7
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	9	0.7
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	4	0.7
(3,25)	1:22:A:ALA:N	1:18:A:GLU:O	3	0.69
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	10	0.69
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	6	0.69
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	6	0.69
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	6	0.69
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	3	0.69
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	4	0.69
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	5	0.69
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	6	0.69
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	6	0.69
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	6	0.69
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	6	0.69
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	6	0.69
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	6	0.69
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	6	0.69
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	6	0.69
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	6	0.69
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	6	0.69
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	6	0.69
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	6	0.69
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	6	0.69
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	6	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	6	0.69
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	6	0.69
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	6	0.69
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	6	0.69
(1,744)	1:123:A:ALA:HB1	1:19:A:TYR:HB3	3	0.69
(1,744)	1:123:A:ALA:HB2	1:19:A:TYR:HB3	3	0.69
(1,744)	1:123:A:ALA:HB3	1:19:A:TYR:HB3	3	0.69
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	5	0.69
(1,572)	1:84:A:LEU:H	1:89:A:LEU:HG	1	0.69
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	6	0.69
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	6	0.69
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	4	0.69
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	4	0.69
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	4	0.69
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	4	0.69
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	4	0.69
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	4	0.69
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	4	0.69
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	4	0.69
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	4	0.69
(1,275)	1:77:A:ASN:HB2	1:70:A:VAL:HA	2	0.69
(1,275)	1:77:A:ASN:HB3	1:70:A:VAL:HA	2	0.69
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	6	0.69
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB1	3	0.69
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB2	3	0.69
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB3	3	0.69
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB2	4	0.69
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB3	4	0.69
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB2	4	0.69
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB3	4	0.69
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	9	0.69
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	9	0.69
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	8	0.69
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	2	0.69
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	2	0.69
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	10	0.68
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	8	0.68
(1,1970)	1:124:A:LYS:HG3	1:14:A:GLU:HB3	9	0.68
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG11	9	0.68
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG12	9	0.68
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG13	9	0.68
(1,1905)	1:27:A:GLN:HA	1:30:A:ILE:HG12	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	7	0.68
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	8	0.68
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	8	0.68
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	8	0.68
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	9	0.68
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	9	0.68
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	9	0.68
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	9	0.68
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	9	0.68
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	9	0.68
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	9	0.68
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	9	0.68
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	9	0.68
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	9	0.68
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	9	0.68
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	9	0.68
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	9	0.68
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	9	0.68
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	9	0.68
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	9	0.68
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	9	0.68
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	9	0.68
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG2	10	0.68
(1,374)	1:80:A:SER:H	1:94:A:GLU:HG3	10	0.68
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	2	0.68
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	2	0.68
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	2	0.68
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	2	0.68
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	2	0.68
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	2	0.68
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	2	0.68
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	2	0.68
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	2	0.68
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	2	0.68
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	2	0.68
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	2	0.68
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	8	0.68
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	4	0.68
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	7	0.67
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	10	0.67
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	10	0.67
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	10	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	10	0.67
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	10	0.67
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	10	0.67
(1,1914)	1:30:A:ILE:HG13	1:34:A:ASN:HB2	6	0.67
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	10	0.67
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	10	0.67
(1,1907)	1:34:A:ASN:HB2	1:30:A:ILE:HG13	6	0.67
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	10	0.67
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	10	0.67
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	2	0.67
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	6	0.67
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	6	0.67
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	6	0.67
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	6	0.67
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	6	0.67
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	6	0.67
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	6	0.67
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	6	0.67
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	6	0.67
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	5	0.67
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	5	0.67
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	5	0.67
(1,387)	1:10:A:LEU:HG	1:38:A:VAL:HB	1	0.67
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG21	2	0.67
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG22	2	0.67
(1,211)	1:127:A:PHE:H	1:113:A:VAL:HG23	2	0.67
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	5	0.67
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	5	0.67
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	5	0.67
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	5	0.67
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	6	0.67
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	7	0.67
(1,139)	1:33:A:ALA:H	1:73:A:THR:HB	8	0.67
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	7	0.67
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	2	0.67
(1,2023)	1:78:A:ILE:HG13	1:93:A:SER:HB3	7	0.66
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	10	0.66
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	10	0.66
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	10	0.66
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	9	0.66
(1,1784)	1:27:A:GLN:HE21	1:29:A:SER:H	9	0.66
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	10	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	10	0.66
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	10	0.66
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	3	0.66
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	3	0.66
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	3	0.66
(1,390)	1:106:A:GLU:HA	1:88:A:LYS:HB3	4	0.66
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	5	0.66
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	5	0.66
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	5	0.66
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	3	0.66
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	3	0.66
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	3	0.66
(1,347)	1:43:A:ILE:H	1:50:A:THR:HB	7	0.66
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	2	0.66
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	5	0.66
(1,1972)	1:27:A:GLN:HA	1:17:A:GLU:HA	4	0.65
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	8	0.65
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	8	0.65
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	8	0.65
(1,1901)	1:32:A:LYS:HE2	1:29:A:SER:HB2	3	0.65
(1,1901)	1:32:A:LYS:HE3	1:29:A:SER:HB2	3	0.65
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	8	0.65
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD11	9	0.65
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD12	9	0.65
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD13	9	0.65
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG11	3	0.65
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG12	3	0.65
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG13	3	0.65
(1,1779)	1:15:A:ASN:HD22	1:18:A:GLU:HB3	9	0.65
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	6	0.65
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	8	0.65
(1,689)	1:79:A:LYS:H	1:95:A:LEU:HA	4	0.65
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	4	0.65
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	4	0.65
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	9	0.65
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	9	0.65
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	9	0.65
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	9	0.65
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	2	0.65
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	2	0.65
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	6	0.65
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:33:A:ALA:H	1:73:A:THR:HB	2	0.65
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	10	0.65
(1,12)	1:130:A:THR:H	1:8:A:TYR:HA	6	0.65
(3,37)	1:61:A:LEU:N	1:51:A:PHE:O	8	0.64
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	9	0.64
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	9	0.64
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	9	0.64
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	5	0.64
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	5	0.64
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	5	0.64
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	5	0.64
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	3	0.64
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	9	0.64
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD11	9	0.64
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD12	9	0.64
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD13	9	0.64
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA2	3	0.64
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA3	3	0.64
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA2	5	0.64
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA3	5	0.64
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	3	0.64
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	9	0.64
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	7	0.64
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	4	0.64
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	4	0.64
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	4	0.64
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	5	0.64
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	4	0.64
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	8	0.64
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	4	0.64
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	6	0.64
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	6	0.64
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	2	0.64
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	5	0.64
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	2	0.64
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	10	0.64
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	3	0.64
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD11	7	0.63
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD12	7	0.63
(1,2036)	1:125:A:ARG:HB3	1:114:A:LEU:HD13	7	0.63
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG11	4	0.63
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG12	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG13	4	0.63
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	6	0.63
(1,1813)	1:3:A:GLN:HE22	1:45:A:ASN:HA	1	0.63
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD11	7	0.63
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD12	7	0.63
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD13	7	0.63
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	7	0.63
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	1	0.63
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	1	0.63
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	1	0.63
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	10	0.63
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	10	0.63
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	10	0.63
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	1	0.63
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	6	0.63
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	6	0.63
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	6	0.63
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	4	0.63
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	4	0.63
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG2	10	0.63
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG3	10	0.63
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB2	5	0.63
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB3	5	0.63
(3,20)	1:19:A:TYR:H	1:15:A:ASN:O	3	0.62
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	9	0.62
(1,2004)	1:93:A:SER:HB2	1:78:A:ILE:HG12	9	0.62
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	8	0.62
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	8	0.62
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	8	0.62
(1,1784)	1:27:A:GLN:HE21	1:29:A:SER:H	2	0.62
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	5	0.62
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	5	0.62
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	5	0.62
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	5	0.62
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	5	0.62
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	5	0.62
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	10	0.62
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	2	0.62
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	8	0.62
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	8	0.62
(1,451)	1:35:A:SER:H	1:31:A:LYS:HA	3	0.62
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	5	0.62
(1,394)	1:126:A:TYR:HB2	1:113:A:VAL:HA	6	0.62
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	2	0.62
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	2	0.62
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	2	0.62
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	4	0.62
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	4	0.62
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	9	0.62
(1,171)	1:92:A:ASN:H	1:91:A:VAL:H	10	0.62
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	7	0.62
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	7	0.62
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	7	0.62
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	7	0.62
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	7	0.62
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	7	0.62
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	7	0.62
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	7	0.62
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	7	0.62
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	7	0.62
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	7	0.62
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	7	0.62
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG2	7	0.62
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG3	7	0.62
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	9	0.62
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	8	0.62
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	2	0.61
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	1	0.61
(1,1935)	1:94:A:GLU:HG2	1:96:A:PRO:HB2	6	0.61
(1,1935)	1:94:A:GLU:HG3	1:96:A:PRO:HB2	6	0.61
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	9	0.61
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	9	0.61
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	9	0.61
(1,1788)	1:47:A:ASN:H	1:45:A:ASN:HB3	7	0.61
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	2	0.61
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	8	0.61
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	8	0.61
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	7	0.61
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	10	0.61
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	10	0.61
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	9	0.6
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	9	0.6
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2026)	1:78:A:ILE:HG13	1:96:A:PRO:HD2	2	0.6
(1,2019)	1:63:A:VAL:HG21	1:89:A:LEU:HB2	6	0.6
(1,2019)	1:63:A:VAL:HG22	1:89:A:LEU:HB2	6	0.6
(1,2019)	1:63:A:VAL:HG23	1:89:A:LEU:HB2	6	0.6
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	6	0.6
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	6	0.6
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	6	0.6
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	6	0.6
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	6	0.6
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	6	0.6
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD21	8	0.6
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD22	8	0.6
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD23	8	0.6
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	5	0.6
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	5	0.6
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	5	0.6
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	7	0.6
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	7	0.6
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	7	0.6
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD11	10	0.6
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD12	10	0.6
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD13	10	0.6
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD11	2	0.6
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD12	2	0.6
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD13	2	0.6
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	10	0.6
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	10	0.6
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	7	0.6
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	7	0.6
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	7	0.6
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	7	0.6
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	7	0.6
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	7	0.6
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	7	0.6
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	7	0.6
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	7	0.6
(1,139)	1:33:A:ALA:H	1:73:A:THR:HB	5	0.6
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	7	0.6
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	8	0.6
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	5	0.6
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	4	0.6
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	7	0.59
(3,10)	1:10:A:LEU:H	1:40:A:TYR:O	3	0.59
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	6	0.59
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	6	0.59
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	6	0.59
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	9	0.59
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	9	0.59
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	9	0.59
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	8	0.59
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	8	0.59
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	8	0.59
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	8	0.59
(1,1862)	1:32:A:LYS:HA	1:31:A:LYS:HG3	5	0.59
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	8	0.59
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	9	0.59
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG2	2	0.59
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG3	2	0.59
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	1	0.59
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	1	0.59
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	1	0.59
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	10	0.59
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	10	0.59
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	10	0.59
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	4	0.59
(1,572)	1:84:A:LEU:H	1:89:A:LEU:HG	10	0.59
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	10	0.59
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	10	0.59
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	10	0.59
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	5	0.59
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	5	0.59
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	5	0.59
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG2	1	0.59
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG3	1	0.59
(1,78)	1:35:A:SER:H	1:33:A:ALA:H	1	0.59
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	1	0.59
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	4	0.59
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	9	0.58
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	7	0.58
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	7	0.58
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG2	9	0.58
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG3	9	0.58
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG2	9	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG3	9	0.58
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG2	9	0.58
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG3	9	0.58
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD21	9	0.58
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD22	9	0.58
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD23	9	0.58
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD21	9	0.58
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD22	9	0.58
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD23	9	0.58
(1,1906)	1:27:A:GLN:HA	1:30:A:ILE:HG13	4	0.58
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	6	0.58
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	6	0.58
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	6	0.58
(1,1799)	1:47:A:ASN:HD21	1:2:A:VAL:HB	2	0.58
(1,1793)	1:87:A:SER:H	1:85:A:GLU:HG2	3	0.58
(1,1793)	1:87:A:SER:H	1:85:A:GLU:HG3	3	0.58
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	3	0.58
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD11	10	0.58
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD12	10	0.58
(1,1244)	1:94:A:GLU:H	1:78:A:ILE:HD13	10	0.58
(1,760)	1:78:A:ILE:HB	1:96:A:PRO:HD2	4	0.58
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	9	0.58
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	1	0.58
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	1	0.58
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	1	0.58
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	1	0.58
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD21	6	0.58
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD22	6	0.58
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD23	6	0.58
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD21	6	0.58
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD22	6	0.58
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD23	6	0.58
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD21	6	0.58
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD22	6	0.58
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD23	6	0.58
(1,387)	1:10:A:LEU:HG	1:38:A:VAL:HB	4	0.58
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	5	0.58
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	5	0.58
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	5	0.58
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	5	0.58
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	5	0.58
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	5	0.58
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	5	0.58
(1,217)	1:116:A:MET:H	1:115:A:THR:HG21	1	0.58
(1,217)	1:116:A:MET:H	1:115:A:THR:HG22	1	0.58
(1,217)	1:116:A:MET:H	1:115:A:THR:HG23	1	0.58
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	9	0.58
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	9	0.58
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	10	0.58
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	5	0.58
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	6	0.58
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG2	3	0.58
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG3	3	0.58
(1,124)	1:53:A:SER:H	1:59:A:SER:H	8	0.58
(1,113)	1:59:A:SER:H	1:53:A:SER:H	8	0.58
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	3	0.58
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	8	0.58
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	8	0.58
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	10	0.57
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	1	0.57
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	1	0.57
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	1	0.57
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	9	0.57
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	9	0.57
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	9	0.57
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG11	3	0.57
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG12	3	0.57
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG13	3	0.57
(1,1991)	1:82:A:THR:HB	1:61:A:LEU:HB2	10	0.57
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG21	1	0.57
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG22	1	0.57
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG23	1	0.57
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	4	0.57
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	4	0.57
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	4	0.57
(1,1909)	1:27:A:GLN:HG2	1:31:A:LYS:HE2	4	0.57
(1,1909)	1:27:A:GLN:HG2	1:31:A:LYS:HE3	4	0.57
(1,1909)	1:27:A:GLN:HG3	1:31:A:LYS:HE2	4	0.57
(1,1909)	1:27:A:GLN:HG3	1:31:A:LYS:HE3	4	0.57
(1,1897)	1:31:A:LYS:HE2	1:27:A:GLN:HG2	4	0.57
(1,1897)	1:31:A:LYS:HE2	1:27:A:GLN:HG3	4	0.57
(1,1897)	1:31:A:LYS:HE3	1:27:A:GLN:HG2	4	0.57
(1,1897)	1:31:A:LYS:HE3	1:27:A:GLN:HG3	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	10	0.57
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	2	0.57
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	9	0.57
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	9	0.57
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	9	0.57
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	10	0.57
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	10	0.57
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	10	0.57
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	10	0.57
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	10	0.57
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	10	0.57
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	10	0.57
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	10	0.57
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	10	0.57
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	10	0.57
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	10	0.57
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	10	0.57
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	10	0.57
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	10	0.57
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	10	0.57
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	10	0.57
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	10	0.57
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	10	0.57
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	6	0.57
(1,743)	1:121:A:MET:HB3	1:18:A:GLU:HG3	4	0.57
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	10	0.57
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	9	0.57
(1,390)	1:106:A:GLU:HA	1:88:A:LYS:HB3	3	0.57
(1,387)	1:10:A:LEU:HG	1:38:A:VAL:HB	9	0.57
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	2	0.57
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	1	0.57
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	1	0.57
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	1	0.57
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	1	0.57
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	1	0.57
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	1	0.57
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	1	0.57
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	1	0.57
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	1	0.57
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	1	0.57
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	1	0.57
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	1	0.57
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	1	0.57
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	8	0.57
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG2	9	0.57
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG3	9	0.57
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	8	0.56
(1,2064)	1:9:A:LYS:HB2	1:130:A:THR:HB	9	0.56
(1,2064)	1:9:A:LYS:HB3	1:130:A:THR:HB	9	0.56
(1,2054)	1:12:A:LYS:HD3	1:126:A:TYR:HE1	1	0.56
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	7	0.56
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	7	0.56
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	7	0.56
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	6	0.56
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	6	0.56
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	6	0.56
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	2	0.56
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	2	0.56
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	2	0.56
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	4	0.56
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	4	0.56
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	4	0.56
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	10	0.56
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	10	0.56
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	10	0.56
(1,1956)	1:130:A:THR:HB	1:9:A:LYS:HB2	9	0.56
(1,1956)	1:130:A:THR:HB	1:9:A:LYS:HB3	9	0.56
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD21	7	0.56
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD22	7	0.56
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD23	7	0.56
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	1	0.56
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	1	0.56
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	1	0.56
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	1	0.56
(1,1770)	1:13:A:ASN:HD21	1:10:A:LEU:HG	2	0.56
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	4	0.56
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	4	0.56
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	4	0.56
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	3	0.56
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	3	0.56
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	3	0.56
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	5	0.56
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	5	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	5	0.56
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	8	0.56
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	8	0.56
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	8	0.56
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	9	0.56
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	9	0.56
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	9	0.56
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	4	0.56
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	4	0.56
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	3	0.56
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	3	0.56
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	3	0.56
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	3	0.56
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	5	0.56
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	4	0.55
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	1	0.55
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	8	0.55
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	8	0.55
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	8	0.55
(1,1957)	1:114:A:LEU:HD21	1:10:A:LEU:HA	2	0.55
(1,1957)	1:114:A:LEU:HD22	1:10:A:LEU:HA	2	0.55
(1,1957)	1:114:A:LEU:HD23	1:10:A:LEU:HA	2	0.55
(1,1921)	1:48:A:LYS:HD2	1:45:A:ASN:HB3	10	0.55
(1,1921)	1:48:A:LYS:HD3	1:45:A:ASN:HB3	10	0.55
(1,1799)	1:47:A:ASN:HD21	1:2:A:VAL:HB	1	0.55
(1,1770)	1:13:A:ASN:HD21	1:10:A:LEU:HG	1	0.55
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB1	10	0.55
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB2	10	0.55
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB3	10	0.55
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB1	10	0.55
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB2	10	0.55
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB3	10	0.55
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	9	0.55
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	9	0.55
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	9	0.55
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	9	0.55
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	9	0.55
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	9	0.55
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	9	0.55
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	9	0.55
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	9	0.55
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	9	0.55
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	9	0.55
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	9	0.55
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	9	0.55
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	9	0.55
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	9	0.55
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	9	0.55
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	9	0.55
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	9	0.55
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	9	0.55
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	9	0.55
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	9	0.55
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	9	0.55
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	9	0.55
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	9	0.55
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	9	0.55
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	9	0.55
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	9	0.55
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	9	0.55
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	9	0.55
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	9	0.55
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	9	0.55
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	9	0.55
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	9	0.55
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	9	0.55
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	9	0.55
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	9	0.55
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	9	0.55
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	9	0.55
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	9	0.55
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	9	0.55
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	9	0.55
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	9	0.55
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	9	0.55
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	9	0.55
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	9	0.55
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	9	0.55
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	9	0.55
(1,1330)	1:82:A:THR:H	1:91:A:VAL:HB	5	0.55
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB2	5	0.55
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB3	5	0.55
(1,793)	1:130:A:THR:H	1:7:A:THR:HB	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	2	0.55
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	2	0.55
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	2	0.55
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	9	0.55
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	6	0.55
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	6	0.55
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	6	0.55
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	6	0.55
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	10	0.55
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	10	0.55
(1,430)	1:24:A:GLY:H	1:20:A:LEU:HA	8	0.55
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	8	0.55
(1,377)	1:74:A:VAL:HG11	1:71:A:LEU:HB2	1	0.55
(1,377)	1:74:A:VAL:HG12	1:71:A:LEU:HB2	1	0.55
(1,377)	1:74:A:VAL:HG13	1:71:A:LEU:HB2	1	0.55
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	10	0.55
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	7	0.55
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	7	0.55
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	8	0.55
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	2	0.54
(3,51)	1:106:A:GLU:N	1:113:A:VAL:O	2	0.54
(1,2056)	1:14:A:GLU:HB3	1:126:A:TYR:HE1	7	0.54
(1,1970)	1:124:A:LYS:HG3	1:14:A:GLU:HB3	4	0.54
(1,1935)	1:94:A:GLU:HG2	1:96:A:PRO:HB2	2	0.54
(1,1935)	1:94:A:GLU:HG3	1:96:A:PRO:HB2	2	0.54
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	8	0.54
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	2	0.54
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	2	0.54
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	2	0.54
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	4	0.54
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	8	0.54
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	2	0.54
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	2	0.54
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	2	0.54
(1,761)	1:78:A:ILE:HB	1:96:A:PRO:HD3	3	0.54
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	1	0.54
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	10	0.54
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	9	0.54
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	9	0.54
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	5	0.54
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	5	0.54
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	5	0.54
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	7	0.54
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	9	0.54
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	9	0.54
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	9	0.54
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD11	5	0.54
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD12	5	0.54
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD13	5	0.54
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	6	0.54
(1,491)	1:41:A:GLU:H	1:51:A:PHE:HA	4	0.54
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	10	0.54
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	7	0.54
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	7	0.54
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG11	5	0.54
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG12	5	0.54
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG13	5	0.54
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG21	5	0.54
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG22	5	0.54
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG23	5	0.54
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	6	0.54
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD2	8	0.54
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD3	8	0.54
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	9	0.54
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	5	0.54
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	3	0.54
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	3	0.54
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	10	0.54
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	10	0.54
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG11	7	0.54
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG12	7	0.54
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG13	7	0.54
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG21	7	0.54
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG22	7	0.54
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG23	7	0.54
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	7	0.54
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	10	0.54
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	8	0.54
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	10	0.54
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB2	6	0.54
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB3	6	0.54
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	1	0.53
(3,10)	1:10:A:LEU:H	1:40:A:TYR:O	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	1:10:A:LEU:H	1:40:A:TYR:O	10	0.53
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	2	0.53
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	10	0.53
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	10	0.53
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	10	0.53
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG11	2	0.53
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG12	2	0.53
(1,1946)	1:48:A:LYS:HA	1:2:A:VAL:HG13	2	0.53
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG11	2	0.53
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG12	2	0.53
(1,1828)	1:35:A:SER:H	1:74:A:VAL:HG13	2	0.53
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD11	6	0.53
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD12	6	0.53
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD13	6	0.53
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	8	0.53
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	7	0.53
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	7	0.53
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	7	0.53
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	7	0.53
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	7	0.53
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	7	0.53
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	10	0.53
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	10	0.53
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	10	0.53
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	10	0.53
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	10	0.53
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	10	0.53
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	10	0.53
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	10	0.53
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	10	0.53
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	10	0.53
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	10	0.53
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	10	0.53
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	10	0.53
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	10	0.53
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	10	0.53
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	10	0.53
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	10	0.53
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	10	0.53
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	10	0.53
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	10	0.53
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	10	0.53
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	10	0.53
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	10	0.53
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	10	0.53
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	10	0.53
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	10	0.53
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	10	0.53
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	10	0.53
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	10	0.53
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	10	0.53
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	10	0.53
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	10	0.53
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	10	0.53
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	10	0.53
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	10	0.53
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	10	0.53
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	10	0.53
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	10	0.53
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	10	0.53
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	10	0.53
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	10	0.53
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	10	0.53
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	10	0.53
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	10	0.53
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	10	0.53
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	10	0.53
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	10	0.53
(1,1531)	1:130:A:THR:HB	1:7:A:THR:HB	9	0.53
(1,1330)	1:82:A:THR:H	1:91:A:VAL:HB	9	0.53
(1,1286)	1:88:A:LYS:H	1:84:A:LEU:HG	9	0.53
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	10	0.53
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	10	0.53
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	10	0.53
(1,451)	1:35:A:SER:H	1:31:A:LYS:HA	8	0.53
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	4	0.53
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	4	0.53
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	4	0.53
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	10	0.53
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	10	0.53
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	10	0.53
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	10	0.53
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	10	0.53
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	10	0.53
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	10	0.53
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	9	0.53
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	9	0.53
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD2	1	0.53
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD3	1	0.53
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	1	0.53
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	9	0.53
(1,217)	1:116:A:MET:H	1:115:A:THR:HG21	6	0.53
(1,217)	1:116:A:MET:H	1:115:A:THR:HG22	6	0.53
(1,217)	1:116:A:MET:H	1:115:A:THR:HG23	6	0.53
(1,215)	1:124:A:LYS:H	1:115:A:THR:HA	10	0.53
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	3	0.53
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	9	0.53
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	4	0.53
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	2	0.53
(3,51)	1:106:A:GLU:N	1:113:A:VAL:O	3	0.52
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	3	0.52
(1,2064)	1:9:A:LYS:HB2	1:130:A:THR:HB	3	0.52
(1,2064)	1:9:A:LYS:HB3	1:130:A:THR:HB	3	0.52
(1,2005)	1:93:A:SER:HB3	1:78:A:ILE:HG12	8	0.52
(1,1991)	1:82:A:THR:HB	1:61:A:LEU:HB2	5	0.52
(1,1956)	1:130:A:THR:HB	1:9:A:LYS:HB2	3	0.52
(1,1956)	1:130:A:THR:HB	1:9:A:LYS:HB3	3	0.52
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB1	2	0.52
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB2	2	0.52
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB3	2	0.52
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	8	0.52
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	8	0.52
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	8	0.52
(1,1737)	1:43:A:ILE:HG12	1:41:A:GLU:HB2	1	0.52
(1,1737)	1:43:A:ILE:HG12	1:41:A:GLU:HB3	1	0.52
(1,1737)	1:43:A:ILE:HG13	1:41:A:GLU:HB2	1	0.52
(1,1737)	1:43:A:ILE:HG13	1:41:A:GLU:HB3	1	0.52
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA2	2	0.52
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA3	2	0.52
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	1	0.52
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	1	0.52
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	1	0.52
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	1	0.52
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	1	0.52
(1,759)	1:78:A:ILE:HB	1:93:A:SER:HB3	10	0.52
(1,754)	1:79:A:LYS:HG3	1:68:A:GLU:HA	1	0.52
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	5	0.52
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	5	0.52
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	5	0.52
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	7	0.52
(1,594)	1:93:A:SER:H	1:101:A:GLY:H	10	0.52
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	1	0.52
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	10	0.52
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	8	0.52
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	8	0.52
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	8	0.52
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	3	0.52
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	3	0.52
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	3	0.52
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	3	0.52
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	3	0.52
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	3	0.52
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	3	0.52
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	3	0.52
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	10	0.52
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	10	0.52
(1,141)	1:75:A:ASN:H	1:74:A:VAL:HG11	1	0.52
(1,141)	1:75:A:ASN:H	1:74:A:VAL:HG12	1	0.52
(1,141)	1:75:A:ASN:H	1:74:A:VAL:HG13	1	0.52
(1,141)	1:75:A:ASN:H	1:74:A:VAL:HG21	1	0.52
(1,141)	1:75:A:ASN:H	1:74:A:VAL:HG22	1	0.52
(1,141)	1:75:A:ASN:H	1:74:A:VAL:HG23	1	0.52
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	10	0.52
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	6	0.52
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	3	0.52
(1,47)	1:19:A:TYR:H	1:19:A:TYR:HE1	7	0.52
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	1	0.51
(1,2032)	1:105:A:TYR:HB2	1:112:A:PHE:HA	6	0.51
(1,2032)	1:105:A:TYR:HB3	1:112:A:PHE:HA	6	0.51
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	9	0.51
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	9	0.51
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	9	0.51
(1,1791)	1:45:A:ASN:HD21	1:48:A:LYS:HG2	5	0.51
(1,907)	1:25:A:VAL:H	1:23:A:LEU:HG	6	0.51
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:89:A:LEU:HA	1:84:A:LEU:HG	4	0.51
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	5	0.51
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	5	0.51
(1,390)	1:106:A:GLU:HA	1:88:A:LYS:HB3	2	0.51
(1,390)	1:106:A:GLU:HA	1:88:A:LYS:HB3	7	0.51
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	1	0.51
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	9	0.51
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD2	6	0.51
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD3	6	0.51
(1,226)	1:118:A:ALA:H	1:122:A:VAL:HA	3	0.51
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	10	0.51
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	10	0.51
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	2	0.51
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	2	0.51
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	9	0.51
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	4	0.51
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	4	0.51
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	7	0.51
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	1	0.51
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	10	0.5
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	1	0.5
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	1	0.5
(1,2022)	1:78:A:ILE:HG13	1:93:A:SER:HB2	7	0.5
(1,1908)	1:27:A:GLN:HG2	1:31:A:LYS:HD2	4	0.5
(1,1908)	1:27:A:GLN:HG2	1:31:A:LYS:HD3	4	0.5
(1,1908)	1:27:A:GLN:HG3	1:31:A:LYS:HD2	4	0.5
(1,1908)	1:27:A:GLN:HG3	1:31:A:LYS:HD3	4	0.5
(1,1896)	1:31:A:LYS:HD2	1:27:A:GLN:HG2	4	0.5
(1,1896)	1:31:A:LYS:HD2	1:27:A:GLN:HG3	4	0.5
(1,1896)	1:31:A:LYS:HD3	1:27:A:GLN:HG2	4	0.5
(1,1896)	1:31:A:LYS:HD3	1:27:A:GLN:HG3	4	0.5
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD11	8	0.5
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD12	8	0.5
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD13	8	0.5
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	8	0.5
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	8	0.5
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	8	0.5
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG11	4	0.5
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG12	4	0.5
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG13	4	0.5
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	8	0.5
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD11	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD12	6	0.5
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD13	6	0.5
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	1	0.5
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	1	0.5
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	1	0.5
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	1	0.5
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	1	0.5
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	1	0.5
(1,1286)	1:88:A:LYS:H	1:84:A:LEU:HG	8	0.5
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG11	3	0.5
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG12	3	0.5
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG13	3	0.5
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG11	3	0.5
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG12	3	0.5
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG13	3	0.5
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG11	3	0.5
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG12	3	0.5
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG13	3	0.5
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	4	0.5
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	4	0.5
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	4	0.5
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	4	0.5
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD11	6	0.5
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD12	6	0.5
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD13	6	0.5
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	9	0.5
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	9	0.5
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	7	0.5
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	7	0.5
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	3	0.5
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	1	0.5
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	1	0.5
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	10	0.5
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	10	0.5
(1,275)	1:77:A:ASN:HB2	1:70:A:VAL:HA	3	0.5
(1,275)	1:77:A:ASN:HB3	1:70:A:VAL:HA	3	0.5
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	6	0.5
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	6	0.5
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	4	0.5
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	4	0.5
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	7	0.5
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	7	0.5
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	7	0.5
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	7	0.5
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	7	0.5
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	1	0.5
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	10	0.5
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	7	0.5
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	1	0.5
(1,1)	1:2:A:VAL:H	1:1:A:MET:HB2	4	0.5
(1,1)	1:2:A:VAL:H	1:1:A:MET:HB3	4	0.5
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	5	0.49
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	10	0.49
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	3	0.49
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	3	0.49
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	3	0.49
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	2	0.49
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	2	0.49
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	2	0.49
(1,1948)	1:44:A:VAL:HB	1:4:A:LEU:HB3	9	0.49
(1,1914)	1:30:A:ILE:HG13	1:34:A:ASN:HB2	4	0.49
(1,1907)	1:34:A:ASN:HB2	1:30:A:ILE:HG13	4	0.49
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	5	0.49
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG21	3	0.49
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG22	3	0.49
(1,1783)	1:22:A:ALA:H	1:25:A:VAL:HG23	3	0.49
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	3	0.49
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	1	0.49
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	1	0.49
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	1	0.49
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	1	0.49
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	10	0.49
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	10	0.49
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	10	0.49
(1,572)	1:84:A:LEU:H	1:89:A:LEU:HG	9	0.49
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	9	0.49
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	2	0.49
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	2	0.49
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	1	0.49
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	1	0.49
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	1	0.49
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	1	0.49
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	1	0.49
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	1	0.49
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	1	0.49
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG11	8	0.49
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG12	8	0.49
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG13	8	0.49
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG21	8	0.49
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG22	8	0.49
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG23	8	0.49
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	4	0.49
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	2	0.49
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	2	0.49
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	2	0.49
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	6	0.49
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	5	0.49
(3,64)	1:129:A:ARG:H	1:109:A:ASP:O	6	0.48
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	6	0.48
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	2	0.48
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE2	6	0.48
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE3	6	0.48
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE2	6	0.48
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE3	6	0.48
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE2	6	0.48
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE3	6	0.48
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE2	6	0.48
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE3	6	0.48
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE2	6	0.48
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE3	6	0.48
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE2	6	0.48
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE3	6	0.48
(1,1991)	1:82:A:THR:HB	1:61:A:LEU:HB2	1	0.48
(1,1935)	1:94:A:GLU:HG2	1:96:A:PRO:HB2	9	0.48
(1,1935)	1:94:A:GLU:HG3	1:96:A:PRO:HB2	9	0.48
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	9	0.48
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	9	0.48
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	9	0.48
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	4	0.48
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG11	7	0.48
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG12	7	0.48
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG13	7	0.48
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG11	7	0.48
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG12	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG13	7	0.48
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG11	7	0.48
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG12	7	0.48
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG13	7	0.48
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG21	4	0.48
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG22	4	0.48
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG23	4	0.48
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	5	0.48
(1,387)	1:10:A:LEU:HG	1:38:A:VAL:HB	5	0.48
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	5	0.48
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	2	0.48
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	2	0.48
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	2	0.48
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	2	0.48
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	2	0.48
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	2	0.48
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	2	0.48
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	2	0.48
(1,257)	1:112:A:PHE:H	1:128:A:ILE:HA	10	0.48
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	10	0.48
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	1	0.48
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	1	0.48
(1,183)	1:99:A:ARG:H	1:99:A:ARG:HD2	9	0.48
(1,183)	1:99:A:ARG:H	1:99:A:ARG:HD3	9	0.48
(1,123)	1:60:A:THR:H	1:59:A:SER:HB2	9	0.48
(1,123)	1:60:A:THR:H	1:59:A:SER:HB3	9	0.48
(1,78)	1:35:A:SER:H	1:33:A:ALA:H	9	0.48
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	6	0.48
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	8	0.48
(3,18)	1:124:A:LYS:H	1:14:A:GLU:O	7	0.47
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	9	0.47
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	3	0.47
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	5	0.47
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	7	0.47
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	7	0.47
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	7	0.47
(1,1967)	1:124:A:LYS:HB2	1:14:A:GLU:HB3	4	0.47
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	5	0.47
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	5	0.47
(1,1914)	1:30:A:ILE:HG13	1:34:A:ASN:HB2	5	0.47
(1,1907)	1:34:A:ASN:HB2	1:30:A:ILE:HG13	5	0.47
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	9	0.47
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	9	0.47
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	9	0.47
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	9	0.47
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	9	0.47
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	6	0.47
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	6	0.47
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	6	0.47
(1,1330)	1:82:A:THR:H	1:91:A:VAL:HB	2	0.47
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA2	7	0.47
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA3	7	0.47
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB2	3	0.47
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB3	3	0.47
(1,691)	1:34:A:ASN:H	1:32:A:LYS:HA	10	0.47
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	2	0.47
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	2	0.47
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	2	0.47
(1,392)	1:79:A:LYS:HE2	1:94:A:GLU:HG2	5	0.47
(1,392)	1:79:A:LYS:HE2	1:94:A:GLU:HG3	5	0.47
(1,392)	1:79:A:LYS:HE3	1:94:A:GLU:HG2	5	0.47
(1,392)	1:79:A:LYS:HE3	1:94:A:GLU:HG3	5	0.47
(1,276)	1:25:A:VAL:HG11	1:74:A:VAL:HB	1	0.47
(1,276)	1:25:A:VAL:HG12	1:74:A:VAL:HB	1	0.47
(1,276)	1:25:A:VAL:HG13	1:74:A:VAL:HB	1	0.47
(1,276)	1:25:A:VAL:HG21	1:74:A:VAL:HB	1	0.47
(1,276)	1:25:A:VAL:HG22	1:74:A:VAL:HB	1	0.47
(1,276)	1:25:A:VAL:HG23	1:74:A:VAL:HB	1	0.47
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG11	1	0.47
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG12	1	0.47
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG13	1	0.47
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG21	1	0.47
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG22	1	0.47
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG23	1	0.47
(1,193)	1:104:A:THR:H	1:104:A:THR:HG21	9	0.47
(1,193)	1:104:A:THR:H	1:104:A:THR:HG22	9	0.47
(1,193)	1:104:A:THR:H	1:104:A:THR:HG23	9	0.47
(1,186)	1:102:A:THR:H	1:102:A:THR:HG21	4	0.47
(1,186)	1:102:A:THR:H	1:102:A:THR:HG22	4	0.47
(1,186)	1:102:A:THR:H	1:102:A:THR:HG23	4	0.47
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	9	0.47
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	9	0.47
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	9	0.47
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	9	0.47
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	9	0.47
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	9	0.47
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	9	0.47
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	9	0.47
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	9	0.47
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	9	0.47
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	9	0.47
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	2	0.47
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	7	0.47
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB2	7	0.47
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB3	7	0.47
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	5	0.47
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	7	0.47
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	8	0.46
(3,18)	1:124:A:LYS:H	1:14:A:GLU:O	2	0.46
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	9	0.46
(1,2051)	1:12:A:LYS:HE2	1:126:A:TYR:HD1	7	0.46
(1,2051)	1:12:A:LYS:HE3	1:126:A:TYR:HD1	7	0.46
(1,1957)	1:114:A:LEU:HD21	1:10:A:LEU:HA	1	0.46
(1,1957)	1:114:A:LEU:HD22	1:10:A:LEU:HA	1	0.46
(1,1957)	1:114:A:LEU:HD23	1:10:A:LEU:HA	1	0.46
(1,1948)	1:44:A:VAL:HB	1:4:A:LEU:HB3	10	0.46
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	1	0.46
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	1	0.46
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	1	0.46
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG11	5	0.46
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG12	5	0.46
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG13	5	0.46
(1,1885)	1:22:A:ALA:HB1	1:18:A:GLU:HB2	10	0.46
(1,1885)	1:22:A:ALA:HB2	1:18:A:GLU:HB2	10	0.46
(1,1885)	1:22:A:ALA:HB3	1:18:A:GLU:HB2	10	0.46
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	9	0.46
(1,1787)	1:29:A:SER:H	1:32:A:LYS:HE2	8	0.46
(1,1787)	1:29:A:SER:H	1:32:A:LYS:HE3	8	0.46
(1,1286)	1:88:A:LYS:H	1:84:A:LEU:HG	4	0.46
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	8	0.46
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	8	0.46
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	8	0.46
(1,729)	1:125:A:ARG:H	1:13:A:ASN:HA	6	0.46
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	5	0.46
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	5	0.46
(1,627)	1:14:A:GLU:H	1:124:A:LYS:H	1	0.46
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	9	0.46
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	9	0.46
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	9	0.46
(1,409)	1:124:A:LYS:H	1:14:A:GLU:H	1	0.46
(1,396)	1:11:A:GLU:HG2	1:128:A:ILE:HG12	8	0.46
(1,396)	1:11:A:GLU:HG3	1:128:A:ILE:HG12	8	0.46
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD21	8	0.46
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD22	8	0.46
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD23	8	0.46
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD21	8	0.46
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD22	8	0.46
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD23	8	0.46
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD21	8	0.46
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD22	8	0.46
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD23	8	0.46
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG11	4	0.46
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG12	4	0.46
(1,378)	1:48:A:LYS:HB2	1:2:A:VAL:HG13	4	0.46
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	3	0.46
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	3	0.46
(1,276)	1:25:A:VAL:HG11	1:74:A:VAL:HB	6	0.46
(1,276)	1:25:A:VAL:HG12	1:74:A:VAL:HB	6	0.46
(1,276)	1:25:A:VAL:HG13	1:74:A:VAL:HB	6	0.46
(1,276)	1:25:A:VAL:HG21	1:74:A:VAL:HB	6	0.46
(1,276)	1:25:A:VAL:HG22	1:74:A:VAL:HB	6	0.46
(1,276)	1:25:A:VAL:HG23	1:74:A:VAL:HB	6	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG11	6	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG12	6	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG13	6	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG21	6	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG22	6	0.46
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG23	6	0.46
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB2	6	0.46
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB3	6	0.46
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB2	6	0.46
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB3	6	0.46
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	1	0.46
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	1	0.46
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	2	0.46
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	10	0.46
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	2	0.46
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	2	0.46
(3,64)	1:129:A:ARG:H	1:109:A:ASP:O	3	0.45
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	3	0.45
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	2	0.45
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	2	0.45
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	2	0.45
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	9	0.45
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	9	0.45
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	9	0.45
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG11	10	0.45
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG12	10	0.45
(1,2002)	1:34:A:ASN:HB3	1:74:A:VAL:HG13	10	0.45
(1,1943)	1:45:A:ASN:HB3	1:2:A:VAL:HA	3	0.45
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	9	0.45
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	9	0.45
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	9	0.45
(1,1906)	1:27:A:GLN:HA	1:30:A:ILE:HG13	9	0.45
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	5	0.45
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	5	0.45
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	5	0.45
(1,1813)	1:3:A:GLN:HE22	1:45:A:ASN:HA	10	0.45
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG2	9	0.45
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG3	9	0.45
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	10	0.45
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	10	0.45
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	10	0.45
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	3	0.45
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	3	0.45
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	3	0.45
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	3	0.45
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	3	0.45
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	3	0.45
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	7	0.45
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	7	0.45
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	7	0.45
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD11	4	0.45
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD12	4	0.45
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD13	4	0.45
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	4	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	4	0.45
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	4	0.45
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	5	0.45
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	5	0.45
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	5	0.45
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	6	0.45
(1,383)	1:36:A:PRO:HG2	1:12:A:LYS:HA	8	0.45
(1,383)	1:36:A:PRO:HG3	1:12:A:LYS:HA	8	0.45
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB1	9	0.45
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB2	9	0.45
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB3	9	0.45
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB1	9	0.45
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB2	9	0.45
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB3	9	0.45
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB1	9	0.45
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB2	9	0.45
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB3	9	0.45
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB2	4	0.45
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB3	4	0.45
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	2	0.45
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	2	0.45
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	5	0.45
(1,68)	1:33:A:ALA:H	1:31:A:LYS:H	7	0.45
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	6	0.45
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	2	0.45
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	2	0.45
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	9	0.44
(3,51)	1:106:A:GLU:N	1:113:A:VAL:O	4	0.44
(3,20)	1:19:A:TYR:H	1:15:A:ASN:O	4	0.44
(1,2056)	1:14:A:GLU:HB3	1:126:A:TYR:HE1	3	0.44
(1,2052)	1:14:A:GLU:HB2	1:126:A:TYR:HD1	7	0.44
(1,2032)	1:105:A:TYR:HB2	1:112:A:PHE:HA	9	0.44
(1,2032)	1:105:A:TYR:HB3	1:112:A:PHE:HA	9	0.44
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	8	0.44
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	8	0.44
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	8	0.44
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE2	4	0.44
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE3	4	0.44
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE2	4	0.44
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE3	4	0.44
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE2	4	0.44
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE3	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE2	4	0.44
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE3	4	0.44
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE2	4	0.44
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE3	4	0.44
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE2	4	0.44
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE3	4	0.44
(1,1991)	1:82:A:THR:HB	1:61:A:LEU:HB2	4	0.44
(1,1958)	1:36:A:PRO:HA	1:10:A:LEU:HB3	4	0.44
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	9	0.44
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	9	0.44
(1,1935)	1:94:A:GLU:HG2	1:96:A:PRO:HB2	8	0.44
(1,1935)	1:94:A:GLU:HG3	1:96:A:PRO:HB2	8	0.44
(1,1885)	1:22:A:ALA:HB1	1:18:A:GLU:HB2	8	0.44
(1,1885)	1:22:A:ALA:HB2	1:18:A:GLU:HB2	8	0.44
(1,1885)	1:22:A:ALA:HB3	1:18:A:GLU:HB2	8	0.44
(1,1781)	1:17:A:GLU:H	1:21:A:ALA:HB1	2	0.44
(1,1781)	1:17:A:GLU:H	1:21:A:ALA:HB2	2	0.44
(1,1781)	1:17:A:GLU:H	1:21:A:ALA:HB3	2	0.44
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	10	0.44
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	6	0.44
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	6	0.44
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	6	0.44
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	6	0.44
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	6	0.44
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	6	0.44
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	3	0.44
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	6	0.44
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	6	0.44
(1,430)	1:24:A:GLY:H	1:20:A:LEU:HA	3	0.44
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG11	7	0.44
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG12	7	0.44
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG13	7	0.44
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	2	0.44
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD2	10	0.44
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD3	10	0.44
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	9	0.44
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	9	0.44
(1,197)	1:89:A:LEU:H	1:106:A:GLU:HA	1	0.44
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	8	0.44
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	8	0.44
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	8	0.44
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	8	0.44
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	8	0.44
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	4	0.44
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	8	0.44
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	1	0.44
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	10	0.44
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	4	0.44
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	9	0.44
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	9	0.44
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG21	10	0.44
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG22	10	0.44
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG23	10	0.44
(3,17)	1:124:A:LYS:N	1:14:A:GLU:O	4	0.43
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	4	0.43
(1,2019)	1:63:A:VAL:HG21	1:89:A:LEU:HB2	9	0.43
(1,2019)	1:63:A:VAL:HG22	1:89:A:LEU:HB2	9	0.43
(1,2019)	1:63:A:VAL:HG23	1:89:A:LEU:HB2	9	0.43
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	4	0.43
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	4	0.43
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	4	0.43
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	5	0.43
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	5	0.43
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	5	0.43
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	5	0.43
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	5	0.43
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	5	0.43
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	5	0.43
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	2	0.43
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	2	0.43
(1,430)	1:24:A:GLY:H	1:20:A:LEU:HA	10	0.43
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	5	0.43
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	5	0.43
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	1	0.43
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	4	0.43
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	4	0.43
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	4	0.43
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	4	0.43
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	4	0.43
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	4	0.43
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	4	0.43
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	4	0.43
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	8	0.43
(1,247)	1:124:A:LYS:H	1:125:A:ARG:H	10	0.43
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	4	0.43
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	10	0.43
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	8	0.43
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	8	0.43
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB2	2	0.43
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB3	2	0.43
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB2	2	0.43
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB3	2	0.43
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	1	0.43
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	1	0.43
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	10	0.43
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	10	0.43
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG11	5	0.43
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG12	5	0.43
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG13	5	0.43
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG21	5	0.43
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG22	5	0.43
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG23	5	0.43
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	9	0.43
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE2	9	0.43
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE3	9	0.43
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	2	0.43
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	3	0.43
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	6	0.43
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	3	0.43
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	10	0.43
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB2	4	0.43
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB3	4	0.43
(3,64)	1:129:A:ARG:H	1:109:A:ASP:O	5	0.42
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG11	9	0.42
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG12	9	0.42
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG13	9	0.42
(1,1784)	1:27:A:GLN:HE21	1:29:A:SER:H	1	0.42
(1,1784)	1:27:A:GLN:HE21	1:29:A:SER:H	6	0.42
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	9	0.42
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB1	4	0.42
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB2	4	0.42
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB3	4	0.42
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB1	4	0.42
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB2	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB3	4	0.42
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	2	0.42
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	2	0.42
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	2	0.42
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	2	0.42
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	2	0.42
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	2	0.42
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	2	0.42
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	2	0.42
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	2	0.42
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	2	0.42
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	2	0.42
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	2	0.42
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	2	0.42
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	2	0.42
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	2	0.42
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	2	0.42
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	2	0.42
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	2	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	4	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	4	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	4	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	4	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	4	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	4	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	6	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	6	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	6	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	6	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	6	0.42
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	6	0.42
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB2	1	0.42
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB3	1	0.42
(1,731)	1:76:A:MET:H	1:71:A:LEU:HD11	8	0.42
(1,731)	1:76:A:MET:H	1:71:A:LEU:HD12	8	0.42
(1,731)	1:76:A:MET:H	1:71:A:LEU:HD13	8	0.42
(1,614)	1:121:A:MET:H	1:118:A:ALA:HA	3	0.42
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE2	7	0.42
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE3	7	0.42
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	8	0.42
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD2	6	0.42
(1,395)	1:115:A:THR:HB	1:124:A:LYS:HD3	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	7	0.42
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	10	0.42
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	5	0.42
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	6	0.42
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG2	10	0.42
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG3	10	0.42
(1,152)	1:92:A:ASN:H	1:82:A:THR:HA	3	0.42
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG2	6	0.42
(1,136)	1:66:A:GLU:H	1:65:A:GLU:HG3	6	0.42
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD11	10	0.42
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD12	10	0.42
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD13	10	0.42
(1,78)	1:35:A:SER:H	1:33:A:ALA:H	4	0.42
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	4	0.42
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	7	0.42
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	7	0.42
(3,16)	1:14:A:GLU:H	1:124:A:LYS:O	4	0.41
(3,10)	1:10:A:LEU:H	1:40:A:TYR:O	6	0.41
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	5	0.41
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	8	0.41
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	7	0.41
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	7	0.41
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	7	0.41
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD21	3	0.41
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD22	3	0.41
(1,1950)	1:87:A:SER:HB2	1:4:A:LEU:HD23	3	0.41
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	9	0.41
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	9	0.41
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	9	0.41
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	9	0.41
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	7	0.41
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	7	0.41
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	7	0.41
(1,1799)	1:47:A:ASN:HD21	1:2:A:VAL:HB	4	0.41
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	6	0.41
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	2	0.41
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD2	10	0.41
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD3	10	0.41
(1,1768)	1:12:A:LYS:H	1:10:A:LEU:HB3	1	0.41
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	1	0.41
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	1	0.41
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	1	0.41
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	1	0.41
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	1	0.41
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	1	0.41
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	1	0.41
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	1	0.41
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	1	0.41
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	1	0.41
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	1	0.41
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	1	0.41
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	1	0.41
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	1	0.41
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	1	0.41
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	1	0.41
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	1	0.41
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA2	8	0.41
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA3	8	0.41
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	8	0.41
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	8	0.41
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	8	0.41
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	8	0.41
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	8	0.41
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	8	0.41
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	6	0.41
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	6	0.41
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	6	0.41
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	2	0.41
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	2	0.41
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	2	0.41
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	8	0.41
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	8	0.41
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	8	0.41
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	8	0.41
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	4	0.41
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	10	0.41
(1,644)	1:126:A:TYR:HB2	1:12:A:LYS:HB2	2	0.41
(1,644)	1:126:A:TYR:HB2	1:12:A:LYS:HB3	2	0.41
(1,644)	1:126:A:TYR:HB3	1:12:A:LYS:HB2	2	0.41
(1,644)	1:126:A:TYR:HB3	1:12:A:LYS:HB3	2	0.41
(1,643)	1:126:A:TYR:HB2	1:12:A:LYS:HB2	2	0.41
(1,643)	1:126:A:TYR:HB2	1:12:A:LYS:HB3	2	0.41
(1,643)	1:126:A:TYR:HB3	1:12:A:LYS:HB2	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:126:A:TYR:HB3	1:12:A:LYS:HB3	2	0.41
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD11	4	0.41
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD12	4	0.41
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD13	4	0.41
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD11	8	0.41
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD12	8	0.41
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD13	8	0.41
(1,614)	1:121:A:MET:H	1:118:A:ALA:HA	5	0.41
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	5	0.41
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	6	0.41
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	9	0.41
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	9	0.41
(1,275)	1:77:A:ASN:HB2	1:70:A:VAL:HA	5	0.41
(1,275)	1:77:A:ASN:HB3	1:70:A:VAL:HA	5	0.41
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB2	10	0.41
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB3	10	0.41
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	6	0.41
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	7	0.41
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	7	0.41
(1,197)	1:89:A:LEU:H	1:106:A:GLU:HA	3	0.41
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	7	0.41
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	7	0.41
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG11	1	0.41
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG12	1	0.41
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG13	1	0.41
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG21	1	0.41
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG22	1	0.41
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG23	1	0.41
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	3	0.41
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	3	0.41
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	3	0.41
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	3	0.41
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	3	0.41
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	3	0.41
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	3	0.41
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	3	0.41
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	3	0.41
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	3	0.41
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	3	0.41
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	3	0.41
(1,139)	1:33:A:ALA:H	1:73:A:THR:HB	10	0.41
(1,130)	1:63:A:VAL:H	1:62:A:ILE:HB	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	1	0.41
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	9	0.41
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	9	0.41
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	1	0.41
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	9	0.41
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	10	0.41
(3,18)	1:124:A:LYS:H	1:14:A:GLU:O	1	0.4
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	7	0.4
(1,2051)	1:12:A:LYS:HE2	1:126:A:TYR:HD1	9	0.4
(1,2051)	1:12:A:LYS:HE3	1:126:A:TYR:HD1	9	0.4
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	2	0.4
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	2	0.4
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	2	0.4
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	10	0.4
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	10	0.4
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	10	0.4
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	2	0.4
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	2	0.4
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	2	0.4
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	10	0.4
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	10	0.4
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	10	0.4
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	4	0.4
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	4	0.4
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	4	0.4
(1,1923)	1:67:A:VAL:HG21	1:65:A:GLU:HB2	2	0.4
(1,1923)	1:67:A:VAL:HG22	1:65:A:GLU:HB2	2	0.4
(1,1923)	1:67:A:VAL:HG23	1:65:A:GLU:HB2	2	0.4
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	3	0.4
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	3	0.4
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	3	0.4
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	2	0.4
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	7	0.4
(1,1628)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	1	0.4
(1,1628)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	1	0.4
(1,1627)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	1	0.4
(1,1627)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	1	0.4
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	2	0.4
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	2	0.4
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	2	0.4
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	2	0.4
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	2	0.4
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	2	0.4
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	2	0.4
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	2	0.4
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	2	0.4
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	2	0.4
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	2	0.4
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	2	0.4
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	2	0.4
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	2	0.4
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	2	0.4
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	2	0.4
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	2	0.4
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	2	0.4
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	2	0.4
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	2	0.4
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	2	0.4
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	2	0.4
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	2	0.4
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	2	0.4
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	2	0.4
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	2	0.4
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	2	0.4
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	2	0.4
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	2	0.4
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	2	0.4
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	2	0.4
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	2	0.4
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	2	0.4
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	2	0.4
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	2	0.4
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	2	0.4
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	2	0.4
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	2	0.4
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	2	0.4
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	2	0.4
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	2	0.4
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	2	0.4
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	2	0.4
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	2	0.4
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	2	0.4
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	2	0.4
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	1	0.4
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	8	0.4
(1,614)	1:121:A:MET:H	1:118:A:ALA:HA	4	0.4
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	10	0.4
(1,394)	1:126:A:TYR:HB2	1:113:A:VAL:HA	3	0.4
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD21	9	0.4
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD22	9	0.4
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD23	9	0.4
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	9	0.4
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	9	0.4
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	9	0.4
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	9	0.4
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	9	0.4
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	9	0.4
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	9	0.4
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	9	0.4
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	9	0.4
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	9	0.4
(1,123)	1:60:A:THR:H	1:59:A:SER:HB2	8	0.4
(1,123)	1:60:A:THR:H	1:59:A:SER:HB3	8	0.4
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	6	0.4
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	10	0.4
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	2	0.4
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB2	3	0.4
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB3	3	0.4
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	6	0.4
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	8	0.4
(3,63)	1:129:A:ARG:N	1:109:A:ASP:O	1	0.39
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	9	0.39
(2,6)	1:39:A:VAL:H	1:54:A:SER:H	4	0.39
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	2	0.39
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	2	0.39
(1,1938)	1:118:A:ALA:HB1	1:122:A:VAL:HB	6	0.39
(1,1938)	1:118:A:ALA:HB2	1:122:A:VAL:HB	6	0.39
(1,1938)	1:118:A:ALA:HB3	1:122:A:VAL:HB	6	0.39
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG11	3	0.39
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG12	3	0.39
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG13	3	0.39
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG11	6	0.39
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG12	6	0.39
(1,1920)	1:42:A:ILE:HG13	1:44:A:VAL:HG13	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1885)	1:22:A:ALA:HB1	1:18:A:GLU:HB2	1	0.39
(1,1885)	1:22:A:ALA:HB2	1:18:A:GLU:HB2	1	0.39
(1,1885)	1:22:A:ALA:HB3	1:18:A:GLU:HB2	1	0.39
(1,766)	1:124:A:LYS:HA	1:115:A:THR:H	2	0.39
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	2	0.39
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	1	0.39
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	4	0.39
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	8	0.39
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	8	0.39
(1,222)	1:120:A:ASP:H	1:118:A:ALA:HA	7	0.39
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	4	0.39
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	4	0.39
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	4	0.39
(1,124)	1:53:A:SER:H	1:59:A:SER:H	7	0.39
(1,113)	1:59:A:SER:H	1:53:A:SER:H	7	0.39
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	3	0.39
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	3	0.39
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	5	0.39
(1,88)	1:54:A:SER:H	1:39:A:VAL:H	4	0.39
(1,73)	1:30:A:ILE:H	1:32:A:LYS:H	5	0.39
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	7	0.39
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	9	0.39
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	5	0.39
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	9	0.39
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	4	0.39
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	7	0.39
(1,22)	1:11:A:GLU:H	1:10:A:LEU:HG	1	0.39
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	4	0.39
(3,18)	1:124:A:LYS:H	1:14:A:GLU:O	8	0.38
(3,10)	1:10:A:LEU:H	1:40:A:TYR:O	9	0.38
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG21	10	0.38
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG22	10	0.38
(1,1985)	1:10:A:LEU:HB2	1:38:A:VAL:HG23	10	0.38
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	1	0.38
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	1	0.38
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	1	0.38
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	10	0.38
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	10	0.38
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	10	0.38
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	10	0.38
(1,1799)	1:47:A:ASN:HD21	1:2:A:VAL:HB	6	0.38
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	4	0.38
(1,1757)	1:64:A:ASN:HD22	1:63:A:VAL:HB	1	0.38
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	1	0.38
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	1	0.38
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	1	0.38
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	1	0.38
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	1	0.38
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	1	0.38
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	1	0.38
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	1	0.38
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	4	0.38
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	4	0.38
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	4	0.38
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	1	0.38
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	1	0.38
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	1	0.38
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	1	0.38
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	1	0.38
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	1	0.38
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	1	0.38
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	1	0.38
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA2	10	0.38
(1,1207)	1:76:A:MET:H	1:72:A:GLY:HA3	10	0.38
(1,907)	1:25:A:VAL:H	1:23:A:LEU:HG	2	0.38
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG11	3	0.38
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG12	3	0.38
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG13	3	0.38
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG11	3	0.38
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG12	3	0.38
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG13	3	0.38
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	8	0.38
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	8	0.38
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	8	0.38
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	6	0.38
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	10	0.38
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	10	0.38
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	1	0.38
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	10	0.38
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	4	0.38
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	7	0.38
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	7	0.38
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB1	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB2	1	0.38
(1,371)	1:32:A:LYS:H	1:33:A:ALA:HB3	1	0.38
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	5	0.38
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	4	0.38
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	4	0.38
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	1	0.38
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	1	0.38
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	1	0.38
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	1	0.38
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	1	0.38
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	1	0.38
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE2	3	0.38
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE3	3	0.38
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	3	0.38
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	5	0.38
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	4	0.38
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	9	0.38
(1,55)	1:24:A:GLY:H	1:23:A:LEU:HB2	8	0.38
(1,55)	1:24:A:GLY:H	1:23:A:LEU:HB3	8	0.38
(1,23)	1:12:A:LYS:H	1:11:A:GLU:HA	3	0.38
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	7	0.38
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	5	0.38
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	6	0.38
(1,1816)	1:39:A:VAL:H	1:54:A:SER:HA	4	0.37
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	2	0.37
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	10	0.37
(1,1628)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	2	0.37
(1,1628)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	2	0.37
(1,1627)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	2	0.37
(1,1627)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	2	0.37
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	8	0.37
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	8	0.37
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	8	0.37
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	8	0.37
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	8	0.37
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	8	0.37
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	8	0.37
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	8	0.37
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	8	0.37
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	8	0.37
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	8	0.37
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	8	0.37
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	8	0.37
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	8	0.37
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	8	0.37
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	8	0.37
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	8	0.37
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	8	0.37
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	8	0.37
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	8	0.37
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	8	0.37
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	8	0.37
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	8	0.37
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	8	0.37
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	8	0.37
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	8	0.37
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	8	0.37
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	8	0.37
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	8	0.37
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	8	0.37
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	8	0.37
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	8	0.37
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	8	0.37
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	8	0.37
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	8	0.37
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	8	0.37
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	8	0.37
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	8	0.37
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	8	0.37
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	8	0.37
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	8	0.37
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	8	0.37
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	8	0.37
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	8	0.37
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	8	0.37
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	8	0.37
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	8	0.37
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD21	3	0.37
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD22	3	0.37
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	5	0.37
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	5	0.37
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	5	0.37
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	5	0.37
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	5	0.37
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	4	0.37
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	4	0.37
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	4	0.37
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	5	0.37
(1,725)	1:29:A:SER:H	1:32:A:LYS:HG2	1	0.37
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	7	0.37
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB2	1	0.37
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB3	1	0.37
(1,646)	1:30:A:ILE:HG21	1:20:A:LEU:HD11	9	0.37
(1,646)	1:30:A:ILE:HG21	1:20:A:LEU:HD12	9	0.37
(1,646)	1:30:A:ILE:HG21	1:20:A:LEU:HD13	9	0.37
(1,646)	1:30:A:ILE:HG21	1:20:A:LEU:HD21	9	0.37
(1,646)	1:30:A:ILE:HG21	1:20:A:LEU:HD22	9	0.37
(1,646)	1:30:A:ILE:HG21	1:20:A:LEU:HD23	9	0.37
(1,646)	1:30:A:ILE:HG22	1:20:A:LEU:HD11	9	0.37
(1,646)	1:30:A:ILE:HG22	1:20:A:LEU:HD12	9	0.37
(1,646)	1:30:A:ILE:HG22	1:20:A:LEU:HD13	9	0.37
(1,646)	1:30:A:ILE:HG22	1:20:A:LEU:HD21	9	0.37
(1,646)	1:30:A:ILE:HG22	1:20:A:LEU:HD22	9	0.37
(1,646)	1:30:A:ILE:HG22	1:20:A:LEU:HD23	9	0.37
(1,646)	1:30:A:ILE:HG23	1:20:A:LEU:HD11	9	0.37
(1,646)	1:30:A:ILE:HG23	1:20:A:LEU:HD12	9	0.37
(1,646)	1:30:A:ILE:HG23	1:20:A:LEU:HD13	9	0.37
(1,646)	1:30:A:ILE:HG23	1:20:A:LEU:HD21	9	0.37
(1,646)	1:30:A:ILE:HG23	1:20:A:LEU:HD22	9	0.37
(1,646)	1:30:A:ILE:HG23	1:20:A:LEU:HD23	9	0.37
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	8	0.37
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	8	0.37
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	8	0.37
(1,428)	1:17:A:GLU:H	1:19:A:TYR:H	5	0.37
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	1	0.37
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	1	0.37
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	1	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	1	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	1	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	1	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	1	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	1	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	1	0.37
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	5	0.37
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	5	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	5	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	5	0.37
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	5	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	5	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	5	0.37
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	5	0.37
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	2	0.37
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	2	0.37
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	2	0.37
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD11	7	0.37
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD12	7	0.37
(1,373)	1:76:A:MET:H	1:71:A:LEU:HD13	7	0.37
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	4	0.37
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	5	0.37
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	6	0.37
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG12	9	0.37
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG13	9	0.37
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	7	0.37
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	7	0.37
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	3	0.37
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	3	0.37
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB2	5	0.37
(1,196)	1:106:A:GLU:H	1:105:A:TYR:HB3	5	0.37
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	7	0.37
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	7	0.37
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	10	0.37
(1,49)	1:23:A:LEU:H	1:21:A:ALA:HA	6	0.37
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	2	0.37
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	6	0.37
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	6	0.37
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	8	0.37
(3,34)	1:48:A:LYS:H	1:45:A:ASN:O	6	0.36
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	3	0.36
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	3	0.36
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	3	0.36
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE2	8	0.36
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE3	8	0.36
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE2	8	0.36
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE3	8	0.36
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE2	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE3	8	0.36
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE2	8	0.36
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE3	8	0.36
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE2	8	0.36
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE3	8	0.36
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE2	8	0.36
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE3	8	0.36
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	7	0.36
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	7	0.36
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	7	0.36
(1,1973)	1:121:A:MET:HB2	1:18:A:GLU:HG3	6	0.36
(1,1755)	1:60:A:THR:H	1:61:A:LEU:HG	9	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	3	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	3	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	3	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	3	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	3	0.36
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	3	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	3	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	3	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	3	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	3	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	3	0.36
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	3	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	3	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	3	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	3	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	3	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	3	0.36
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	3	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	3	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	3	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	3	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	3	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	3	0.36
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	3	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	3	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	3	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	3	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	3	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	3	0.36
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	3	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	3	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	3	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	3	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	3	0.36
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	3	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	3	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	3	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	3	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	3	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	3	0.36
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	3	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	3	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	3	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	3	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	3	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	3	0.36
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	3	0.36
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	3	0.36
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	3	0.36
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	3	0.36
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB2	10	0.36
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB3	10	0.36
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	8	0.36
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	2	0.36
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	2	0.36
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	2	0.36
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	2	0.36
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	7	0.36
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	6	0.36
(1,286)	1:23:A:LEU:HG	1:95:A:LEU:HG	7	0.36
(1,273)	1:50:A:THR:HB	1:43:A:ILE:HG12	7	0.36
(1,273)	1:50:A:THR:HB	1:43:A:ILE:HG13	7	0.36
(1,272)	1:50:A:THR:HB	1:43:A:ILE:HG12	7	0.36
(1,272)	1:50:A:THR:HB	1:43:A:ILE:HG13	7	0.36
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	10	0.36
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	10	0.36
(1,217)	1:116:A:MET:H	1:115:A:THR:HG21	10	0.36
(1,217)	1:116:A:MET:H	1:115:A:THR:HG22	10	0.36
(1,217)	1:116:A:MET:H	1:115:A:THR:HG23	10	0.36
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	3	0.36
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	3	0.36
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	3	0.36
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	3	0.36
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	3	0.36
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	1	0.36
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	7	0.36
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	3	0.36
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	3	0.36
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB2	1	0.36
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB3	1	0.36
(1,12)	1:130:A:THR:H	1:8:A:TYR:HA	2	0.36
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	2	0.36
(1,2055)	1:14:A:GLU:HB2	1:126:A:TYR:HE1	7	0.35
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	6	0.35
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	6	0.35
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	6	0.35
(1,2019)	1:63:A:VAL:HG21	1:89:A:LEU:HB2	3	0.35
(1,2019)	1:63:A:VAL:HG22	1:89:A:LEU:HB2	3	0.35
(1,2019)	1:63:A:VAL:HG23	1:89:A:LEU:HB2	3	0.35
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	7	0.35
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	7	0.35
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	7	0.35
(1,1978)	1:74:A:VAL:HG21	1:29:A:SER:HB3	6	0.35
(1,1978)	1:74:A:VAL:HG22	1:29:A:SER:HB3	6	0.35
(1,1978)	1:74:A:VAL:HG23	1:29:A:SER:HB3	6	0.35
(1,1973)	1:121:A:MET:HB2	1:18:A:GLU:HG3	10	0.35
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD21	7	0.35
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD22	7	0.35
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD23	7	0.35
(1,725)	1:29:A:SER:H	1:32:A:LYS:HG2	3	0.35
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	5	0.35
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	1	0.35
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	1	0.35
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	8	0.35
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	8	0.35
(1,614)	1:121:A:MET:H	1:118:A:ALA:HA	1	0.35
(1,430)	1:24:A:GLY:H	1:20:A:LEU:HA	9	0.35
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	1	0.35
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD21	10	0.35
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD22	10	0.35
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD23	10	0.35
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	6	0.35
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	7	0.35
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	7	0.35
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	1	0.35
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	1	0.35
(1,246)	1:125:A:ARG:H	1:125:A:ARG:HG2	2	0.35
(1,246)	1:125:A:ARG:H	1:125:A:ARG:HG3	2	0.35
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	3	0.35
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	3	0.35
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG11	8	0.35
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG12	8	0.35
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG13	8	0.35
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG21	8	0.35
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG22	8	0.35
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG23	8	0.35
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG11	8	0.35
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG12	8	0.35
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG13	8	0.35
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG21	8	0.35
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG22	8	0.35
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG23	8	0.35
(1,228)	1:123:A:ALA:H	1:122:A:VAL:HB	7	0.35
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	10	0.35
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	7	0.35
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	8	0.35
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	5	0.35
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	5	0.35
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	8	0.35
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	8	0.35
(1,157)	1:85:A:GLU:H	1:86:A:GLY:H	8	0.35
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	6	0.35
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	8	0.35
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	8	0.35
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	3	0.35
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	5	0.35
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	8	0.35
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB2	10	0.35
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB3	10	0.35
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	1	0.35
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	3	0.35
(3,21)	1:20:A:LEU:N	1:16:A:PHE:O	4	0.34
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	10	0.34
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	10	0.34
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	10	0.34
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	4	0.34
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	4	0.34
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	4	0.34
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG21	6	0.34
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG22	6	0.34
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG23	6	0.34
(1,1885)	1:22:A:ALA:HB1	1:18:A:GLU:HB2	7	0.34
(1,1885)	1:22:A:ALA:HB2	1:18:A:GLU:HB2	7	0.34
(1,1885)	1:22:A:ALA:HB3	1:18:A:GLU:HB2	7	0.34
(1,1790)	1:45:A:ASN:HD21	1:48:A:LYS:HD2	9	0.34
(1,1790)	1:45:A:ASN:HD21	1:48:A:LYS:HD3	9	0.34
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	4	0.34
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	8	0.34
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	2	0.34
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	2	0.34
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	2	0.34
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	2	0.34
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	2	0.34
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	2	0.34
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	2	0.34
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	2	0.34
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	2	0.34
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	2	0.34
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	2	0.34
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	2	0.34
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	2	0.34
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	2	0.34
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	2	0.34
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	2	0.34
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD11	10	0.34
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD12	10	0.34
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD13	10	0.34
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD21	10	0.34
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD22	10	0.34
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD23	10	0.34
(1,1322)	1:105:A:TYR:H	1:89:A:LEU:HG	1	0.34
(1,1053)	1:48:A:LYS:H	1:45:A:ASN:HA	6	0.34
(1,764)	1:12:A:LYS:HE2	1:126:A:TYR:HE1	7	0.34
(1,764)	1:12:A:LYS:HE3	1:126:A:TYR:HE1	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:85:A:GLU:H	1:89:A:LEU:HG	7	0.34
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	3	0.34
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB2	10	0.34
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB3	10	0.34
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE2	6	0.34
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE3	6	0.34
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	1	0.34
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	1	0.34
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	9	0.34
(1,390)	1:106:A:GLU:HA	1:88:A:LYS:HB3	8	0.34
(1,386)	1:31:A:LYS:HB2	1:28:A:ASP:HA	5	0.34
(1,386)	1:31:A:LYS:HB3	1:28:A:ASP:HA	5	0.34
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	9	0.34
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	9	0.34
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	9	0.34
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	9	0.34
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	9	0.34
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	9	0.34
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	9	0.34
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	9	0.34
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	9	0.34
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG21	5	0.34
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG22	5	0.34
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG23	5	0.34
(1,276)	1:25:A:VAL:HG11	1:74:A:VAL:HB	9	0.34
(1,276)	1:25:A:VAL:HG12	1:74:A:VAL:HB	9	0.34
(1,276)	1:25:A:VAL:HG13	1:74:A:VAL:HB	9	0.34
(1,276)	1:25:A:VAL:HG21	1:74:A:VAL:HB	9	0.34
(1,276)	1:25:A:VAL:HG22	1:74:A:VAL:HB	9	0.34
(1,276)	1:25:A:VAL:HG23	1:74:A:VAL:HB	9	0.34
(1,269)	1:28:A:ASP:HA	1:31:A:LYS:HB2	5	0.34
(1,269)	1:28:A:ASP:HA	1:31:A:LYS:HB3	5	0.34
(1,268)	1:31:A:LYS:HB2	1:28:A:ASP:HA	5	0.34
(1,268)	1:31:A:LYS:HB3	1:28:A:ASP:HA	5	0.34
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG11	9	0.34
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG12	9	0.34
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG13	9	0.34
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG21	9	0.34
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG22	9	0.34
(1,267)	1:74:A:VAL:HB	1:25:A:VAL:HG23	9	0.34
(1,186)	1:102:A:THR:H	1:102:A:THR:HG21	5	0.34
(1,186)	1:102:A:THR:H	1:102:A:THR:HG22	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:102:A:THR:H	1:102:A:THR:HG23	5	0.34
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD2	3	0.34
(1,181)	1:95:A:LEU:H	1:96:A:PRO:HD3	3	0.34
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	5	0.34
(1,139)	1:33:A:ALA:H	1:73:A:THR:HB	7	0.34
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	3	0.34
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	3	0.34
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	3	0.34
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	2	0.34
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	6	0.34
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	10	0.34
(1,12)	1:130:A:THR:H	1:8:A:TYR:HA	5	0.34
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	7	0.33
(1,2059)	1:11:A:GLU:HA	1:127:A:PHE:HA	10	0.33
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	5	0.33
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	5	0.33
(1,1970)	1:124:A:LYS:HG3	1:14:A:GLU:HB3	7	0.33
(1,1965)	1:114:A:LEU:HD21	1:13:A:ASN:HB2	9	0.33
(1,1965)	1:114:A:LEU:HD22	1:13:A:ASN:HB2	9	0.33
(1,1965)	1:114:A:LEU:HD23	1:13:A:ASN:HB2	9	0.33
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	9	0.33
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	9	0.33
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	9	0.33
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG2	10	0.33
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG3	10	0.33
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG2	10	0.33
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG3	10	0.33
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG2	10	0.33
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG3	10	0.33
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD21	10	0.33
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD22	10	0.33
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD23	10	0.33
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD21	10	0.33
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD22	10	0.33
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD23	10	0.33
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG11	5	0.33
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG12	5	0.33
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG13	5	0.33
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD2	4	0.33
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD3	4	0.33
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD11	8	0.33
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD12	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:13:A:ASN:H	1:10:A:LEU:HD13	8	0.33
(1,1757)	1:64:A:ASN:HD22	1:63:A:VAL:HB	5	0.33
(1,1639)	1:7:A:THR:H	1:130:A:THR:H	9	0.33
(1,1638)	1:130:A:THR:H	1:7:A:THR:H	9	0.33
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	7	0.33
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	7	0.33
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	7	0.33
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	7	0.33
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	7	0.33
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	7	0.33
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	7	0.33
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	7	0.33
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	7	0.33
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	7	0.33
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	7	0.33
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	7	0.33
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	7	0.33
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	7	0.33
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	7	0.33
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	7	0.33
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	7	0.33
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	7	0.33
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	7	0.33
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	7	0.33
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	7	0.33
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	7	0.33
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	7	0.33
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	7	0.33
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	7	0.33
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	7	0.33
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	7	0.33
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	7	0.33
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	7	0.33
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	7	0.33
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	7	0.33
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	7	0.33
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	7	0.33
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	7	0.33
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	7	0.33
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	7	0.33
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	7	0.33
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	7	0.33
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	7	0.33
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	7	0.33
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	7	0.33
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	7	0.33
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	7	0.33
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	7	0.33
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	7	0.33
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	7	0.33
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	7	0.33
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	2	0.33
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	7	0.33
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	7	0.33
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	7	0.33
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	9	0.33
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	9	0.33
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	9	0.33
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	4	0.33
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	4	0.33
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	9	0.33
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	9	0.33
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	9	0.33
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	9	0.33
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	2	0.33
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD11	10	0.33
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD12	10	0.33
(1,634)	1:112:A:PHE:H	1:128:A:ILE:HD13	10	0.33
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	4	0.33
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	8	0.33
(1,594)	1:93:A:SER:H	1:101:A:GLY:H	3	0.33
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	7	0.33
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	7	0.33
(1,441)	1:29:A:SER:H	1:27:A:GLN:HA	1	0.33
(1,418)	1:19:A:TYR:H	1:17:A:GLU:HA	4	0.33
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG11	4	0.33
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG12	4	0.33
(1,369)	1:3:A:GLN:H	1:2:A:VAL:HG13	4	0.33
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	5	0.33
(1,275)	1:77:A:ASN:HB2	1:70:A:VAL:HA	10	0.33
(1,275)	1:77:A:ASN:HB3	1:70:A:VAL:HA	10	0.33
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG12	2	0.33
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG13	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	5	0.33
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	6	0.33
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	6	0.33
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	9	0.33
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	9	0.33
(1,48)	1:21:A:ALA:H	1:20:A:LEU:HA	8	0.33
(1,42)	1:19:A:TYR:H	1:18:A:GLU:HA	3	0.33
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG21	1	0.33
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG22	1	0.33
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG23	1	0.33
(3,34)	1:48:A:LYS:H	1:45:A:ASN:O	1	0.32
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	6	0.32
(1,2028)	1:91:A:VAL:HA	1:103:A:ARG:HB2	9	0.32
(1,1989)	1:39:A:VAL:HG21	1:54:A:SER:HA	2	0.32
(1,1989)	1:39:A:VAL:HG22	1:54:A:SER:HA	2	0.32
(1,1989)	1:39:A:VAL:HG23	1:54:A:SER:HA	2	0.32
(1,1957)	1:114:A:LEU:HD21	1:10:A:LEU:HA	7	0.32
(1,1957)	1:114:A:LEU:HD22	1:10:A:LEU:HA	7	0.32
(1,1957)	1:114:A:LEU:HD23	1:10:A:LEU:HA	7	0.32
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	3	0.32
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD11	8	0.32
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD12	8	0.32
(1,1933)	1:97:A:ASP:HB3	1:95:A:LEU:HD13	8	0.32
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG2	1	0.32
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG3	1	0.32
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG2	1	0.32
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG3	1	0.32
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG2	1	0.32
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG3	1	0.32
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD21	1	0.32
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD22	1	0.32
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD23	1	0.32
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD21	1	0.32
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD22	1	0.32
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD23	1	0.32
(1,1911)	1:28:A:ASP:HA	1:32:A:LYS:HE2	7	0.32
(1,1911)	1:28:A:ASP:HA	1:32:A:LYS:HE3	7	0.32
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	4	0.32
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	4	0.32
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	4	0.32
(1,1789)	1:48:A:LYS:H	1:45:A:ASN:HD21	4	0.32
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	5	0.32
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	5	0.32
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	5	0.32
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	5	0.32
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	5	0.32
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	5	0.32
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	5	0.32
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	5	0.32
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	5	0.32
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	5	0.32
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	5	0.32
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	5	0.32
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	5	0.32
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	5	0.32
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	5	0.32
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	5	0.32
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	5	0.32
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	2	0.32
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	2	0.32
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	2	0.32
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	2	0.32
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	2	0.32
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	2	0.32
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	9	0.32
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	1	0.32
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	4	0.32
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	3	0.32
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	8	0.32
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	10	0.32
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	10	0.32
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	10	0.32
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	10	0.32
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	10	0.32
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	10	0.32
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	4	0.32
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	10	0.32
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	3	0.32
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	4	0.32
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	5	0.32
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	3	0.32
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	2	0.32
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB2	5	0.32
(1,34)	1:124:A:LYS:H	1:14:A:GLU:HB3	5	0.32
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG21	8	0.32
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG22	8	0.32
(1,10)	1:8:A:TYR:H	1:7:A:THR:HG23	8	0.32
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	10	0.32
(1,2032)	1:105:A:TYR:HB2	1:112:A:PHE:HA	2	0.31
(1,2032)	1:105:A:TYR:HB3	1:112:A:PHE:HA	2	0.31
(1,1991)	1:82:A:THR:HB	1:61:A:LEU:HB2	6	0.31
(1,1991)	1:82:A:THR:HB	1:61:A:LEU:HB2	9	0.31
(1,1978)	1:74:A:VAL:HG21	1:29:A:SER:HB3	7	0.31
(1,1978)	1:74:A:VAL:HG22	1:29:A:SER:HB3	7	0.31
(1,1978)	1:74:A:VAL:HG23	1:29:A:SER:HB3	7	0.31
(1,1967)	1:124:A:LYS:HB2	1:14:A:GLU:HB3	10	0.31
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	1	0.31
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	1	0.31
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	1	0.31
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	7	0.31
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	7	0.31
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	7	0.31
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG21	4	0.31
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG22	4	0.31
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG23	4	0.31
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	3	0.31
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	3	0.31
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	3	0.31
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG11	4	0.31
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG12	4	0.31
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG13	4	0.31
(1,1885)	1:22:A:ALA:HB1	1:18:A:GLU:HB2	4	0.31
(1,1885)	1:22:A:ALA:HB2	1:18:A:GLU:HB2	4	0.31
(1,1885)	1:22:A:ALA:HB3	1:18:A:GLU:HB2	4	0.31
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD11	1	0.31
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD12	1	0.31
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD13	1	0.31
(1,1810)	1:13:A:ASN:HD22	1:34:A:ASN:HA	9	0.31
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	4	0.31
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	4	0.31
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	4	0.31
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	4	0.31
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	4	0.31
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	4	0.31
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	4	0.31
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	4	0.31
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	4	0.31
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	4	0.31
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	4	0.31
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	4	0.31
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	4	0.31
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	2	0.31
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	2	0.31
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	2	0.31
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	7	0.31
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	7	0.31
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	7	0.31
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	4	0.31
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	4	0.31
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	4	0.31
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	4	0.31
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	4	0.31
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	4	0.31
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	4	0.31
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	4	0.31
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	2	0.31
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	6	0.31
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	6	0.31
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	3	0.31
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	7	0.31
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	7	0.31
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	7	0.31
(1,572)	1:84:A:LEU:H	1:89:A:LEU:HG	6	0.31
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	3	0.31
(1,383)	1:36:A:PRO:HG2	1:12:A:LYS:HA	3	0.31
(1,383)	1:36:A:PRO:HG3	1:12:A:LYS:HA	3	0.31
(1,275)	1:77:A:ASN:HB2	1:70:A:VAL:HA	6	0.31
(1,275)	1:77:A:ASN:HB3	1:70:A:VAL:HA	6	0.31
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	5	0.31
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	5	0.31
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	4	0.31
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	4	0.31
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	8	0.31
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	8	0.31
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB2	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB3	8	0.31
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB2	8	0.31
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB3	8	0.31
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	1	0.31
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	9	0.31
(1,192)	1:104:A:THR:H	1:104:A:THR:HB	6	0.31
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	5	0.31
(1,124)	1:53:A:SER:H	1:59:A:SER:H	3	0.31
(1,113)	1:59:A:SER:H	1:53:A:SER:H	3	0.31
(1,110)	1:41:A:GLU:H	1:53:A:SER:HA	9	0.31
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	1	0.31
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	1	0.31
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	4	0.31
(1,66)	1:29:A:SER:H	1:31:A:LYS:H	9	0.31
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB2	3	0.31
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB3	3	0.31
(3,49)	1:101:A:GLY:N	1:93:A:SER:O	10	0.3
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	5	0.3
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	4	0.3
(1,2051)	1:12:A:LYS:HE2	1:126:A:TYR:HD1	5	0.3
(1,2051)	1:12:A:LYS:HE3	1:126:A:TYR:HD1	5	0.3
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD2	6	0.3
(1,1785)	1:27:A:GLN:HE22	1:31:A:LYS:HD3	6	0.3
(1,1778)	1:15:A:ASN:H	1:18:A:GLU:HB3	2	0.3
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	1	0.3
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	1	0.3
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	1	0.3
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	1	0.3
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	1	0.3
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	1	0.3
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	1	0.3
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	1	0.3
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	1	0.3
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	1	0.3
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	1	0.3
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	1	0.3
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	1	0.3
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	1	0.3
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	1	0.3
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	1	0.3
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	1	0.3
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	1	0.3
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	1	0.3
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	1	0.3
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	1	0.3
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	1	0.3
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	1	0.3
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	1	0.3
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	1	0.3
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	1	0.3
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	1	0.3
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	1	0.3
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	1	0.3
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	1	0.3
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	1	0.3
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	1	0.3
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	1	0.3
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	1	0.3
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	1	0.3
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	1	0.3
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	1	0.3
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	1	0.3
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	1	0.3
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	1	0.3
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	1	0.3
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	1	0.3
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	1	0.3
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	1	0.3
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	1	0.3
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	1	0.3
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	1	0.3
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD11	7	0.3
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD12	7	0.3
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD13	7	0.3
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD21	7	0.3
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD22	7	0.3
(1,1578)	1:73:A:THR:HG21	1:71:A:LEU:HD23	7	0.3
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD11	7	0.3
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD12	7	0.3
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD13	7	0.3
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD21	7	0.3
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD22	7	0.3
(1,1578)	1:73:A:THR:HG22	1:71:A:LEU:HD23	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD11	7	0.3
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD12	7	0.3
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD13	7	0.3
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD21	7	0.3
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD22	7	0.3
(1,1578)	1:73:A:THR:HG23	1:71:A:LEU:HD23	7	0.3
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	10	0.3
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB2	6	0.3
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB3	6	0.3
(1,1186)	1:77:A:ASN:HD21	1:70:A:VAL:HA	3	0.3
(1,1186)	1:77:A:ASN:HD22	1:70:A:VAL:HA	3	0.3
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG11	5	0.3
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG12	5	0.3
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG13	5	0.3
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG11	5	0.3
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG12	5	0.3
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG13	5	0.3
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG11	5	0.3
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG12	5	0.3
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG13	5	0.3
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	3	0.3
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	3	0.3
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	3	0.3
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	7	0.3
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	7	0.3
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	7	0.3
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB2	6	0.3
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB3	6	0.3
(1,614)	1:121:A:MET:H	1:118:A:ALA:HA	8	0.3
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	3	0.3
(1,345)	1:43:A:ILE:HG21	1:7:A:THR:HG21	1	0.3
(1,345)	1:43:A:ILE:HG21	1:7:A:THR:HG22	1	0.3
(1,345)	1:43:A:ILE:HG21	1:7:A:THR:HG23	1	0.3
(1,345)	1:43:A:ILE:HG22	1:7:A:THR:HG21	1	0.3
(1,345)	1:43:A:ILE:HG22	1:7:A:THR:HG22	1	0.3
(1,345)	1:43:A:ILE:HG22	1:7:A:THR:HG23	1	0.3
(1,345)	1:43:A:ILE:HG23	1:7:A:THR:HG21	1	0.3
(1,345)	1:43:A:ILE:HG23	1:7:A:THR:HG22	1	0.3
(1,345)	1:43:A:ILE:HG23	1:7:A:THR:HG23	1	0.3
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG11	8	0.3
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG12	8	0.3
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG13	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG21	8	0.3
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG22	8	0.3
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG23	8	0.3
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	7	0.3
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	5	0.3
(1,192)	1:104:A:THR:H	1:104:A:THR:HB	7	0.3
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	8	0.3
(1,78)	1:35:A:SER:H	1:33:A:ALA:H	8	0.3
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	7	0.3
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	8	0.3
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	9	0.3
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	4	0.3
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	4	0.3
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	6	0.3
(3,64)	1:129:A:ARG:H	1:109:A:ASP:O	4	0.29
(3,34)	1:48:A:LYS:H	1:45:A:ASN:O	5	0.29
(3,9)	1:10:A:LEU:N	1:40:A:TYR:O	8	0.29
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	6	0.29
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG2	7	0.29
(1,2063)	1:111:A:GLY:HA3	1:129:A:ARG:HG3	7	0.29
(1,2041)	1:93:A:SER:HB2	1:116:A:MET:HG3	7	0.29
(1,1822)	1:34:A:ASN:HD21	1:71:A:LEU:HB2	9	0.29
(1,1566)	1:43:A:ILE:HB	1:7:A:THR:HB	6	0.29
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD11	4	0.29
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD12	4	0.29
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD13	4	0.29
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD21	4	0.29
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD22	4	0.29
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD23	4	0.29
(1,1356)	1:99:A:ARG:H	1:95:A:LEU:HG	2	0.29
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	7	0.29
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	7	0.29
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	7	0.29
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	7	0.29
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	7	0.29
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	7	0.29
(1,725)	1:29:A:SER:H	1:32:A:LYS:HG2	5	0.29
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	4	0.29
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	2	0.29
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	2	0.29
(1,636)	1:129:A:ARG:H	1:128:A:ILE:HG12	1	0.29
(1,636)	1:129:A:ARG:H	1:128:A:ILE:HG13	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	3	0.29
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	3	0.29
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	3	0.29
(1,627)	1:14:A:GLU:H	1:124:A:LYS:H	9	0.29
(1,599)	1:127:A:PHE:H	1:112:A:PHE:HA	9	0.29
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	2	0.29
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	2	0.29
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	1	0.29
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	1	0.29
(1,491)	1:41:A:GLU:H	1:51:A:PHE:HA	8	0.29
(1,450)	1:32:A:LYS:H	1:30:A:ILE:H	6	0.29
(1,436)	1:19:A:TYR:H	1:21:A:ALA:H	2	0.29
(1,409)	1:124:A:LYS:H	1:14:A:GLU:H	9	0.29
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	3	0.29
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	8	0.29
(1,353)	1:6:A:GLY:H	1:5:A:ALA:HA	3	0.29
(1,349)	1:77:A:ASN:HB2	1:70:A:VAL:HG11	2	0.29
(1,349)	1:77:A:ASN:HB2	1:70:A:VAL:HG12	2	0.29
(1,349)	1:77:A:ASN:HB2	1:70:A:VAL:HG13	2	0.29
(1,349)	1:77:A:ASN:HB2	1:70:A:VAL:HG21	2	0.29
(1,349)	1:77:A:ASN:HB2	1:70:A:VAL:HG22	2	0.29
(1,349)	1:77:A:ASN:HB2	1:70:A:VAL:HG23	2	0.29
(1,349)	1:77:A:ASN:HB3	1:70:A:VAL:HG11	2	0.29
(1,349)	1:77:A:ASN:HB3	1:70:A:VAL:HG12	2	0.29
(1,349)	1:77:A:ASN:HB3	1:70:A:VAL:HG13	2	0.29
(1,349)	1:77:A:ASN:HB3	1:70:A:VAL:HG21	2	0.29
(1,349)	1:77:A:ASN:HB3	1:70:A:VAL:HG22	2	0.29
(1,349)	1:77:A:ASN:HB3	1:70:A:VAL:HG23	2	0.29
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD2	7	0.29
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD3	7	0.29
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	9	0.29
(1,193)	1:104:A:THR:H	1:104:A:THR:HG21	8	0.29
(1,193)	1:104:A:THR:H	1:104:A:THR:HG22	8	0.29
(1,193)	1:104:A:THR:H	1:104:A:THR:HG23	8	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	5	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	5	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	5	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	5	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	5	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	5	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	6	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	6	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	6	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	6	0.29
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	6	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	6	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	6	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	6	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	6	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	6	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	6	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	10	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	10	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	10	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	10	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	10	0.29
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	10	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	6	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	6	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	6	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	6	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	6	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	6	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	10	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	10	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	10	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	10	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	10	0.29
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	10	0.29
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	5	0.29
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	5	0.29
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	5	0.29
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	1	0.29
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	1	0.29
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	9	0.29
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	9	0.29
(1,75)	1:34:A:ASN:H	1:33:A:ALA:HA	9	0.29
(1,5)	1:5:A:ALA:H	1:4:A:LEU:HB2	10	0.29
(1,5)	1:5:A:ALA:H	1:4:A:LEU:HB3	10	0.29
(1,2051)	1:12:A:LYS:HE2	1:126:A:TYR:HD1	4	0.28
(1,2051)	1:12:A:LYS:HE3	1:126:A:TYR:HD1	4	0.28
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG21	2	0.28
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG22	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1947)	1:47:A:ASN:HA	1:2:A:VAL:HG23	2	0.28
(1,1935)	1:94:A:GLU:HG2	1:96:A:PRO:HB2	7	0.28
(1,1935)	1:94:A:GLU:HG3	1:96:A:PRO:HB2	7	0.28
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD11	10	0.28
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD12	10	0.28
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD13	10	0.28
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG11	2	0.28
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG12	2	0.28
(1,1801)	1:45:A:ASN:HD22	1:2:A:VAL:HG13	2	0.28
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	5	0.28
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	4	0.28
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG2	3	0.28
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG3	3	0.28
(1,1628)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	6	0.28
(1,1628)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	6	0.28
(1,1627)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	6	0.28
(1,1627)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	6	0.28
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	1	0.28
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	7	0.28
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG11	8	0.28
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG12	8	0.28
(1,750)	1:4:A:LEU:HD11	1:44:A:VAL:HG13	8	0.28
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG11	8	0.28
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG12	8	0.28
(1,750)	1:4:A:LEU:HD12	1:44:A:VAL:HG13	8	0.28
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG11	8	0.28
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG12	8	0.28
(1,750)	1:4:A:LEU:HD13	1:44:A:VAL:HG13	8	0.28
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	2	0.28
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	2	0.28
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	2	0.28
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD11	7	0.28
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD12	7	0.28
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD13	7	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG11	2	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG12	2	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG13	2	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG21	2	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG22	2	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG23	2	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG11	10	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG12	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG13	10	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG21	10	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG22	10	0.28
(1,693)	1:61:A:LEU:HA	1:67:A:VAL:HG23	10	0.28
(1,394)	1:126:A:TYR:HB2	1:113:A:VAL:HA	8	0.28
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD11	4	0.28
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD12	4	0.28
(1,384)	1:25:A:VAL:HG11	1:20:A:LEU:HD13	4	0.28
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD11	4	0.28
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD12	4	0.28
(1,384)	1:25:A:VAL:HG12	1:20:A:LEU:HD13	4	0.28
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD11	4	0.28
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD12	4	0.28
(1,384)	1:25:A:VAL:HG13	1:20:A:LEU:HD13	4	0.28
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD21	2	0.28
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD22	2	0.28
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD23	2	0.28
(1,347)	1:43:A:ILE:H	1:50:A:THR:HB	10	0.28
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	8	0.28
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	8	0.28
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB1	10	0.28
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB2	10	0.28
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB3	10	0.28
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB1	10	0.28
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB2	10	0.28
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB3	10	0.28
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB1	10	0.28
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB2	10	0.28
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB3	10	0.28
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	2	0.28
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	2	0.28
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB2	6	0.28
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB3	6	0.28
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB1	10	0.28
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB2	10	0.28
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB3	10	0.28
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB2	2	0.28
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB3	2	0.28
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB2	3	0.28
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB3	3	0.28
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	4	0.28
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	1	0.28
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD11	4	0.28
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD12	4	0.28
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD13	4	0.28
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD21	4	0.28
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD22	4	0.28
(1,156)	1:89:A:LEU:H	1:84:A:LEU:HD23	4	0.28
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD11	4	0.28
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD12	4	0.28
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD13	4	0.28
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD21	4	0.28
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD22	4	0.28
(1,155)	1:89:A:LEU:H	1:84:A:LEU:HD23	4	0.28
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	5	0.28
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB2	5	0.28
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB3	5	0.28
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	3	0.28
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	3	0.28
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	8	0.27
(1,2047)	1:113:A:VAL:HG21	1:124:A:LYS:HB2	4	0.27
(1,2047)	1:113:A:VAL:HG22	1:124:A:LYS:HB2	4	0.27
(1,2047)	1:113:A:VAL:HG23	1:124:A:LYS:HB2	4	0.27
(1,2033)	1:126:A:TYR:HA	1:113:A:VAL:HB	4	0.27
(1,2019)	1:63:A:VAL:HG21	1:89:A:LEU:HB2	7	0.27
(1,2019)	1:63:A:VAL:HG22	1:89:A:LEU:HB2	7	0.27
(1,2019)	1:63:A:VAL:HG23	1:89:A:LEU:HB2	7	0.27
(1,1943)	1:45:A:ASN:HB3	1:2:A:VAL:HA	9	0.27
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG11	6	0.27
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG12	6	0.27
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG13	6	0.27
(1,1885)	1:22:A:ALA:HB1	1:18:A:GLU:HB2	3	0.27
(1,1885)	1:22:A:ALA:HB2	1:18:A:GLU:HB2	3	0.27
(1,1885)	1:22:A:ALA:HB3	1:18:A:GLU:HB2	3	0.27
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG11	1	0.27
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG12	1	0.27
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG13	1	0.27
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	10	0.27
(1,1639)	1:7:A:THR:H	1:130:A:THR:H	5	0.27
(1,1638)	1:130:A:THR:H	1:7:A:THR:H	5	0.27
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	4	0.27
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	4	0.27
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	4	0.27
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	4	0.27
(1,1605)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	4	0.27
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	4	0.27
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	4	0.27
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	4	0.27
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	4	0.27
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	4	0.27
(1,1605)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	4	0.27
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	4	0.27
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	4	0.27
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	4	0.27
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	4	0.27
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	4	0.27
(1,1604)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	4	0.27
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	4	0.27
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	4	0.27
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	4	0.27
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	4	0.27
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	4	0.27
(1,1604)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	4	0.27
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	4	0.27
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	4	0.27
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	4	0.27
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	4	0.27
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	4	0.27
(1,1603)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	4	0.27
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	4	0.27
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	4	0.27
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	4	0.27
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	4	0.27
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	4	0.27
(1,1603)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	4	0.27
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD11	4	0.27
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD12	4	0.27
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD13	4	0.27
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD21	4	0.27
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD22	4	0.27
(1,1602)	1:99:A:ARG:HD2	1:95:A:LEU:HD23	4	0.27
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD11	4	0.27
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD12	4	0.27
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD13	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD21	4	0.27
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD22	4	0.27
(1,1602)	1:99:A:ARG:HD3	1:95:A:LEU:HD23	4	0.27
(1,1459)	1:125:A:ARG:H	1:114:A:LEU:HG	9	0.27
(1,1459)	1:125:A:ARG:H	1:114:A:LEU:HG	10	0.27
(1,1356)	1:99:A:ARG:H	1:95:A:LEU:HG	8	0.27
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB2	1	0.27
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB3	1	0.27
(1,907)	1:25:A:VAL:H	1:23:A:LEU:HG	9	0.27
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD11	8	0.27
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD12	8	0.27
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD13	8	0.27
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD11	8	0.27
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD12	8	0.27
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD13	8	0.27
(1,554)	1:84:A:LEU:H	1:83:A:LYS:HG2	3	0.27
(1,554)	1:84:A:LEU:H	1:83:A:LYS:HG3	3	0.27
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE2	5	0.27
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE3	5	0.27
(1,430)	1:24:A:GLY:H	1:20:A:LEU:HA	7	0.27
(1,356)	1:63:A:VAL:H	1:62:A:ILE:HA	2	0.27
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	6	0.27
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	6	0.27
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	6	0.27
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	6	0.27
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	6	0.27
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	6	0.27
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	6	0.27
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	6	0.27
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB2	4	0.27
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB3	4	0.27
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	6	0.27
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG2	1	0.27
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG3	1	0.27
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG2	4	0.27
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG3	4	0.27
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	2	0.27
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	2	0.27
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	2	0.27
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	2	0.27
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	2	0.27
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD11	4	0.27
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD12	4	0.27
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD13	4	0.27
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	9	0.27
(1,45)	1:23:A:LEU:H	1:19:A:TYR:HA	2	0.27
(1,4)	1:5:A:ALA:H	1:4:A:LEU:HA	9	0.27
(2,8)	1:41:A:GLU:H	1:52:A:LYS:H	9	0.26
(2,7)	1:52:A:LYS:H	1:41:A:GLU:H	9	0.26
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	1	0.26
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	3	0.26
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	3	0.26
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	3	0.26
(1,2017)	1:63:A:VAL:HG11	1:89:A:LEU:HA	4	0.26
(1,2017)	1:63:A:VAL:HG12	1:89:A:LEU:HA	4	0.26
(1,2017)	1:63:A:VAL:HG13	1:89:A:LEU:HA	4	0.26
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE2	10	0.26
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE3	10	0.26
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE2	10	0.26
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE3	10	0.26
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE2	10	0.26
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE3	10	0.26
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE2	10	0.26
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE3	10	0.26
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE2	10	0.26
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE3	10	0.26
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE2	10	0.26
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE3	10	0.26
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG11	2	0.26
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG12	2	0.26
(1,2001)	1:34:A:ASN:HB2	1:74:A:VAL:HG13	2	0.26
(1,1935)	1:94:A:GLU:HG2	1:96:A:PRO:HB2	4	0.26
(1,1935)	1:94:A:GLU:HG3	1:96:A:PRO:HB2	4	0.26
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG11	7	0.26
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG12	7	0.26
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG13	7	0.26
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG21	7	0.26
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG22	7	0.26
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG23	7	0.26
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	10	0.26
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	3	0.26
(1,1628)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	8	0.26
(1,1628)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	8	0.26
(1,1627)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	8	0.26
(1,1210)	1:72:A:GLY:H	1:74:A:VAL:HB	9	0.26
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD11	7	0.26
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD12	7	0.26
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD13	7	0.26
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD21	7	0.26
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD22	7	0.26
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD23	7	0.26
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD11	7	0.26
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD12	7	0.26
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD13	7	0.26
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD21	7	0.26
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD22	7	0.26
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD23	7	0.26
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD11	7	0.26
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD12	7	0.26
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD13	7	0.26
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD21	7	0.26
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD22	7	0.26
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD23	7	0.26
(1,723)	1:16:A:PHE:H	1:14:A:GLU:HB2	1	0.26
(1,554)	1:84:A:LEU:H	1:83:A:LYS:HG2	7	0.26
(1,554)	1:84:A:LEU:H	1:83:A:LYS:HG3	7	0.26
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	8	0.26
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	8	0.26
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	8	0.26
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	8	0.26
(1,392)	1:79:A:LYS:HE2	1:94:A:GLU:HG2	6	0.26
(1,392)	1:79:A:LYS:HE2	1:94:A:GLU:HG3	6	0.26
(1,392)	1:79:A:LYS:HE3	1:94:A:GLU:HG2	6	0.26
(1,392)	1:79:A:LYS:HE3	1:94:A:GLU:HG3	6	0.26
(1,392)	1:79:A:LYS:HE2	1:94:A:GLU:HG2	7	0.26
(1,392)	1:79:A:LYS:HE2	1:94:A:GLU:HG3	7	0.26
(1,392)	1:79:A:LYS:HE3	1:94:A:GLU:HG2	7	0.26
(1,392)	1:79:A:LYS:HE3	1:94:A:GLU:HG3	7	0.26
(1,348)	1:116:A:MET:HA	1:103:A:ARG:HG2	1	0.26
(1,348)	1:116:A:MET:HA	1:103:A:ARG:HG3	1	0.26
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	9	0.26
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	9	0.26
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG11	10	0.26
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG12	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG13	10	0.26
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG21	10	0.26
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG22	10	0.26
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG23	10	0.26
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG11	10	0.26
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG12	10	0.26
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG13	10	0.26
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG21	10	0.26
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG22	10	0.26
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG23	10	0.26
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB2	6	0.26
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB3	6	0.26
(1,197)	1:89:A:LEU:H	1:106:A:GLU:HA	10	0.26
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG2	5	0.26
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG3	5	0.26
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB2	7	0.26
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB3	7	0.26
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	4	0.26
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	4	0.26
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	4	0.26
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	4	0.26
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	4	0.26
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	4	0.26
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG11	3	0.26
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG12	3	0.26
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG13	3	0.26
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG21	3	0.26
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG22	3	0.26
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG23	3	0.26
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	2	0.26
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	5	0.26
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	5	0.26
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	2	0.26
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	6	0.26
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	6	0.26
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	8	0.26
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	8	0.26
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	10	0.26
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	10	0.26
(3,51)	1:106:A:GLU:N	1:113:A:VAL:O	7	0.25
(3,51)	1:106:A:GLU:N	1:113:A:VAL:O	8	0.25
(3,51)	1:106:A:GLU:N	1:113:A:VAL:O	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	1:12:A:LYS:N	1:126:A:TYR:O	10	0.25
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	4	0.25
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	9	0.25
(1,1981)	1:25:A:VAL:HB	1:30:A:ILE:HG12	2	0.25
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG2	4	0.25
(1,1928)	1:84:A:LEU:HD21	1:88:A:LYS:HG3	4	0.25
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG2	4	0.25
(1,1928)	1:84:A:LEU:HD22	1:88:A:LYS:HG3	4	0.25
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG2	4	0.25
(1,1928)	1:84:A:LEU:HD23	1:88:A:LYS:HG3	4	0.25
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD21	4	0.25
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD22	4	0.25
(1,1927)	1:88:A:LYS:HG2	1:84:A:LEU:HD23	4	0.25
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD21	4	0.25
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD22	4	0.25
(1,1927)	1:88:A:LYS:HG3	1:84:A:LEU:HD23	4	0.25
(1,1923)	1:67:A:VAL:HG21	1:65:A:GLU:HB2	5	0.25
(1,1923)	1:67:A:VAL:HG22	1:65:A:GLU:HB2	5	0.25
(1,1923)	1:67:A:VAL:HG23	1:65:A:GLU:HB2	5	0.25
(1,1921)	1:48:A:LYS:HD2	1:45:A:ASN:HB3	3	0.25
(1,1921)	1:48:A:LYS:HD3	1:45:A:ASN:HB3	3	0.25
(1,1901)	1:32:A:LYS:HE2	1:29:A:SER:HB2	1	0.25
(1,1901)	1:32:A:LYS:HE3	1:29:A:SER:HB2	1	0.25
(1,1793)	1:87:A:SER:H	1:85:A:GLU:HG2	7	0.25
(1,1793)	1:87:A:SER:H	1:85:A:GLU:HG3	7	0.25
(1,1755)	1:60:A:THR:H	1:61:A:LEU:HG	10	0.25
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	7	0.25
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	7	0.25
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	7	0.25
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	7	0.25
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	7	0.25
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	7	0.25
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	7	0.25
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	7	0.25
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	7	0.25
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	7	0.25
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	7	0.25
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	7	0.25
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	7	0.25
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	7	0.25
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	7	0.25
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:115:A:THR:H	1:114:A:LEU:HG	5	0.25
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG21	8	0.25
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG22	8	0.25
(1,1249)	1:94:A:GLU:H	1:78:A:ILE:HG23	8	0.25
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	8	0.25
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD21	1	0.25
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD22	1	0.25
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD23	1	0.25
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG21	4	0.25
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG22	4	0.25
(1,289)	1:92:A:ASN:HA	1:102:A:THR:HG23	4	0.25
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	8	0.25
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	8	0.25
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	8	0.25
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	8	0.25
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	8	0.25
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	8	0.25
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	8	0.25
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	8	0.25
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB2	9	0.25
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB3	9	0.25
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB2	9	0.25
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB3	9	0.25
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA2	3	0.25
(1,205)	1:129:A:ARG:H	1:111:A:GLY:HA3	3	0.25
(1,197)	1:89:A:LEU:H	1:106:A:GLU:HA	6	0.25
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG11	9	0.25
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG12	9	0.25
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG13	9	0.25
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG21	9	0.25
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG22	9	0.25
(1,170)	1:92:A:ASN:H	1:91:A:VAL:HG23	9	0.25
(1,164)	1:81:A:PHE:H	1:91:A:VAL:HA	2	0.25
(1,158)	1:88:A:LYS:H	1:87:A:SER:H	3	0.25
(1,157)	1:85:A:GLU:H	1:86:A:GLY:H	9	0.25
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	10	0.25
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	10	0.25
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	2	0.25
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	2	0.25
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	2	0.25
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	2	0.25
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	2	0.25
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	2	0.25
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	2	0.25
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	7	0.25
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	1	0.24
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	5	0.24
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	10	0.24
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	2	0.24
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	3	0.24
(1,2059)	1:11:A:GLU:HA	1:127:A:PHE:HA	1	0.24
(1,2052)	1:14:A:GLU:HB2	1:126:A:TYR:HD1	6	0.24
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	8	0.24
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	8	0.24
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	8	0.24
(1,2030)	1:113:A:VAL:HG11	1:106:A:GLU:HB2	3	0.24
(1,2030)	1:113:A:VAL:HG11	1:106:A:GLU:HB3	3	0.24
(1,2030)	1:113:A:VAL:HG12	1:106:A:GLU:HB2	3	0.24
(1,2030)	1:113:A:VAL:HG12	1:106:A:GLU:HB3	3	0.24
(1,2030)	1:113:A:VAL:HG13	1:106:A:GLU:HB2	3	0.24
(1,2030)	1:113:A:VAL:HG13	1:106:A:GLU:HB3	3	0.24
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG11	8	0.24
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG12	8	0.24
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG13	8	0.24
(1,1823)	1:34:A:ASN:HD22	1:71:A:LEU:HB2	3	0.24
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD11	1	0.24
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD12	1	0.24
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD13	1	0.24
(1,1788)	1:47:A:ASN:H	1:45:A:ASN:HB3	6	0.24
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	8	0.24
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	8	0.24
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	8	0.24
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	8	0.24
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	8	0.24
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	8	0.24
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	8	0.24
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	8	0.24
(1,1639)	1:7:A:THR:H	1:130:A:THR:H	2	0.24
(1,1638)	1:130:A:THR:H	1:7:A:THR:H	2	0.24
(1,1632)	1:9:A:LYS:HA	1:127:A:PHE:HD1	8	0.24
(1,1632)	1:9:A:LYS:HA	1:127:A:PHE:HD2	8	0.24
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	8	0.24
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	8	0.24
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	8	0.24
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	8	0.24
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	8	0.24
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	8	0.24
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	8	0.24
(1,1566)	1:43:A:ILE:HB	1:7:A:THR:HB	2	0.24
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD11	2	0.24
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD12	2	0.24
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD13	2	0.24
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD21	2	0.24
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD22	2	0.24
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD23	2	0.24
(1,724)	1:17:A:GLU:H	1:20:A:LEU:HB2	7	0.24
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	3	0.24
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	3	0.24
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	8	0.24
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	8	0.24
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	9	0.24
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	9	0.24
(1,521)	1:69:A:GLU:H	1:68:A:GLU:HG2	10	0.24
(1,521)	1:69:A:GLU:H	1:68:A:GLU:HG3	10	0.24
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	4	0.24
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	4	0.24
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	6	0.24
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	6	0.24
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	9	0.24
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	9	0.24
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	10	0.24
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	10	0.24
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	4	0.24
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	4	0.24
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	6	0.24
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	6	0.24
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	9	0.24
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	9	0.24
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	10	0.24
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	10	0.24
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	5	0.24
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	5	0.24
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	7	0.24
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	10	0.24
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	10	0.24
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	5	0.24
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	5	0.24
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	7	0.24
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	7	0.24
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	10	0.24
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	10	0.24
(1,448)	1:31:A:LYS:H	1:30:A:ILE:HG12	10	0.24
(1,448)	1:31:A:LYS:H	1:30:A:ILE:HG13	10	0.24
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	6	0.24
(1,265)	1:130:A:THR:H	1:130:A:THR:HG21	9	0.24
(1,265)	1:130:A:THR:H	1:130:A:THR:HG22	9	0.24
(1,265)	1:130:A:THR:H	1:130:A:THR:HG23	9	0.24
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG11	2	0.24
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG12	2	0.24
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG13	2	0.24
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG21	2	0.24
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG22	2	0.24
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG23	2	0.24
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG11	2	0.24
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG12	2	0.24
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG13	2	0.24
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG21	2	0.24
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG22	2	0.24
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG23	2	0.24
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	3	0.24
(1,214)	1:125:A:ARG:H	1:114:A:LEU:H	7	0.24
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	2	0.24
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	2	0.24
(1,183)	1:99:A:ARG:H	1:99:A:ARG:HD2	10	0.24
(1,183)	1:99:A:ARG:H	1:99:A:ARG:HD3	10	0.24
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB2	10	0.24
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB3	10	0.24
(1,140)	1:73:A:THR:H	1:73:A:THR:HB	1	0.24
(1,129)	1:51:A:PHE:H	1:62:A:ILE:HA	3	0.24
(1,123)	1:60:A:THR:H	1:59:A:SER:HB2	2	0.24
(1,123)	1:60:A:THR:H	1:59:A:SER:HB3	2	0.24
(1,123)	1:60:A:THR:H	1:59:A:SER:HB2	4	0.24
(1,123)	1:60:A:THR:H	1:59:A:SER:HB3	4	0.24
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB2	4	0.24
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB3	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	3	0.24
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	3	0.24
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	5	0.24
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	5	0.24
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	6	0.24
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	6	0.24
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	7	0.24
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	7	0.24
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	8	0.24
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	8	0.24
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	9	0.24
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	9	0.24
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	10	0.24
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	10	0.24
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	3	0.24
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	3	0.24
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	5	0.24
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	5	0.24
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	6	0.24
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	6	0.24
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	7	0.24
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	7	0.24
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	8	0.24
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	8	0.24
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	9	0.24
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	9	0.24
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	10	0.24
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	10	0.24
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	3	0.24
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	3	0.24
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	5	0.24
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	5	0.24
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	6	0.24
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	6	0.24
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	7	0.24
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	7	0.24
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	8	0.24
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	8	0.24
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	9	0.24
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	9	0.24
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	10	0.24
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	3	0.24
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	3	0.24
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	5	0.24
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	5	0.24
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	6	0.24
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	6	0.24
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	7	0.24
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	7	0.24
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	8	0.24
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	8	0.24
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	9	0.24
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	9	0.24
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	10	0.24
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	10	0.24
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	4	0.24
(1,43)	1:22:A:ALA:H	1:18:A:GLU:HA	2	0.24
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	4	0.24
(1,5)	1:5:A:ALA:H	1:4:A:LEU:HB2	9	0.24
(1,5)	1:5:A:ALA:H	1:4:A:LEU:HB3	9	0.24
(1,2052)	1:14:A:GLU:HB2	1:126:A:TYR:HD1	9	0.23
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	3	0.23
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	3	0.23
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	8	0.23
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	8	0.23
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	8	0.23
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB1	7	0.23
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB2	7	0.23
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB3	7	0.23
(1,1779)	1:15:A:ASN:HD22	1:18:A:GLU:HB3	6	0.23
(1,1631)	1:113:A:VAL:HG21	1:126:A:TYR:HE1	1	0.23
(1,1631)	1:113:A:VAL:HG22	1:126:A:TYR:HE1	1	0.23
(1,1631)	1:113:A:VAL:HG23	1:126:A:TYR:HE1	1	0.23
(1,1356)	1:99:A:ARG:H	1:95:A:LEU:HG	10	0.23
(1,1322)	1:105:A:TYR:H	1:89:A:LEU:HG	7	0.23
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB2	2	0.23
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB3	2	0.23
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD11	8	0.23
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD12	8	0.23
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD13	8	0.23
(1,627)	1:14:A:GLU:H	1:124:A:LYS:H	2	0.23
(1,583)	1:101:A:GLY:H	1:93:A:SER:HB2	1	0.23
(1,583)	1:101:A:GLY:H	1:93:A:SER:HB3	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE2	8	0.23
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE3	8	0.23
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	1	0.23
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	1	0.23
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	2	0.23
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	2	0.23
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	3	0.23
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	3	0.23
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	7	0.23
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	7	0.23
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	8	0.23
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	8	0.23
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	1	0.23
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	1	0.23
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	2	0.23
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	2	0.23
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	3	0.23
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	3	0.23
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	7	0.23
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	7	0.23
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	8	0.23
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	8	0.23
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	1	0.23
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	1	0.23
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	2	0.23
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	2	0.23
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	3	0.23
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	3	0.23
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	4	0.23
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	4	0.23
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	6	0.23
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	6	0.23
(1,465)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	9	0.23
(1,465)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	9	0.23
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	1	0.23
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	1	0.23
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	2	0.23
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	2	0.23
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	3	0.23
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	3	0.23
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	4	0.23
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	6	0.23
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	6	0.23
(1,464)	1:34:A:ASN:HD21	1:34:A:ASN:HD22	9	0.23
(1,464)	1:34:A:ASN:HD22	1:34:A:ASN:HD21	9	0.23
(1,447)	1:30:A:ILE:H	1:30:A:ILE:HD11	2	0.23
(1,447)	1:30:A:ILE:H	1:30:A:ILE:HD12	2	0.23
(1,447)	1:30:A:ILE:H	1:30:A:ILE:HD13	2	0.23
(1,409)	1:124:A:LYS:H	1:14:A:GLU:H	2	0.23
(1,394)	1:126:A:TYR:HB2	1:113:A:VAL:HA	7	0.23
(1,394)	1:126:A:TYR:HB2	1:113:A:VAL:HA	9	0.23
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	8	0.23
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	8	0.23
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	8	0.23
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	8	0.23
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	8	0.23
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	8	0.23
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	8	0.23
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	8	0.23
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	8	0.23
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	1	0.23
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	1	0.23
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	1	0.23
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	3	0.23
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	3	0.23
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	3	0.23
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	7	0.23
(1,347)	1:43:A:ILE:H	1:50:A:THR:HB	5	0.23
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB1	7	0.23
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB2	7	0.23
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB3	7	0.23
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB1	7	0.23
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB2	7	0.23
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB3	7	0.23
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB1	7	0.23
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB2	7	0.23
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB3	7	0.23
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB1	2	0.23
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB2	2	0.23
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB3	2	0.23
(1,214)	1:125:A:ARG:H	1:114:A:LEU:H	2	0.23
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB2	3	0.23
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB3	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB2	3	0.23
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB3	3	0.23
(1,192)	1:104:A:THR:H	1:104:A:THR:HB	10	0.23
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	8	0.23
(1,140)	1:73:A:THR:H	1:73:A:THR:HB	6	0.23
(1,139)	1:33:A:ALA:H	1:73:A:THR:HB	6	0.23
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	4	0.23
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	4	0.23
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	4	0.23
(1,124)	1:53:A:SER:H	1:59:A:SER:H	5	0.23
(1,113)	1:59:A:SER:H	1:53:A:SER:H	5	0.23
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	1	0.23
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	1	0.23
(1,96)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	4	0.23
(1,96)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	4	0.23
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	1	0.23
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	1	0.23
(1,95)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	4	0.23
(1,95)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	4	0.23
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	1	0.23
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	1	0.23
(1,94)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	4	0.23
(1,94)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	4	0.23
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	1	0.23
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	1	0.23
(1,93)	1:45:A:ASN:HD21	1:45:A:ASN:HD22	4	0.23
(1,93)	1:45:A:ASN:HD22	1:45:A:ASN:HD21	4	0.23
(1,25)	1:128:A:ILE:H	1:11:A:GLU:HG2	3	0.23
(1,25)	1:128:A:ILE:H	1:11:A:GLU:HG3	3	0.23
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	10	0.22
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	10	0.22
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD21	10	0.22
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD22	10	0.22
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD23	10	0.22
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	9	0.22
(1,1813)	1:3:A:GLN:HE22	1:45:A:ASN:HA	4	0.22
(1,1799)	1:47:A:ASN:HD21	1:2:A:VAL:HB	10	0.22
(1,1786)	1:31:A:LYS:H	1:27:A:GLN:HB2	6	0.22
(1,1760)	1:77:A:ASN:HD21	1:76:A:MET:HB2	2	0.22
(1,1703)	1:104:A:THR:H	1:115:A:THR:HB	5	0.22
(1,1646)	1:14:A:GLU:H	1:124:A:LYS:HB2	8	0.22
(1,1646)	1:14:A:GLU:H	1:124:A:LYS:HB3	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1645)	1:14:A:GLU:H	1:124:A:LYS:HB2	8	0.22
(1,1645)	1:14:A:GLU:H	1:124:A:LYS:HB3	8	0.22
(1,1628)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	7	0.22
(1,1628)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	7	0.22
(1,1627)	1:12:A:LYS:HG2	1:126:A:TYR:HD1	7	0.22
(1,1627)	1:12:A:LYS:HG3	1:126:A:TYR:HD1	7	0.22
(1,1356)	1:99:A:ARG:H	1:95:A:LEU:HG	1	0.22
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG11	4	0.22
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG12	4	0.22
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG13	4	0.22
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG11	4	0.22
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG12	4	0.22
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG13	4	0.22
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG11	10	0.22
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG12	10	0.22
(1,732)	1:33:A:ALA:H	1:74:A:VAL:HG13	10	0.22
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB2	3	0.22
(1,713)	1:51:A:PHE:H	1:61:A:LEU:HB3	3	0.22
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG21	1	0.22
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG22	1	0.22
(1,708)	1:43:A:ILE:HB	1:7:A:THR:HG23	1	0.22
(1,649)	1:44:A:VAL:HB	1:49:A:PHE:HA	7	0.22
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	9	0.22
(1,594)	1:93:A:SER:H	1:101:A:GLY:H	1	0.22
(1,568)	1:85:A:GLU:H	1:88:A:LYS:HG2	9	0.22
(1,568)	1:85:A:GLU:H	1:88:A:LYS:HG3	9	0.22
(1,499)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	5	0.22
(1,499)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	5	0.22
(1,498)	1:58:A:ASN:HD21	1:58:A:ASN:HD22	5	0.22
(1,498)	1:58:A:ASN:HD22	1:58:A:ASN:HD21	5	0.22
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	6	0.22
(1,264)	1:129:A:ARG:H	1:129:A:ARG:HD2	10	0.22
(1,264)	1:129:A:ARG:H	1:129:A:ARG:HD3	10	0.22
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD2	5	0.22
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD3	5	0.22
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB2	10	0.22
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB3	10	0.22
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB2	10	0.22
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB3	10	0.22
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	2	0.22
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	3	0.22
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:110:A:LYS:H	1:109:A:ASP:HB2	5	0.22
(1,201)	1:110:A:LYS:H	1:109:A:ASP:HB3	5	0.22
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	2	0.22
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	1	0.22
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	3	0.22
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	5	0.22
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	5	0.22
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	8	0.22
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	8	0.22
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	9	0.22
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	9	0.22
(3,49)	1:101:A:GLY:N	1:93:A:SER:O	1	0.21
(3,33)	1:48:A:LYS:N	1:45:A:ASN:O	4	0.21
(3,24)	1:21:A:ALA:H	1:17:A:GLU:O	2	0.21
(3,11)	1:12:A:LYS:N	1:126:A:TYR:O	1	0.21
(1,2039)	1:125:A:ARG:HB3	1:114:A:LEU:HG	10	0.21
(1,2032)	1:105:A:TYR:HB2	1:112:A:PHE:HA	1	0.21
(1,2032)	1:105:A:TYR:HB3	1:112:A:PHE:HA	1	0.21
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	3	0.21
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	3	0.21
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	3	0.21
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	3	0.21
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB1	5	0.21
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB2	5	0.21
(1,1845)	1:17:A:GLU:H	1:123:A:ALA:HB3	5	0.21
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG11	8	0.21
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG12	8	0.21
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG13	8	0.21
(1,1799)	1:47:A:ASN:HD21	1:2:A:VAL:HB	8	0.21
(1,1792)	1:72:A:GLY:H	1:75:A:ASN:HA	7	0.21
(1,1765)	1:3:A:GLN:HE22	1:5:A:ALA:HB1	5	0.21
(1,1765)	1:3:A:GLN:HE22	1:5:A:ALA:HB2	5	0.21
(1,1765)	1:3:A:GLN:HE22	1:5:A:ALA:HB3	5	0.21
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	10	0.21
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	10	0.21
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	10	0.21
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	10	0.21
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	10	0.21
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	10	0.21
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	10	0.21
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	10	0.21
(1,1632)	1:9:A:LYS:HA	1:127:A:PHE:HD1	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:9:A:LYS:HA	1:127:A:PHE:HD2	4	0.21
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	10	0.21
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	10	0.21
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	10	0.21
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	10	0.21
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	10	0.21
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	10	0.21
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	10	0.21
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	10	0.21
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD11	8	0.21
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD12	8	0.21
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD13	8	0.21
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD21	8	0.21
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD22	8	0.21
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD23	8	0.21
(1,1285)	1:86:A:GLY:H	1:84:A:LEU:HG	2	0.21
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD21	6	0.21
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD22	6	0.21
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD11	2	0.21
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD12	2	0.21
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD13	2	0.21
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD21	2	0.21
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD22	2	0.21
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD23	2	0.21
(1,790)	1:44:A:VAL:H	1:6:A:GLY:HA2	6	0.21
(1,790)	1:44:A:VAL:H	1:6:A:GLY:HA3	6	0.21
(1,753)	1:79:A:LYS:HG2	1:68:A:GLU:HA	4	0.21
(1,725)	1:29:A:SER:H	1:32:A:LYS:HG2	8	0.21
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD11	4	0.21
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD12	4	0.21
(1,706)	1:65:A:GLU:HB2	1:62:A:ILE:HD13	4	0.21
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD11	4	0.21
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD12	4	0.21
(1,706)	1:65:A:GLU:HB3	1:62:A:ILE:HD13	4	0.21
(1,695)	1:51:A:PHE:H	1:61:A:LEU:HG	7	0.21
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD11	10	0.21
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD12	10	0.21
(1,635)	1:129:A:ARG:H	1:128:A:ILE:HD13	10	0.21
(1,627)	1:14:A:GLU:H	1:124:A:LYS:H	5	0.21
(1,572)	1:84:A:LEU:H	1:89:A:LEU:HG	8	0.21
(1,409)	1:124:A:LYS:H	1:14:A:GLU:H	5	0.21
(1,377)	1:74:A:VAL:HG11	1:71:A:LEU:HB2	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:74:A:VAL:HG12	1:71:A:LEU:HB2	9	0.21
(1,377)	1:74:A:VAL:HG13	1:71:A:LEU:HB2	9	0.21
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	10	0.21
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD2	6	0.21
(1,240)	1:124:A:LYS:H	1:124:A:LYS:HD3	6	0.21
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	4	0.21
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	7	0.21
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG2	7	0.21
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG3	7	0.21
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB2	8	0.21
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB3	8	0.21
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	1	0.21
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	8	0.21
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	1	0.21
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	9	0.21
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	6	0.21
(1,64)	1:33:A:ALA:H	1:31:A:LYS:HA	5	0.21
(1,19)	1:128:A:ILE:H	1:10:A:LEU:HA	1	0.21
(3,33)	1:48:A:LYS:N	1:45:A:ASN:O	1	0.2
(2,3)	1:59:A:SER:H	1:54:A:SER:HA	8	0.2
(1,2052)	1:14:A:GLU:HB2	1:126:A:TYR:HD1	8	0.2
(1,2051)	1:12:A:LYS:HE2	1:126:A:TYR:HD1	6	0.2
(1,2051)	1:12:A:LYS:HE3	1:126:A:TYR:HD1	6	0.2
(1,2045)	1:19:A:TYR:HA	1:121:A:MET:HB2	3	0.2
(1,2044)	1:122:A:VAL:HG21	1:117:A:CYS:HB2	5	0.2
(1,2044)	1:122:A:VAL:HG22	1:117:A:CYS:HB2	5	0.2
(1,2044)	1:122:A:VAL:HG23	1:117:A:CYS:HB2	5	0.2
(1,2023)	1:78:A:ILE:HG13	1:93:A:SER:HB3	4	0.2
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG11	9	0.2
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG12	9	0.2
(1,1976)	1:75:A:ASN:HB2	1:25:A:VAL:HG13	9	0.2
(1,1974)	1:121:A:MET:HB2	1:19:A:TYR:HA	3	0.2
(1,1957)	1:114:A:LEU:HD21	1:10:A:LEU:HA	5	0.2
(1,1957)	1:114:A:LEU:HD22	1:10:A:LEU:HA	5	0.2
(1,1957)	1:114:A:LEU:HD23	1:10:A:LEU:HA	5	0.2
(1,1921)	1:48:A:LYS:HD2	1:45:A:ASN:HB3	2	0.2
(1,1921)	1:48:A:LYS:HD3	1:45:A:ASN:HB3	2	0.2
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	1	0.2
(1,1807)	1:122:A:VAL:H	1:15:A:ASN:HD21	1	0.2
(1,1786)	1:31:A:LYS:H	1:27:A:GLN:HB2	1	0.2
(1,1527)	1:47:A:ASN:HA	1:2:A:VAL:HB	5	0.2
(1,1494)	1:124:A:LYS:H	1:124:A:LYS:HE2	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1494)	1:124:A:LYS:H	1:124:A:LYS:HE3	8	0.2
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB2	2	0.2
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB3	2	0.2
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD21	4	0.2
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD22	4	0.2
(1,1053)	1:48:A:LYS:H	1:45:A:ASN:HA	1	0.2
(1,1053)	1:48:A:LYS:H	1:45:A:ASN:HA	5	0.2
(1,1036)	1:50:A:THR:H	1:43:A:ILE:HB	7	0.2
(1,766)	1:124:A:LYS:HA	1:115:A:THR:H	5	0.2
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG11	7	0.2
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG12	7	0.2
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG13	7	0.2
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG11	7	0.2
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG12	7	0.2
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG13	7	0.2
(1,725)	1:29:A:SER:H	1:32:A:LYS:HG2	6	0.2
(1,648)	1:50:A:THR:HB	1:43:A:ILE:HB	6	0.2
(1,644)	1:126:A:TYR:HB2	1:12:A:LYS:HB2	8	0.2
(1,644)	1:126:A:TYR:HB2	1:12:A:LYS:HB3	8	0.2
(1,644)	1:126:A:TYR:HB3	1:12:A:LYS:HB2	8	0.2
(1,644)	1:126:A:TYR:HB3	1:12:A:LYS:HB3	8	0.2
(1,643)	1:126:A:TYR:HB2	1:12:A:LYS:HB2	8	0.2
(1,643)	1:126:A:TYR:HB2	1:12:A:LYS:HB3	8	0.2
(1,643)	1:126:A:TYR:HB3	1:12:A:LYS:HB2	8	0.2
(1,643)	1:126:A:TYR:HB3	1:12:A:LYS:HB3	8	0.2
(1,614)	1:121:A:MET:H	1:118:A:ALA:HA	6	0.2
(1,441)	1:29:A:SER:H	1:27:A:GLN:HA	6	0.2
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	2	0.2
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	2	0.2
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	2	0.2
(1,347)	1:43:A:ILE:H	1:50:A:THR:HB	8	0.2
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	5	0.2
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	5	0.2
(1,257)	1:112:A:PHE:H	1:128:A:ILE:HA	5	0.2
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG11	5	0.2
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG12	5	0.2
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG13	5	0.2
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG21	5	0.2
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG22	5	0.2
(1,230)	1:123:A:ALA:H	1:122:A:VAL:HG23	5	0.2
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG11	5	0.2
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG12	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG13	5	0.2
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG21	5	0.2
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG22	5	0.2
(1,229)	1:123:A:ALA:H	1:122:A:VAL:HG23	5	0.2
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB2	8	0.2
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB3	8	0.2
(1,208)	1:127:A:PHE:H	1:112:A:PHE:HB2	3	0.2
(1,208)	1:127:A:PHE:H	1:112:A:PHE:HB3	3	0.2
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	10	0.2
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	8	0.2
(1,142)	1:75:A:ASN:H	1:75:A:ASN:HB2	7	0.2
(1,142)	1:75:A:ASN:H	1:75:A:ASN:HB3	7	0.2
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	7	0.2
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	7	0.2
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	7	0.2
(1,128)	1:51:A:PHE:H	1:61:A:LEU:H	10	0.2
(1,124)	1:53:A:SER:H	1:59:A:SER:H	1	0.2
(1,113)	1:59:A:SER:H	1:53:A:SER:H	1	0.2
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	8	0.2
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	10	0.2
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	1	0.2
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	1	0.2
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	3	0.2
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	3	0.2
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	6	0.19
(1,1975)	1:33:A:ALA:HB1	1:20:A:LEU:HD11	2	0.19
(1,1975)	1:33:A:ALA:HB1	1:20:A:LEU:HD12	2	0.19
(1,1975)	1:33:A:ALA:HB1	1:20:A:LEU:HD13	2	0.19
(1,1975)	1:33:A:ALA:HB2	1:20:A:LEU:HD11	2	0.19
(1,1975)	1:33:A:ALA:HB2	1:20:A:LEU:HD12	2	0.19
(1,1975)	1:33:A:ALA:HB2	1:20:A:LEU:HD13	2	0.19
(1,1975)	1:33:A:ALA:HB3	1:20:A:LEU:HD11	2	0.19
(1,1975)	1:33:A:ALA:HB3	1:20:A:LEU:HD12	2	0.19
(1,1975)	1:33:A:ALA:HB3	1:20:A:LEU:HD13	2	0.19
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD1	6	0.19
(1,1953)	1:111:A:GLY:HA3	1:8:A:TYR:HD2	6	0.19
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD21	5	0.19
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD22	5	0.19
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD23	5	0.19
(1,1877)	1:3:A:GLN:HB3	1:6:A:GLY:HA2	2	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG11	6	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG12	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG13	6	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG21	6	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG22	6	0.19
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG23	6	0.19
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG11	9	0.19
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG12	9	0.19
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG13	9	0.19
(1,1771)	1:16:A:PHE:H	1:14:A:GLU:HB3	9	0.19
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	6	0.19
(1,1706)	1:77:A:ASN:H	1:96:A:PRO:HG2	10	0.19
(1,1706)	1:77:A:ASN:H	1:96:A:PRO:HG3	10	0.19
(1,1494)	1:124:A:LYS:H	1:124:A:LYS:HE2	3	0.19
(1,1494)	1:124:A:LYS:H	1:124:A:LYS:HE3	3	0.19
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB2	7	0.19
(1,972)	1:35:A:SER:H	1:31:A:LYS:HB3	7	0.19
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG11	6	0.19
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG12	6	0.19
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG13	6	0.19
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG11	6	0.19
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG12	6	0.19
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG13	6	0.19
(1,725)	1:29:A:SER:H	1:32:A:LYS:HG2	4	0.19
(1,627)	1:14:A:GLU:H	1:124:A:LYS:H	7	0.19
(1,627)	1:14:A:GLU:H	1:124:A:LYS:H	10	0.19
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	10	0.19
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	10	0.19
(1,409)	1:124:A:LYS:H	1:14:A:GLU:H	7	0.19
(1,409)	1:124:A:LYS:H	1:14:A:GLU:H	10	0.19
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG12	4	0.19
(1,261)	1:112:A:PHE:H	1:128:A:ILE:HG13	4	0.19
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB2	8	0.19
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB3	8	0.19
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB2	8	0.19
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB3	8	0.19
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB2	4	0.19
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB3	4	0.19
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB2	5	0.19
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB3	5	0.19
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB2	6	0.19
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB3	6	0.19
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB2	4	0.19
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB3	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB2	5	0.19
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB3	5	0.19
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB2	6	0.19
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB3	6	0.19
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	2	0.19
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB2	9	0.19
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB3	9	0.19
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB2	6	0.19
(1,202)	1:111:A:GLY:H	1:110:A:LYS:HB3	6	0.19
(1,193)	1:104:A:THR:H	1:104:A:THR:HG21	6	0.19
(1,193)	1:104:A:THR:H	1:104:A:THR:HG22	6	0.19
(1,193)	1:104:A:THR:H	1:104:A:THR:HG23	6	0.19
(1,190)	1:91:A:VAL:H	1:104:A:THR:HA	6	0.19
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG2	3	0.19
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG3	3	0.19
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB2	6	0.19
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB3	6	0.19
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	3	0.19
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	7	0.19
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	3	0.19
(1,125)	1:53:A:SER:H	1:60:A:THR:HA	7	0.19
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	2	0.19
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	4	0.19
(1,65)	1:34:A:ASN:H	1:31:A:LYS:HA	5	0.19
(1,55)	1:24:A:GLY:H	1:23:A:LEU:HB2	3	0.19
(1,55)	1:24:A:GLY:H	1:23:A:LEU:HB3	3	0.19
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	5	0.19
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	5	0.19
(1,2051)	1:12:A:LYS:HE2	1:126:A:TYR:HD1	10	0.18
(1,2051)	1:12:A:LYS:HE3	1:126:A:TYR:HD1	10	0.18
(1,2050)	1:12:A:LYS:HD3	1:126:A:TYR:HD1	7	0.18
(1,2028)	1:91:A:VAL:HA	1:103:A:ARG:HB2	6	0.18
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	6	0.18
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	6	0.18
(1,1901)	1:32:A:LYS:HE2	1:29:A:SER:HB2	10	0.18
(1,1901)	1:32:A:LYS:HE3	1:29:A:SER:HB2	10	0.18
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD11	7	0.18
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD12	7	0.18
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD13	7	0.18
(1,1822)	1:34:A:ASN:HD21	1:71:A:LEU:HB2	3	0.18
(1,1821)	1:77:A:ASN:HD21	1:70:A:VAL:HB	3	0.18
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD21	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD22	6	0.18
(1,1817)	1:81:A:PHE:H	1:61:A:LEU:HD23	6	0.18
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	7	0.18
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	8	0.18
(1,1448)	1:127:A:PHE:H	1:113:A:VAL:HG11	4	0.18
(1,1448)	1:127:A:PHE:H	1:113:A:VAL:HG12	4	0.18
(1,1448)	1:127:A:PHE:H	1:113:A:VAL:HG13	4	0.18
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB2	4	0.18
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB3	4	0.18
(1,1091)	1:48:A:LYS:H	1:48:A:LYS:HD2	2	0.18
(1,1091)	1:48:A:LYS:H	1:48:A:LYS:HD3	2	0.18
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG11	1	0.18
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG12	1	0.18
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG13	1	0.18
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG11	1	0.18
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG12	1	0.18
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG13	1	0.18
(1,694)	1:51:A:PHE:HB2	1:42:A:ILE:HB	6	0.18
(1,694)	1:51:A:PHE:HB3	1:42:A:ILE:HB	6	0.18
(1,649)	1:44:A:VAL:HB	1:49:A:PHE:HA	8	0.18
(1,627)	1:14:A:GLU:H	1:124:A:LYS:H	8	0.18
(1,409)	1:124:A:LYS:H	1:14:A:GLU:H	8	0.18
(1,394)	1:126:A:TYR:HB2	1:113:A:VAL:HA	4	0.18
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD21	6	0.18
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD22	6	0.18
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD23	6	0.18
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	4	0.18
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	9	0.18
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB1	5	0.18
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB2	5	0.18
(1,233)	1:19:A:TYR:H	1:123:A:ALA:HB3	5	0.18
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	9	0.18
(1,216)	1:125:A:ARG:H	1:115:A:THR:HA	10	0.18
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB2	5	0.18
(1,179)	1:97:A:ASP:H	1:95:A:LEU:HB3	5	0.18
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	10	0.18
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	2	0.18
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	2	0.18
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	7	0.18
(1,63)	1:32:A:LYS:H	1:31:A:LYS:HA	8	0.18
(1,59)	1:27:A:GLN:H	1:26:A:PRO:HB2	1	0.18
(1,59)	1:27:A:GLN:H	1:26:A:PRO:HB3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:48:A:LYS:H	1:45:A:ASN:O	10	0.17
(3,10)	1:10:A:LEU:H	1:40:A:TYR:O	7	0.17
(1,2047)	1:113:A:VAL:HG21	1:124:A:LYS:HB2	6	0.17
(1,2047)	1:113:A:VAL:HG22	1:124:A:LYS:HB2	6	0.17
(1,2047)	1:113:A:VAL:HG23	1:124:A:LYS:HB2	6	0.17
(1,2033)	1:126:A:TYR:HA	1:113:A:VAL:HB	3	0.17
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE2	7	0.17
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE3	7	0.17
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE2	7	0.17
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE3	7	0.17
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE2	7	0.17
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE3	7	0.17
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE2	7	0.17
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE3	7	0.17
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE2	7	0.17
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE3	7	0.17
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE2	7	0.17
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE3	7	0.17
(1,1992)	1:80:A:SER:HB2	1:61:A:LEU:HB3	3	0.17
(1,1992)	1:80:A:SER:HB3	1:61:A:LEU:HB3	3	0.17
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD21	2	0.17
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD22	2	0.17
(1,1951)	1:87:A:SER:HB3	1:4:A:LEU:HD23	2	0.17
(1,1942)	1:124:A:LYS:HB3	1:126:A:TYR:HE1	6	0.17
(1,1823)	1:34:A:ASN:HD22	1:71:A:LEU:HB2	1	0.17
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG11	5	0.17
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG12	5	0.17
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG13	5	0.17
(1,1761)	1:75:A:ASN:H	1:76:A:MET:HB3	8	0.17
(1,1757)	1:64:A:ASN:HD22	1:63:A:VAL:HB	7	0.17
(1,1755)	1:60:A:THR:H	1:61:A:LEU:HG	5	0.17
(1,1168)	1:66:A:GLU:H	1:65:A:GLU:HB2	6	0.17
(1,1168)	1:66:A:GLU:H	1:65:A:GLU:HB3	6	0.17
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD11	4	0.17
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD12	4	0.17
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD13	4	0.17
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD21	4	0.17
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD22	4	0.17
(1,757)	1:61:A:LEU:HD21	1:89:A:LEU:HD23	4	0.17
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD11	4	0.17
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD12	4	0.17
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD13	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD21	4	0.17
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD22	4	0.17
(1,757)	1:61:A:LEU:HD22	1:89:A:LEU:HD23	4	0.17
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD11	4	0.17
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD12	4	0.17
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD13	4	0.17
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD21	4	0.17
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD22	4	0.17
(1,757)	1:61:A:LEU:HD23	1:89:A:LEU:HD23	4	0.17
(1,583)	1:101:A:GLY:H	1:93:A:SER:HB2	3	0.17
(1,583)	1:101:A:GLY:H	1:93:A:SER:HB3	3	0.17
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD2	7	0.17
(1,551)	1:83:A:LYS:H	1:83:A:LYS:HD3	7	0.17
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	5	0.17
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD21	5	0.17
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD22	5	0.17
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD23	5	0.17
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB2	2	0.17
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB3	2	0.17
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB2	2	0.17
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB3	2	0.17
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD2	9	0.17
(1,245)	1:125:A:ARG:H	1:125:A:ARG:HD3	9	0.17
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	4	0.17
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	2	0.17
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	7	0.17
(1,135)	1:66:A:GLU:H	1:65:A:GLU:HB2	6	0.17
(1,135)	1:66:A:GLU:H	1:65:A:GLU:HB3	6	0.17
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	1	0.17
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	1	0.17
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	10	0.17
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	10	0.17
(1,91)	1:8:A:TYR:H	1:43:A:ILE:HA	2	0.17
(3,64)	1:129:A:ARG:H	1:109:A:ASP:O	7	0.16
(3,33)	1:48:A:LYS:N	1:45:A:ASN:O	6	0.16
(3,33)	1:48:A:LYS:N	1:45:A:ASN:O	10	0.16
(3,26)	1:22:A:ALA:H	1:18:A:GLU:O	3	0.16
(1,1991)	1:82:A:THR:HB	1:61:A:LEU:HB2	8	0.16
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD21	1	0.16
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD22	1	0.16
(1,1949)	1:87:A:SER:HA	1:4:A:LEU:HD23	1	0.16
(1,1932)	1:96:A:PRO:HA	1:94:A:GLU:HG2	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1932)	1:96:A:PRO:HA	1:94:A:GLU:HG3	2	0.16
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG21	1	0.16
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG22	1	0.16
(1,1924)	1:65:A:GLU:HB3	1:67:A:VAL:HG23	1	0.16
(1,1910)	1:27:A:GLN:HG2	1:31:A:LYS:HG2	4	0.16
(1,1910)	1:27:A:GLN:HG3	1:31:A:LYS:HG2	4	0.16
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG2	4	0.16
(1,1898)	1:31:A:LYS:HG2	1:27:A:GLN:HG3	4	0.16
(1,1822)	1:34:A:ASN:HD21	1:71:A:LEU:HB2	5	0.16
(1,1814)	1:50:A:THR:H	1:45:A:ASN:H	3	0.16
(1,1639)	1:7:A:THR:H	1:130:A:THR:H	8	0.16
(1,1638)	1:130:A:THR:H	1:7:A:THR:H	8	0.16
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD11	9	0.16
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD12	9	0.16
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD13	9	0.16
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD21	9	0.16
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD22	9	0.16
(1,1456)	1:104:A:THR:H	1:114:A:LEU:HD23	9	0.16
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	10	0.16
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	10	0.16
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	10	0.16
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	10	0.16
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	10	0.16
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	10	0.16
(1,766)	1:124:A:LYS:HA	1:115:A:THR:H	1	0.16
(1,766)	1:124:A:LYS:HA	1:115:A:THR:H	7	0.16
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG11	6	0.16
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG12	6	0.16
(1,749)	1:54:A:SER:HA	1:39:A:VAL:HG13	6	0.16
(1,566)	1:86:A:GLY:H	1:87:A:SER:H	3	0.16
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD21	7	0.16
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD22	7	0.16
(1,370)	1:5:A:ALA:H	1:4:A:LEU:HD23	7	0.16
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB2	5	0.16
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB3	5	0.16
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB2	5	0.16
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB3	5	0.16
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	2	0.16
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	2	0.16
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	10	0.16
(1,192)	1:104:A:THR:H	1:104:A:THR:HB	5	0.16
(1,188)	1:104:A:THR:H	1:103:A:ARG:HB2	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:104:A:THR:H	1:103:A:ARG:HB3	6	0.16
(1,187)	1:104:A:THR:H	1:103:A:ARG:HB2	6	0.16
(1,187)	1:104:A:THR:H	1:103:A:ARG:HB3	6	0.16
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	9	0.16
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE2	5	0.16
(1,159)	1:88:A:LYS:H	1:88:A:LYS:HE3	5	0.16
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	4	0.16
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	7	0.16
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	7	0.16
(1,55)	1:24:A:GLY:H	1:23:A:LEU:HB2	10	0.16
(1,55)	1:24:A:GLY:H	1:23:A:LEU:HB3	10	0.16
(1,12)	1:130:A:THR:H	1:8:A:TYR:HA	4	0.16
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	3	0.15
(3,11)	1:12:A:LYS:N	1:126:A:TYR:O	5	0.15
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	7	0.15
(1,2059)	1:11:A:GLU:HA	1:127:A:PHE:HA	5	0.15
(1,2057)	1:113:A:VAL:HG11	1:126:A:TYR:HE1	7	0.15
(1,2057)	1:113:A:VAL:HG12	1:126:A:TYR:HE1	7	0.15
(1,2057)	1:113:A:VAL:HG13	1:126:A:TYR:HE1	7	0.15
(1,1849)	1:8:A:TYR:H	1:129:A:ARG:HB2	1	0.15
(1,1849)	1:8:A:TYR:H	1:129:A:ARG:HB3	1	0.15
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD11	5	0.15
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD12	5	0.15
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD13	5	0.15
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD11	6	0.15
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD12	6	0.15
(1,1824)	1:77:A:ASN:H	1:71:A:LEU:HD13	6	0.15
(1,1822)	1:34:A:ASN:HD21	1:71:A:LEU:HB2	10	0.15
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG11	1	0.15
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG12	1	0.15
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG13	1	0.15
(1,1786)	1:31:A:LYS:H	1:27:A:GLN:HB2	5	0.15
(1,1773)	1:18:A:GLU:H	1:15:A:ASN:H	2	0.15
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD11	10	0.15
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD12	10	0.15
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD13	10	0.15
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD21	10	0.15
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD22	10	0.15
(1,1651)	1:65:A:GLU:H	1:84:A:LEU:HD23	10	0.15
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG2	1	0.15
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG3	1	0.15
(1,1630)	1:113:A:VAL:HG11	1:126:A:TYR:HE1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	1:113:A:VAL:HG12	1:126:A:TYR:HE1	7	0.15
(1,1630)	1:113:A:VAL:HG13	1:126:A:TYR:HE1	7	0.15
(1,1566)	1:43:A:ILE:HB	1:7:A:THR:HB	5	0.15
(1,1356)	1:99:A:ARG:H	1:95:A:LEU:HG	5	0.15
(1,821)	1:12:A:LYS:H	1:12:A:LYS:HE2	4	0.15
(1,821)	1:12:A:LYS:H	1:12:A:LYS:HE3	4	0.15
(1,766)	1:124:A:LYS:HA	1:115:A:THR:H	6	0.15
(1,764)	1:12:A:LYS:HE2	1:126:A:TYR:HE1	10	0.15
(1,764)	1:12:A:LYS:HE3	1:126:A:TYR:HE1	10	0.15
(1,763)	1:18:A:GLU:HB3	1:121:A:MET:HB3	7	0.15
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG11	8	0.15
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG12	8	0.15
(1,747)	1:9:A:LYS:HB2	1:39:A:VAL:HG13	8	0.15
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG11	8	0.15
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG12	8	0.15
(1,747)	1:9:A:LYS:HB3	1:39:A:VAL:HG13	8	0.15
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB2	7	0.15
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB3	7	0.15
(1,572)	1:84:A:LEU:H	1:89:A:LEU:HG	3	0.15
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD21	9	0.15
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD22	9	0.15
(1,389)	1:33:A:ALA:HB1	1:71:A:LEU:HD23	9	0.15
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD21	9	0.15
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD22	9	0.15
(1,389)	1:33:A:ALA:HB2	1:71:A:LEU:HD23	9	0.15
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD21	9	0.15
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD22	9	0.15
(1,389)	1:33:A:ALA:HB3	1:71:A:LEU:HD23	9	0.15
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	9	0.15
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	9	0.15
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	9	0.15
(1,356)	1:63:A:VAL:H	1:62:A:ILE:HA	8	0.15
(1,348)	1:116:A:MET:HA	1:103:A:ARG:HG2	4	0.15
(1,348)	1:116:A:MET:HA	1:103:A:ARG:HG3	4	0.15
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG11	1	0.15
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG12	1	0.15
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG13	1	0.15
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG21	1	0.15
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG22	1	0.15
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG23	1	0.15
(1,275)	1:77:A:ASN:HB2	1:70:A:VAL:HA	8	0.15
(1,275)	1:77:A:ASN:HB3	1:70:A:VAL:HA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB1	4	0.15
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB2	4	0.15
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB3	4	0.15
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB1	4	0.15
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB2	4	0.15
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB3	4	0.15
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB1	4	0.15
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB2	4	0.15
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB3	4	0.15
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB2	1	0.15
(1,221)	1:118:A:ALA:H	1:117:A:CYS:HB3	1	0.15
(1,219)	1:104:A:THR:H	1:116:A:MET:HA	1	0.15
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB2	5	0.15
(1,213)	1:125:A:ARG:H	1:114:A:LEU:HB3	5	0.15
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB2	5	0.15
(1,212)	1:125:A:ARG:H	1:114:A:LEU:HB3	5	0.15
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	1	0.15
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG2	8	0.15
(1,189)	1:104:A:THR:H	1:103:A:ARG:HG3	8	0.15
(1,176)	1:101:A:GLY:H	1:94:A:GLU:HA	9	0.15
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	1	0.15
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	1	0.15
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	1	0.15
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	7	0.15
(1,59)	1:27:A:GLN:H	1:26:A:PRO:HB2	3	0.15
(1,59)	1:27:A:GLN:H	1:26:A:PRO:HB3	3	0.15
(1,59)	1:27:A:GLN:H	1:26:A:PRO:HB2	10	0.15
(1,59)	1:27:A:GLN:H	1:26:A:PRO:HB3	10	0.15
(3,61)	1:116:A:MET:N	1:123:A:ALA:O	6	0.14
(3,19)	1:19:A:TYR:N	1:15:A:ASN:O	7	0.14
(1,2056)	1:14:A:GLU:HB3	1:126:A:TYR:HE1	8	0.14
(1,2033)	1:126:A:TYR:HA	1:113:A:VAL:HB	10	0.14
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE2	5	0.14
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE3	5	0.14
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE2	5	0.14
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE3	5	0.14
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE2	5	0.14
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE3	5	0.14
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE2	5	0.14
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE3	5	0.14
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE2	5	0.14
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE2	5	0.14
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE3	5	0.14
(1,1895)	1:30:A:ILE:HG12	1:27:A:GLN:HA	10	0.14
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD11	4	0.14
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD12	4	0.14
(1,1808)	1:33:A:ALA:H	1:20:A:LEU:HD13	4	0.14
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG11	2	0.14
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG12	2	0.14
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG13	2	0.14
(1,1799)	1:47:A:ASN:HD21	1:2:A:VAL:HB	5	0.14
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG11	1	0.14
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG12	1	0.14
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG13	1	0.14
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG21	1	0.14
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG22	1	0.14
(1,1795)	1:92:A:ASN:HD21	1:90:A:VAL:HG23	1	0.14
(1,1791)	1:45:A:ASN:HD21	1:48:A:LYS:HG2	2	0.14
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG11	6	0.14
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG12	6	0.14
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG13	6	0.14
(1,1753)	1:27:A:GLN:H	1:26:A:PRO:HD2	5	0.14
(1,1737)	1:43:A:ILE:HG12	1:41:A:GLU:HB2	7	0.14
(1,1737)	1:43:A:ILE:HG12	1:41:A:GLU:HB3	7	0.14
(1,1737)	1:43:A:ILE:HG13	1:41:A:GLU:HB2	7	0.14
(1,1737)	1:43:A:ILE:HG13	1:41:A:GLU:HB3	7	0.14
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	9	0.14
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	9	0.14
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	9	0.14
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	9	0.14
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	9	0.14
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	9	0.14
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	9	0.14
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	9	0.14
(1,1703)	1:104:A:THR:H	1:115:A:THR:HB	1	0.14
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	9	0.14
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	9	0.14
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	9	0.14
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	9	0.14
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	9	0.14
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	9	0.14
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	9	0.14
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1459)	1:125:A:ARG:H	1:114:A:LEU:HG	8	0.14
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG11	9	0.14
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG12	9	0.14
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG13	9	0.14
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG21	9	0.14
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG22	9	0.14
(1,1049)	1:48:A:LYS:H	1:44:A:VAL:HG23	9	0.14
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG11	7	0.14
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG12	7	0.14
(1,728)	1:45:A:ASN:H	1:2:A:VAL:HG13	7	0.14
(1,725)	1:29:A:SER:H	1:32:A:LYS:HG2	7	0.14
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB2	3	0.14
(1,710)	1:51:A:PHE:HB2	1:61:A:LEU:HB3	3	0.14
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB2	3	0.14
(1,710)	1:51:A:PHE:HB3	1:61:A:LEU:HB3	3	0.14
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD11	5	0.14
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD12	5	0.14
(1,703)	1:69:A:GLU:H	1:78:A:ILE:HD13	5	0.14
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB2	2	0.14
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB3	2	0.14
(1,649)	1:44:A:VAL:HB	1:49:A:PHE:HA	2	0.14
(1,607)	1:114:A:LEU:H	1:114:A:LEU:HD11	8	0.14
(1,607)	1:114:A:LEU:H	1:114:A:LEU:HD12	8	0.14
(1,607)	1:114:A:LEU:H	1:114:A:LEU:HD13	8	0.14
(1,607)	1:114:A:LEU:H	1:114:A:LEU:HD21	8	0.14
(1,607)	1:114:A:LEU:H	1:114:A:LEU:HD22	8	0.14
(1,607)	1:114:A:LEU:H	1:114:A:LEU:HD23	8	0.14
(1,606)	1:114:A:LEU:H	1:114:A:LEU:HD11	8	0.14
(1,606)	1:114:A:LEU:H	1:114:A:LEU:HD12	8	0.14
(1,606)	1:114:A:LEU:H	1:114:A:LEU:HD13	8	0.14
(1,606)	1:114:A:LEU:H	1:114:A:LEU:HD21	8	0.14
(1,606)	1:114:A:LEU:H	1:114:A:LEU:HD22	8	0.14
(1,606)	1:114:A:LEU:H	1:114:A:LEU:HD23	8	0.14
(1,448)	1:31:A:LYS:H	1:30:A:ILE:HG12	1	0.14
(1,448)	1:31:A:LYS:H	1:30:A:ILE:HG13	1	0.14
(1,448)	1:31:A:LYS:H	1:30:A:ILE:HG12	8	0.14
(1,448)	1:31:A:LYS:H	1:30:A:ILE:HG13	8	0.14
(1,430)	1:24:A:GLY:H	1:20:A:LEU:HA	1	0.14
(1,383)	1:36:A:PRO:HG2	1:12:A:LYS:HA	6	0.14
(1,383)	1:36:A:PRO:HG3	1:12:A:LYS:HA	6	0.14
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB2	2	0.14
(1,281)	1:84:A:LEU:HA	1:89:A:LEU:HB3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB1	1	0.14
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB2	1	0.14
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB3	1	0.14
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB1	1	0.14
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB2	1	0.14
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB3	1	0.14
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB1	1	0.14
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB2	1	0.14
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB3	1	0.14
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB2	1	0.14
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB3	1	0.14
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB2	9	0.14
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB3	9	0.14
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB2	1	0.14
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB3	1	0.14
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB2	9	0.14
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB3	9	0.14
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB2	2	0.14
(1,239)	1:125:A:ARG:H	1:124:A:LYS:HB3	2	0.14
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB2	7	0.14
(1,238)	1:124:A:LYS:H	1:124:A:LYS:HB3	7	0.14
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB2	7	0.14
(1,237)	1:124:A:LYS:H	1:124:A:LYS:HB3	7	0.14
(1,210)	1:127:A:PHE:H	1:113:A:VAL:HA	7	0.14
(1,197)	1:89:A:LEU:H	1:106:A:GLU:HA	4	0.14
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD11	2	0.14
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD12	2	0.14
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD13	2	0.14
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB2	3	0.14
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB3	3	0.14
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB2	5	0.14
(1,99)	1:45:A:ASN:H	1:48:A:LYS:HB3	5	0.14
(1,70)	1:33:A:ALA:H	1:32:A:LYS:HA	10	0.14
(1,39)	1:17:A:GLU:H	1:15:A:ASN:H	9	0.14
(3,61)	1:116:A:MET:N	1:123:A:ALA:O	10	0.13
(3,33)	1:48:A:LYS:N	1:45:A:ASN:O	5	0.13
(1,2019)	1:63:A:VAL:HG21	1:89:A:LEU:HB2	10	0.13
(1,2019)	1:63:A:VAL:HG22	1:89:A:LEU:HB2	10	0.13
(1,2019)	1:63:A:VAL:HG23	1:89:A:LEU:HB2	10	0.13
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD21	9	0.13
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD22	9	0.13
(1,1963)	1:125:A:ARG:HB2	1:10:A:LEU:HD23	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1957)	1:114:A:LEU:HD21	1:10:A:LEU:HA	4	0.13
(1,1957)	1:114:A:LEU:HD22	1:10:A:LEU:HA	4	0.13
(1,1957)	1:114:A:LEU:HD23	1:10:A:LEU:HA	4	0.13
(1,1923)	1:67:A:VAL:HG21	1:65:A:GLU:HB2	9	0.13
(1,1923)	1:67:A:VAL:HG22	1:65:A:GLU:HB2	9	0.13
(1,1923)	1:67:A:VAL:HG23	1:65:A:GLU:HB2	9	0.13
(1,1875)	1:98:A:GLY:HA3	1:99:A:ARG:HB3	9	0.13
(1,1791)	1:45:A:ASN:HD21	1:48:A:LYS:HG2	1	0.13
(1,1755)	1:60:A:THR:H	1:61:A:LEU:HG	3	0.13
(1,1706)	1:77:A:ASN:H	1:96:A:PRO:HG2	6	0.13
(1,1706)	1:77:A:ASN:H	1:96:A:PRO:HG3	6	0.13
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB1	3	0.13
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB2	3	0.13
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB3	3	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB1	3	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB2	3	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB3	3	0.13
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB1	7	0.13
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB2	7	0.13
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB3	7	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB1	7	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB2	7	0.13
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB3	7	0.13
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG2	7	0.13
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG3	7	0.13
(1,1566)	1:43:A:ILE:HB	1:7:A:THR:HB	9	0.13
(1,1356)	1:99:A:ARG:H	1:95:A:LEU:HG	6	0.13
(1,1322)	1:105:A:TYR:H	1:89:A:LEU:HG	3	0.13
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD21	5	0.13
(1,1219)	1:76:A:MET:H	1:75:A:ASN:HD22	5	0.13
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD11	4	0.13
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD12	4	0.13
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD13	4	0.13
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD21	4	0.13
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD22	4	0.13
(1,883)	1:19:A:TYR:H	1:20:A:LEU:HD23	4	0.13
(1,852)	1:15:A:ASN:H	1:16:A:PHE:HB2	6	0.13
(1,852)	1:15:A:ASN:H	1:16:A:PHE:HB3	6	0.13
(1,722)	1:5:A:ALA:H	1:3:A:GLN:HG2	4	0.13
(1,722)	1:5:A:ALA:H	1:3:A:GLN:HG3	4	0.13
(1,553)	1:83:A:LYS:H	1:83:A:LYS:HG2	2	0.13
(1,553)	1:83:A:LYS:H	1:83:A:LYS:HG3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:79:A:LYS:H	1:79:A:LYS:HD2	1	0.13
(1,542)	1:79:A:LYS:H	1:79:A:LYS:HD3	1	0.13
(1,542)	1:79:A:LYS:H	1:79:A:LYS:HD2	6	0.13
(1,542)	1:79:A:LYS:H	1:79:A:LYS:HD3	6	0.13
(1,386)	1:31:A:LYS:HB2	1:28:A:ASP:HA	3	0.13
(1,386)	1:31:A:LYS:HB3	1:28:A:ASP:HA	3	0.13
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG11	6	0.13
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG12	6	0.13
(1,385)	1:33:A:ALA:HB1	1:25:A:VAL:HG13	6	0.13
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG11	6	0.13
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG12	6	0.13
(1,385)	1:33:A:ALA:HB2	1:25:A:VAL:HG13	6	0.13
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG11	6	0.13
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG12	6	0.13
(1,385)	1:33:A:ALA:HB3	1:25:A:VAL:HG13	6	0.13
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	1	0.13
(1,376)	1:106:A:GLU:H	1:113:A:VAL:HB	2	0.13
(1,269)	1:28:A:ASP:HA	1:31:A:LYS:HB2	3	0.13
(1,269)	1:28:A:ASP:HA	1:31:A:LYS:HB3	3	0.13
(1,268)	1:31:A:LYS:HB2	1:28:A:ASP:HA	3	0.13
(1,268)	1:31:A:LYS:HB3	1:28:A:ASP:HA	3	0.13
(1,265)	1:130:A:THR:H	1:130:A:THR:HG21	3	0.13
(1,265)	1:130:A:THR:H	1:130:A:THR:HG22	3	0.13
(1,265)	1:130:A:THR:H	1:130:A:THR:HG23	3	0.13
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB2	7	0.13
(1,255)	1:128:A:ILE:H	1:127:A:PHE:HB3	7	0.13
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB2	7	0.13
(1,254)	1:128:A:ILE:H	1:127:A:PHE:HB3	7	0.13
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB2	10	0.13
(1,253)	1:112:A:PHE:H	1:127:A:PHE:HB3	10	0.13
(1,214)	1:125:A:ARG:H	1:114:A:LEU:H	4	0.13
(1,192)	1:104:A:THR:H	1:104:A:THR:HB	2	0.13
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG11	6	0.13
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG12	6	0.13
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG13	6	0.13
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG21	6	0.13
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG22	6	0.13
(1,169)	1:81:A:PHE:H	1:91:A:VAL:HG23	6	0.13
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	7	0.13
(1,145)	1:94:A:GLU:H	1:79:A:LYS:H	10	0.13
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	6	0.13
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	6	0.13
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	9	0.13
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	9	0.13
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	9	0.13
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD11	1	0.13
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD12	1	0.13
(1,131)	1:63:A:VAL:H	1:62:A:ILE:HD13	1	0.13
(1,124)	1:53:A:SER:H	1:59:A:SER:H	2	0.13
(1,123)	1:60:A:THR:H	1:59:A:SER:HB2	10	0.13
(1,123)	1:60:A:THR:H	1:59:A:SER:HB3	10	0.13
(1,113)	1:59:A:SER:H	1:53:A:SER:H	2	0.13
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG2	6	0.13
(1,109)	1:53:A:SER:H	1:52:A:LYS:HG3	6	0.13
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB2	7	0.13
(1,37)	1:16:A:PHE:H	1:15:A:ASN:HB3	7	0.13
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB2	7	0.13
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB3	7	0.13
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB2	9	0.13
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB3	9	0.13
(3,51)	1:106:A:GLU:N	1:113:A:VAL:O	5	0.12
(3,49)	1:101:A:GLY:N	1:93:A:SER:O	5	0.12
(3,33)	1:48:A:LYS:N	1:45:A:ASN:O	8	0.12
(3,13)	1:126:A:TYR:N	1:12:A:LYS:O	3	0.12
(3,11)	1:12:A:LYS:N	1:126:A:TYR:O	9	0.12
(1,2004)	1:93:A:SER:HB2	1:78:A:ILE:HG12	10	0.12
(1,1978)	1:74:A:VAL:HG21	1:29:A:SER:HB3	3	0.12
(1,1978)	1:74:A:VAL:HG22	1:29:A:SER:HB3	3	0.12
(1,1978)	1:74:A:VAL:HG23	1:29:A:SER:HB3	3	0.12
(1,1978)	1:74:A:VAL:HG21	1:29:A:SER:HB3	8	0.12
(1,1978)	1:74:A:VAL:HG22	1:29:A:SER:HB3	8	0.12
(1,1978)	1:74:A:VAL:HG23	1:29:A:SER:HB3	8	0.12
(1,1971)	1:123:A:ALA:HB1	1:15:A:ASN:HD22	6	0.12
(1,1971)	1:123:A:ALA:HB2	1:15:A:ASN:HD22	6	0.12
(1,1971)	1:123:A:ALA:HB3	1:15:A:ASN:HD22	6	0.12
(1,1935)	1:94:A:GLU:HG2	1:96:A:PRO:HB2	1	0.12
(1,1935)	1:94:A:GLU:HG3	1:96:A:PRO:HB2	1	0.12
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD21	2	0.12
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD22	2	0.12
(1,1934)	1:99:A:ARG:HA	1:95:A:LEU:HD23	2	0.12
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG11	7	0.12
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG12	7	0.12
(1,1922)	1:65:A:GLU:HG2	1:63:A:VAL:HG13	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1843)	1:15:A:ASN:HD22	1:123:A:ALA:HB1	6	0.12
(1,1843)	1:15:A:ASN:HD22	1:123:A:ALA:HB2	6	0.12
(1,1843)	1:15:A:ASN:HD22	1:123:A:ALA:HB3	6	0.12
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG2	5	0.12
(1,1647)	1:14:A:GLU:H	1:124:A:LYS:HG3	5	0.12
(1,1646)	1:14:A:GLU:H	1:124:A:LYS:HB2	4	0.12
(1,1646)	1:14:A:GLU:H	1:124:A:LYS:HB3	4	0.12
(1,1645)	1:14:A:GLU:H	1:124:A:LYS:HB2	4	0.12
(1,1645)	1:14:A:GLU:H	1:124:A:LYS:HB3	4	0.12
(1,1531)	1:130:A:THR:HB	1:7:A:THR:HB	5	0.12
(1,1479)	1:118:A:ALA:H	1:121:A:MET:HB2	3	0.12
(1,1479)	1:118:A:ALA:H	1:121:A:MET:HB3	3	0.12
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD11	7	0.12
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD12	7	0.12
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD13	7	0.12
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD21	7	0.12
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD22	7	0.12
(1,1352)	1:98:A:GLY:H	1:95:A:LEU:HD23	7	0.12
(1,1272)	1:82:A:THR:H	1:83:A:LYS:HB2	2	0.12
(1,1272)	1:82:A:THR:H	1:83:A:LYS:HB3	2	0.12
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB2	8	0.12
(1,971)	1:28:A:ASP:H	1:31:A:LYS:HB3	8	0.12
(1,852)	1:15:A:ASN:H	1:16:A:PHE:HB2	1	0.12
(1,852)	1:15:A:ASN:H	1:16:A:PHE:HB3	1	0.12
(1,852)	1:15:A:ASN:H	1:16:A:PHE:HB2	7	0.12
(1,852)	1:15:A:ASN:H	1:16:A:PHE:HB3	7	0.12
(1,741)	1:44:A:VAL:HG21	1:4:A:LEU:HD11	7	0.12
(1,741)	1:44:A:VAL:HG21	1:4:A:LEU:HD12	7	0.12
(1,741)	1:44:A:VAL:HG21	1:4:A:LEU:HD13	7	0.12
(1,741)	1:44:A:VAL:HG22	1:4:A:LEU:HD11	7	0.12
(1,741)	1:44:A:VAL:HG22	1:4:A:LEU:HD12	7	0.12
(1,741)	1:44:A:VAL:HG22	1:4:A:LEU:HD13	7	0.12
(1,741)	1:44:A:VAL:HG23	1:4:A:LEU:HD11	7	0.12
(1,741)	1:44:A:VAL:HG23	1:4:A:LEU:HD12	7	0.12
(1,741)	1:44:A:VAL:HG23	1:4:A:LEU:HD13	7	0.12
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB2	9	0.12
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB3	9	0.12
(1,614)	1:121:A:MET:H	1:118:A:ALA:HA	10	0.12
(1,602)	1:114:A:LEU:H	1:113:A:VAL:HB	4	0.12
(1,553)	1:83:A:LYS:H	1:83:A:LYS:HG2	9	0.12
(1,553)	1:83:A:LYS:H	1:83:A:LYS:HG3	9	0.12
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:83:A:LYS:H	1:83:A:LYS:HE3	4	0.12
(1,542)	1:79:A:LYS:H	1:79:A:LYS:HD2	2	0.12
(1,542)	1:79:A:LYS:H	1:79:A:LYS:HD3	2	0.12
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB2	3	0.12
(1,493)	1:56:A:GLY:H	1:57:A:MET:HB3	3	0.12
(1,429)	1:22:A:ALA:H	1:20:A:LEU:HA	10	0.12
(1,382)	1:36:A:PRO:HB2	1:10:A:LEU:HG	10	0.12
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG11	6	0.12
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG12	6	0.12
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG13	6	0.12
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG21	6	0.12
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG22	6	0.12
(1,296)	1:6:A:GLY:H	1:44:A:VAL:HG23	6	0.12
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	7	0.12
(1,285)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	7	0.12
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	7	0.12
(1,285)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	7	0.12
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB2	7	0.12
(1,284)	1:23:A:LEU:HB2	1:95:A:LEU:HB3	7	0.12
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB2	7	0.12
(1,284)	1:23:A:LEU:HB3	1:95:A:LEU:HB3	7	0.12
(1,257)	1:112:A:PHE:H	1:128:A:ILE:HA	7	0.12
(1,223)	1:121:A:MET:H	1:118:A:ALA:H	6	0.12
(1,220)	1:123:A:ALA:H	1:117:A:CYS:HA	6	0.12
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG21	10	0.12
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG22	10	0.12
(1,132)	1:63:A:VAL:H	1:62:A:ILE:HG23	10	0.12
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	8	0.12
(1,119)	1:56:A:GLY:H	1:57:A:MET:H	9	0.12
(1,112)	1:54:A:SER:H	1:53:A:SER:HB2	3	0.12
(1,112)	1:54:A:SER:H	1:53:A:SER:HB3	3	0.12
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB2	7	0.12
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB3	7	0.12
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB2	8	0.12
(1,102)	1:50:A:THR:H	1:49:A:PHE:HB3	8	0.12
(1,25)	1:128:A:ILE:H	1:11:A:GLU:HG2	5	0.12
(1,25)	1:128:A:ILE:H	1:11:A:GLU:HG3	5	0.12
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB2	5	0.12
(1,24)	1:128:A:ILE:H	1:11:A:GLU:HB3	5	0.12
(3,33)	1:48:A:LYS:N	1:45:A:ASN:O	3	0.11
(3,18)	1:124:A:LYS:H	1:14:A:GLU:O	9	0.11
(3,15)	1:14:A:GLU:N	1:124:A:LYS:O	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:80:A:SER:H	1:67:A:VAL:H	7	0.11
(1,2057)	1:113:A:VAL:HG11	1:126:A:TYR:HE1	4	0.11
(1,2057)	1:113:A:VAL:HG12	1:126:A:TYR:HE1	4	0.11
(1,2057)	1:113:A:VAL:HG13	1:126:A:TYR:HE1	4	0.11
(1,2057)	1:113:A:VAL:HG11	1:126:A:TYR:HE1	6	0.11
(1,2057)	1:113:A:VAL:HG12	1:126:A:TYR:HE1	6	0.11
(1,2057)	1:113:A:VAL:HG13	1:126:A:TYR:HE1	6	0.11
(1,2028)	1:91:A:VAL:HA	1:103:A:ARG:HB2	3	0.11
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE2	9	0.11
(1,2014)	1:89:A:LEU:HD11	1:83:A:LYS:HE3	9	0.11
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE2	9	0.11
(1,2014)	1:89:A:LEU:HD12	1:83:A:LYS:HE3	9	0.11
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE2	9	0.11
(1,2014)	1:89:A:LEU:HD13	1:83:A:LYS:HE3	9	0.11
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE2	9	0.11
(1,2014)	1:89:A:LEU:HD21	1:83:A:LYS:HE3	9	0.11
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE2	9	0.11
(1,2014)	1:89:A:LEU:HD22	1:83:A:LYS:HE3	9	0.11
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE2	9	0.11
(1,2014)	1:89:A:LEU:HD23	1:83:A:LYS:HE3	9	0.11
(1,2012)	1:89:A:LEU:HD11	1:82:A:THR:H	4	0.11
(1,2012)	1:89:A:LEU:HD12	1:82:A:THR:H	4	0.11
(1,2012)	1:89:A:LEU:HD13	1:82:A:THR:H	4	0.11
(1,2012)	1:89:A:LEU:HD21	1:82:A:THR:H	4	0.11
(1,2012)	1:89:A:LEU:HD22	1:82:A:THR:H	4	0.11
(1,2012)	1:89:A:LEU:HD23	1:82:A:THR:H	4	0.11
(1,1978)	1:74:A:VAL:HG21	1:29:A:SER:HB3	10	0.11
(1,1978)	1:74:A:VAL:HG22	1:29:A:SER:HB3	10	0.11
(1,1978)	1:74:A:VAL:HG23	1:29:A:SER:HB3	10	0.11
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG11	2	0.11
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG12	2	0.11
(1,1812)	1:49:A:PHE:H	1:44:A:VAL:HG13	2	0.11
(1,1788)	1:47:A:ASN:H	1:45:A:ASN:HB3	1	0.11
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG11	7	0.11
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG12	7	0.11
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG13	7	0.11
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	6	0.11
(1,1718)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	6	0.11
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	6	0.11
(1,1718)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	6	0.11
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG2	6	0.11
(1,1717)	1:126:A:TYR:HB2	1:12:A:LYS:HG3	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG2	6	0.11
(1,1717)	1:126:A:TYR:HB3	1:12:A:LYS:HG3	6	0.11
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB1	2	0.11
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB2	2	0.11
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB3	2	0.11
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB1	2	0.11
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB2	2	0.11
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB3	2	0.11
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB1	9	0.11
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB2	9	0.11
(1,1654)	1:16:A:PHE:HB2	1:33:A:ALA:HB3	9	0.11
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB1	9	0.11
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB2	9	0.11
(1,1654)	1:16:A:PHE:HB3	1:33:A:ALA:HB3	9	0.11
(1,1630)	1:113:A:VAL:HG11	1:126:A:TYR:HE1	4	0.11
(1,1630)	1:113:A:VAL:HG12	1:126:A:TYR:HE1	4	0.11
(1,1630)	1:113:A:VAL:HG13	1:126:A:TYR:HE1	4	0.11
(1,1630)	1:113:A:VAL:HG11	1:126:A:TYR:HE1	6	0.11
(1,1630)	1:113:A:VAL:HG12	1:126:A:TYR:HE1	6	0.11
(1,1630)	1:113:A:VAL:HG13	1:126:A:TYR:HE1	6	0.11
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	6	0.11
(1,1626)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	6	0.11
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	6	0.11
(1,1626)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	6	0.11
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB2	6	0.11
(1,1625)	1:12:A:LYS:HG2	1:126:A:TYR:HB3	6	0.11
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB2	6	0.11
(1,1625)	1:12:A:LYS:HG3	1:126:A:TYR:HB3	6	0.11
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB2	5	0.11
(1,1337)	1:79:A:LYS:H	1:93:A:SER:HB3	5	0.11
(1,1286)	1:88:A:LYS:H	1:84:A:LEU:HG	2	0.11
(1,1168)	1:66:A:GLU:H	1:65:A:GLU:HB2	3	0.11
(1,1168)	1:66:A:GLU:H	1:65:A:GLU:HB3	3	0.11
(1,1036)	1:50:A:THR:H	1:43:A:ILE:HB	2	0.11
(1,888)	1:21:A:ALA:H	1:20:A:LEU:HG	4	0.11
(1,722)	1:5:A:ALA:H	1:3:A:GLN:HG2	10	0.11
(1,722)	1:5:A:ALA:H	1:3:A:GLN:HG3	10	0.11
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB2	8	0.11
(1,667)	1:88:A:LYS:HA	1:106:A:GLU:HB3	8	0.11
(1,381)	1:39:A:VAL:HG11	1:9:A:LYS:HG2	7	0.11
(1,381)	1:39:A:VAL:HG12	1:9:A:LYS:HG2	7	0.11
(1,381)	1:39:A:VAL:HG13	1:9:A:LYS:HG2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:88:A:LYS:H	1:85:A:GLU:H	2	0.11
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB1	2	0.11
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB2	2	0.11
(1,270)	1:73:A:THR:HG21	1:33:A:ALA:HB3	2	0.11
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB1	2	0.11
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB2	2	0.11
(1,270)	1:73:A:THR:HG22	1:33:A:ALA:HB3	2	0.11
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB1	2	0.11
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB2	2	0.11
(1,270)	1:73:A:THR:HG23	1:33:A:ALA:HB3	2	0.11
(1,188)	1:104:A:THR:H	1:103:A:ARG:HB2	4	0.11
(1,188)	1:104:A:THR:H	1:103:A:ARG:HB3	4	0.11
(1,188)	1:104:A:THR:H	1:103:A:ARG:HB2	9	0.11
(1,188)	1:104:A:THR:H	1:103:A:ARG:HB3	9	0.11
(1,187)	1:104:A:THR:H	1:103:A:ARG:HB2	4	0.11
(1,187)	1:104:A:THR:H	1:103:A:ARG:HB3	4	0.11
(1,187)	1:104:A:THR:H	1:103:A:ARG:HB2	9	0.11
(1,187)	1:104:A:THR:H	1:103:A:ARG:HB3	9	0.11
(1,165)	1:83:A:LYS:H	1:91:A:VAL:HA	3	0.11
(1,135)	1:66:A:GLU:H	1:65:A:GLU:HB2	3	0.11
(1,135)	1:66:A:GLU:H	1:65:A:GLU:HB3	3	0.11
(1,129)	1:51:A:PHE:H	1:62:A:ILE:HA	8	0.11
(1,129)	1:51:A:PHE:H	1:62:A:ILE:HA	9	0.11
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	1	0.11
(1,126)	1:60:A:THR:H	1:60:A:THR:HB	5	0.11
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD21	7	0.11
(1,38)	1:15:A:ASN:H	1:15:A:ASN:HD22	7	0.11
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB2	2	0.11
(1,29)	1:14:A:GLU:H	1:13:A:ASN:HB3	2	0.11
(3,46)	1:90:A:VAL:H	1:83:A:LYS:O	5	0.1
(2,5)	1:94:A:GLU:H	1:80:A:SER:HA	1	0.1
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG11	10	0.1
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG12	10	0.1
(1,1800)	1:45:A:ASN:HD21	1:2:A:VAL:HG13	10	0.1
(1,1793)	1:87:A:SER:H	1:85:A:GLU:HG2	6	0.1
(1,1793)	1:87:A:SER:H	1:85:A:GLU:HG3	6	0.1
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG11	8	0.1
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG12	8	0.1
(1,1782)	1:27:A:GLN:H	1:25:A:VAL:HG13	8	0.1
(1,1494)	1:124:A:LYS:H	1:124:A:LYS:HE2	10	0.1
(1,1494)	1:124:A:LYS:H	1:124:A:LYS:HE3	10	0.1
(1,659)	1:84:A:LEU:HG	1:89:A:LEU:HD11	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:84:A:LEU:HG	1:89:A:LEU:HD12	4	0.1
(1,659)	1:84:A:LEU:HG	1:89:A:LEU:HD13	4	0.1
(1,659)	1:84:A:LEU:HG	1:89:A:LEU:HD21	4	0.1
(1,659)	1:84:A:LEU:HG	1:89:A:LEU:HD22	4	0.1
(1,659)	1:84:A:LEU:HG	1:89:A:LEU:HD23	4	0.1
(1,649)	1:44:A:VAL:HB	1:49:A:PHE:HA	1	0.1
(1,649)	1:44:A:VAL:HB	1:49:A:PHE:HA	5	0.1
(1,168)	1:92:A:ASN:H	1:91:A:VAL:HB	6	0.1

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

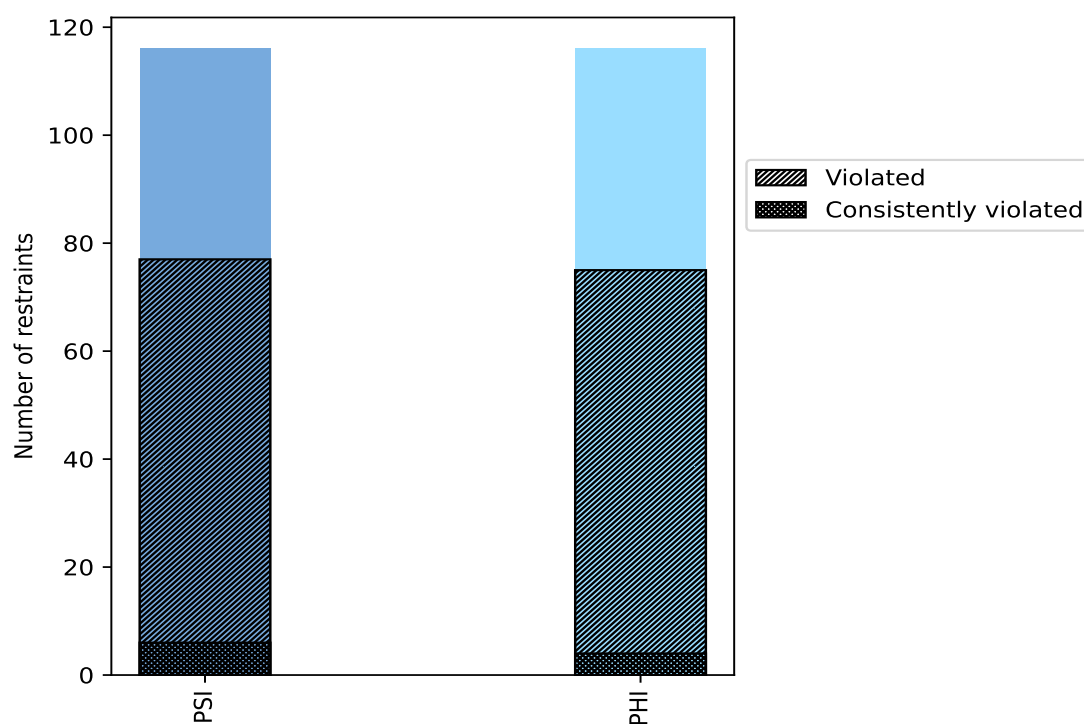
10.1 Summary of dihedral-angle violations [i](#)

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	116	50.0	77	66.4	33.2	6	5.2	2.6
PHI	116	50.0	75	64.7	32.3	4	3.4	1.7
Total	232	100.0	152	65.5	65.5	10	4.3	4.3

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

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



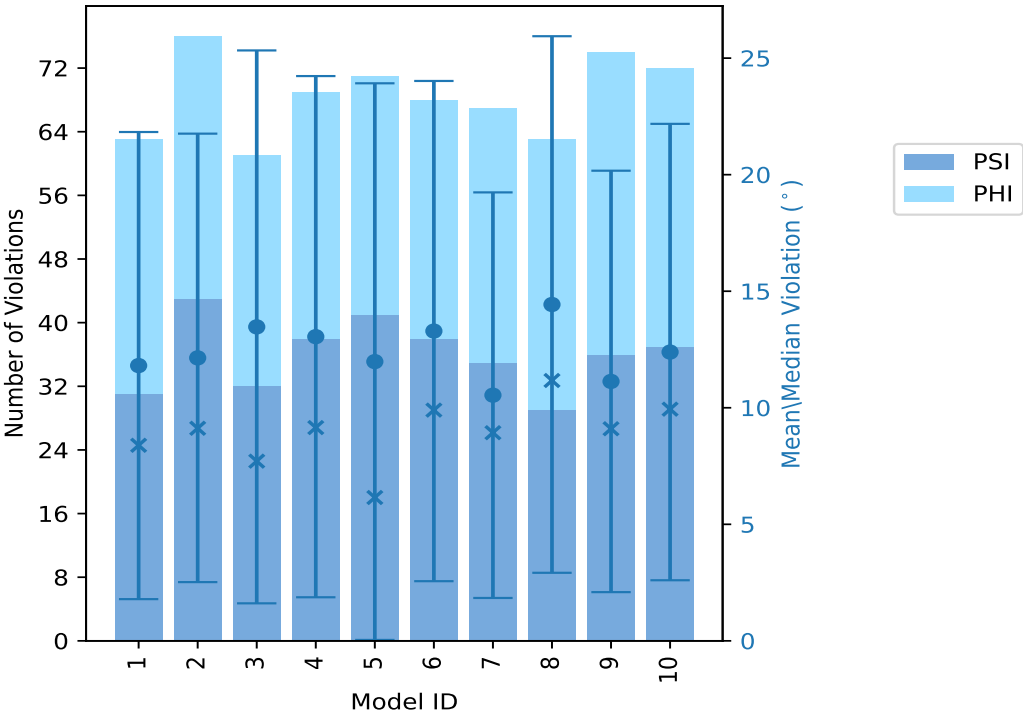
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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	31	32	63	11.81	53.38	10.02	8.39
2	43	33	76	12.14	54.37	9.62	9.12
3	32	29	61	13.47	54.01	11.86	7.71
4	38	31	69	13.05	59.14	11.18	9.15
5	41	30	71	11.98	51.74	11.94	6.15
6	38	30	68	13.29	50.78	10.73	9.9
7	35	32	67	10.54	39.8	8.7	8.93
8	29	34	63	14.43	55.51	11.51	11.17
9	36	38	74	11.13	49.27	9.04	9.1
10	37	35	72	12.39	52.06	9.79	9.94

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

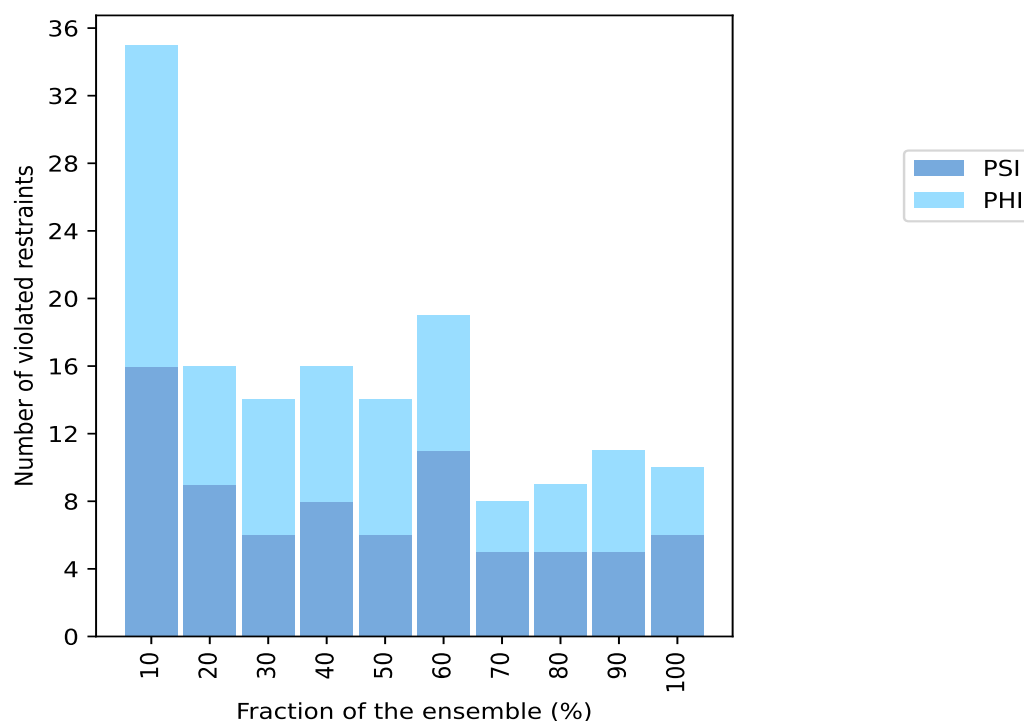
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
16	19	35	1	10.0
9	7	16	2	20.0
6	8	14	3	30.0
8	8	16	4	40.0
6	8	14	5	50.0
11	8	19	6	60.0
5	3	8	7	70.0
5	4	9	8	80.0
5	6	11	9	90.0
6	4	10	10	100.0

¹ Number of models with violations

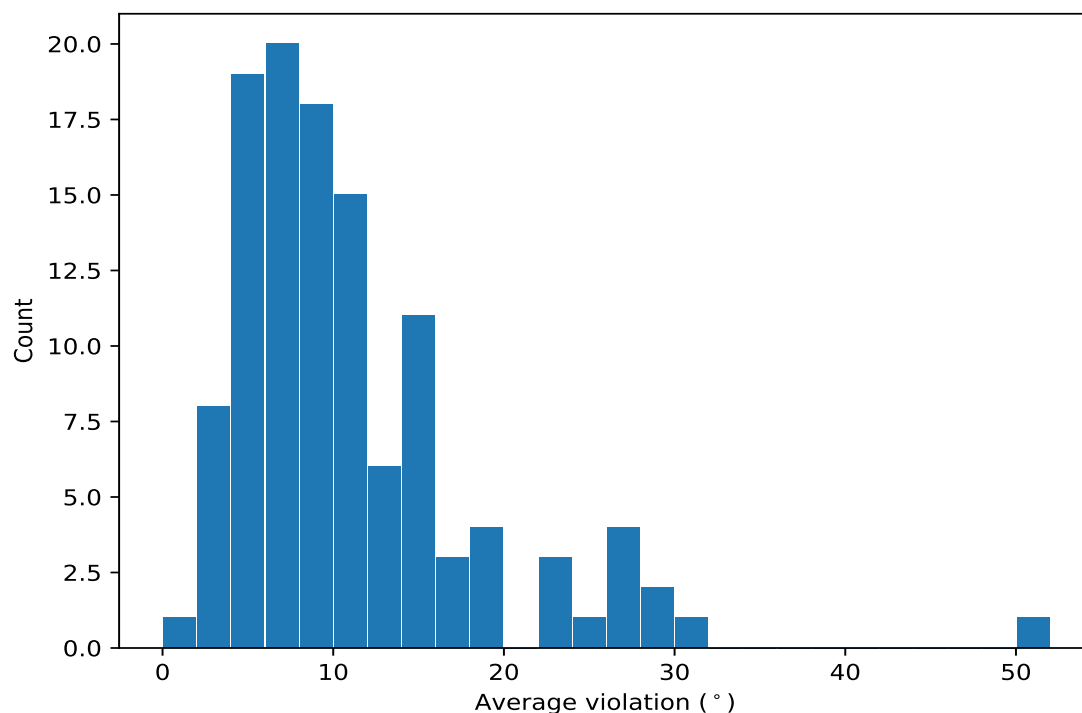
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	10	50.41	6.31	51.9
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	10	30.98	17.18	31.34
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	10	26.21	6.21	24.64
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	10	26.2	6.49	26.58
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	10	25.84	8.23	25.91
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	10	16.67	9.2	19.22
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	10	15.6	8.09	13.49
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	10	15.41	5.95	17.4
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	10	10.15	4.77	11.23
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	10	8.89	5.11	8.14
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	9	23.03	11.58	23.02
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	9	22.82	7.11	22.37
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	9	15.0	9.32	10.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	9	14.77	7.44	13.84
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	9	14.07	7.07	17.21
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	9	12.64	5.66	10.61
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	9	11.33	5.68	12.74
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	9	10.91	6.55	9.6
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	9	10.69	3.77	9.89
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	9	7.4	3.75	6.98
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	9	6.48	4.96	5.16
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	8	23.94	13.2	17.13
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	8	18.92	9.18	22.2
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	8	16.69	8.06	18.1
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	8	14.76	10.66	14.56
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	8	10.86	9.87	5.78
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	8	10.68	6.1	7.46
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	8	9.35	7.61	5.88
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	8	8.97	4.72	8.59
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	8	8.07	5.18	6.78
(1,202)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	7	27.12	10.64	32.3
(1,116)	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1:66:A:GLU:N	7	15.23	9.06	13.53
(1,191)	1:105:A:TYR:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	7	10.43	6.92	6.37
(1,3)	1:2:A:VAL:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	7	9.18	5.35	7.41
(1,165)	1:91:A:VAL:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	7	8.01	2.9	7.46
(1,134)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:MET:N	7	7.93	3.93	8.23
(1,102)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:MET:N	7	7.67	4.93	6.38
(1,230)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ARG:N	7	7.46	3.99	6.15
(1,70)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	6	27.95	8.06	26.73
(1,41)	1:23:A:LEU:C	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	6	19.07	15.95	17.22
(1,58)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ALA:N	6	15.88	7.07	14.98
(1,126)	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	1:71:A:LEU:N	6	13.86	7.3	18.02
(1,59)	1:32:A:LYS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	6	13.36	5.06	13.98
(1,100)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLY:N	6	12.48	8.39	10.56
(1,80)	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	1:46:A:GLY:N	6	10.81	6.78	10.4
(1,177)	1:97:A:ASP:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	6	10.79	6.07	11.28
(1,68)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:TYR:N	6	10.77	7.24	11.1
(1,1)	1:1:A:MET:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	6	10.73	5.64	10.04
(1,206)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:THR:N	6	9.14	3.49	8.58
(1,163)	1:90:A:VAL:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	6	9.11	5.79	9.86
(1,109)	1:59:A:SER:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	6	8.9	3.8	10.22
(1,184)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:ARG:N	6	7.75	3.6	7.56
(1,79)	1:44:A:VAL:C	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	6	6.89	3.81	6.64
(1,119)	1:66:A:GLU:C	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	6	6.8	3.6	6.28
(1,160)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:90:A:VAL:N	6	6.79	4.76	6.86
(1,224)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:TYR:N	6	5.85	2.87	5.42
(1,140)	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1:80:A:SER:N	6	3.32	1.68	3.03
(1,131)	1:73:A:THR:C	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	5	14.53	7.99	16.25
(1,8)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:GLY:N	5	14.03	8.43	13.33
(1,208)	1:115:A:THR:N	1:115:A:THR:CA	1:115:A:THR:C	1:116:A:MET:N	5	13.86	5.44	11.67
(1,65)	1:37:A:GLY:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	5	12.44	3.33	13.14
(1,147)	1:82:A:THR:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	5	9.29	4.82	12.01
(1,192)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:PHE:N	5	8.44	3.88	8.81
(1,216)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:MET:N	5	8.0	8.26	3.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,71)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	5	7.75	4.07	8.07
(1,56)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:LYS:N	5	7.48	3.79	9.5
(1,74)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:ILE:N	5	6.61	3.97	7.45
(1,217)	1:121:A:MET:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	5	5.84	5.71	1.57
(1,211)	1:116:A:MET:C	1:117:A:CYS:N	1:117:A:CYS:CA	1:117:A:CYS:C	5	5.52	3.66	5.53
(1,13)	1:8:A:TYR:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	5	5.44	3.19	5.96
(1,123)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	5	4.03	1.52	4.17
(1,201)	1:111:A:GLY:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	4	19.11	13.0	18.49
(1,40)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:GLY:N	4	16.24	7.59	19.06
(1,135)	1:75:A:ASN:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	4	14.44	3.36	14.34
(1,50)	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	1:29:A:SER:N	4	9.43	3.77	10.94
(1,84)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	4	8.56	2.74	8.84
(1,86)	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1:49:A:PHE:N	4	8.2	4.69	7.5
(1,178)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	4	8.06	4.82	8.96
(1,219)	1:122:A:VAL:C	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	4	7.95	3.24	7.04
(1,77)	1:43:A:ILE:C	1:44:A:VAL:N	1:44:A:VAL:CA	1:44:A:VAL:C	4	6.47	1.95	6.76
(1,60)	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	1:34:A:ASN:N	4	6.36	1.45	6.8
(1,17)	1:10:A:LEU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	4	5.74	5.36	2.94
(1,51)	1:28:A:ASP:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	4	5.15	2.1	5.98
(1,42)	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	1:25:A:VAL:N	4	4.68	2.95	3.21
(1,83)	1:46:A:GLY:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	4	4.46	1.66	3.94
(1,171)	1:94:A:GLU:C	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	4	4.25	1.66	3.98
(1,130)	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	1:74:A:VAL:N	4	3.74	2.62	2.96
(1,193)	1:106:A:GLU:C	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	3	29.02	18.31	39.88
(1,179)	1:98:A:GLY:C	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	3	10.68	5.46	11.99
(1,166)	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	1:93:A:SER:N	3	6.88	3.15	5.09
(1,205)	1:113:A:VAL:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	3	6.51	1.87	6.22
(1,157)	1:87:A:SER:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	3	6.14	4.67	4.45
(1,175)	1:96:A:PRO:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	3	5.96	2.85	5.97
(1,188)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:TYR:N	3	5.86	1.2	5.19
(1,127)	1:71:A:LEU:C	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	3	5.79	3.35	4.97
(1,156)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	3	5.72	5.2	2.12
(1,204)	1:113:A:VAL:N	1:113:A:VAL:CA	1:113:A:VAL:C	1:114:A:LEU:N	3	5.7	2.03	5.59
(1,94)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:SER:N	3	3.86	2.0	3.38
(1,81)	1:45:A:ASN:C	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	3	3.77	3.07	2.15
(1,53)	1:29:A:SER:C	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	3	3.68	0.75	3.59
(1,164)	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	1:92:A:ASN:N	3	2.72	1.63	2.06
(1,76)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:VAL:N	2	29.23	3.26	29.23
(1,32)	1:19:A:TYR:N	1:19:A:TYR:CA	1:19:A:TYR:C	1:20:A:LEU:N	2	19.15	11.34	19.15
(1,57)	1:31:A:LYS:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	2	11.94	10.66	11.94
(1,221)	1:123:A:ALA:C	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	2	11.21	3.24	11.21
(1,49)	1:27:A:GLN:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	2	10.71	4.81	10.71
(1,218)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:ALA:N	2	9.71	7.11	9.71
(1,10)	1:7:A:THR:N	1:7:A:THR:CA	1:7:A:THR:C	1:8:A:TYR:N	2	8.49	4.62	8.49
(1,35)	1:20:A:LEU:C	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	2	6.38	1.78	6.38
(1,30)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:TYR:N	2	6.34	1.38	6.34
(1,12)	1:8:A:TYR:N	1:8:A:TYR:CA	1:8:A:TYR:C	1:9:A:LYS:N	2	5.58	0.54	5.58
(1,101)	1:55:A:SER:C	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	2	4.88	3.56	4.88
(1,146)	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	1:83:A:LYS:N	2	4.11	1.86	4.11
(1,15)	1:9:A:LYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	2	4.06	0.15	4.06
(1,122)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	2	3.09	1.51	3.09

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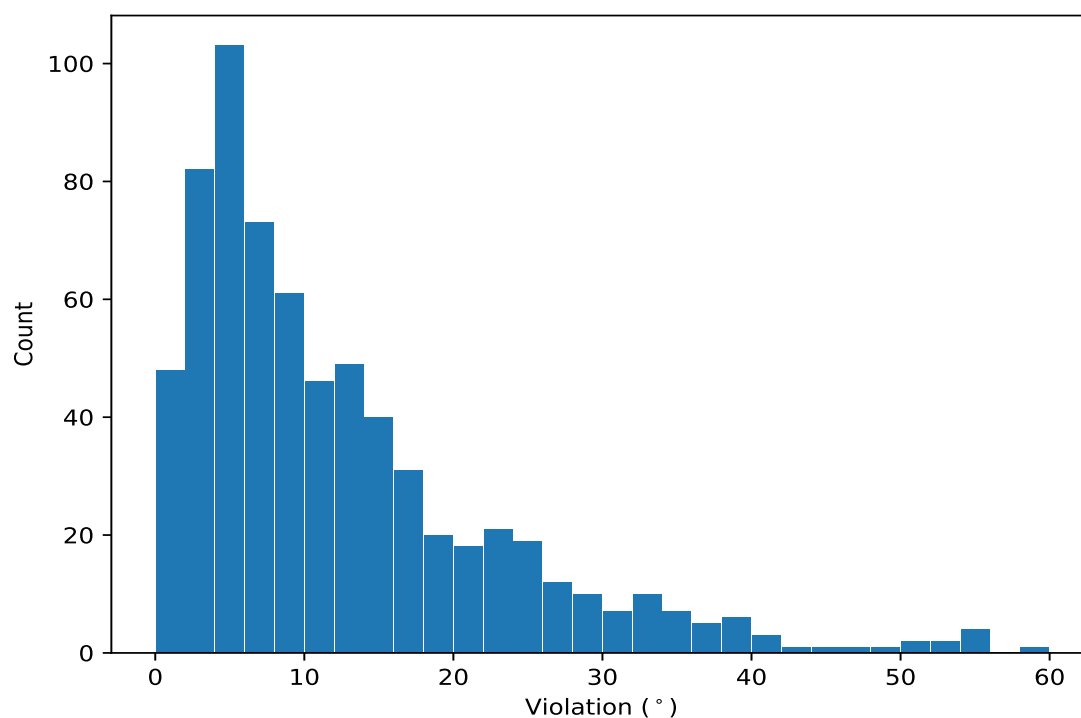
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,210)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:CYS:N	2	2.96	1.7	2.96
(1,115)	1:64:A:ASN:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	2	1.94	0.22	1.94

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 (°)
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	4	59.14
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	8	55.51
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	8	55.48
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	2	54.37
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	3	54.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1	53.38
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	10	52.06
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	5	51.74
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	6	50.78
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	9	49.27
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	5	47.62
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	3	45.72
(1,193)	1:106:A:GLU:C	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	4	43.96
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	6	41.42
(1,41)	1:23:A:LEU:C	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	5	40.25
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	2	40.12
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	1	39.91
(1,193)	1:106:A:GLU:C	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	3	39.88
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	7	39.8
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	6	38.96
(1,70)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	7	38.33
(1,97)	1:53:A:SER:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	3	38.03
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	5	37.08
(1,70)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	9	37.07
(1,201)	1:111:A:GLY:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	9	36.69
(1,202)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	10	36.6
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	10	36.3
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	8	35.44
(1,41)	1:23:A:LEU:C	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	4	35.43
(1,202)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	3	35.35
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	4	34.86
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	5	34.83
(1,202)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	4	34.44
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	5	34.22
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	2	33.86
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	10	33.58
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	6	33.4
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	6	32.56
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1	32.53
(1,76)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:VAL:N	2	32.49
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	4	32.45
(1,202)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	5	32.3
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	7	32.19
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	6	32.09
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1	31.45
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	7	30.94
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	3	30.73
(1,32)	1:19:A:TYR:N	1:19:A:TYR:CA	1:19:A:TYR:C	1:20:A:LEU:N	2	30.49
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	10	30.48
(1,116)	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1:66:A:GLU:N	3	30.29
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	8	30.11
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	6	29.97
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	7	29.3
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	1	29.23
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	8	29.02
(1,100)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLY:N	6	28.98

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	5	28.93
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	4	28.9
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	2	28.19
(1,202)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	8	28.19
(1,8)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:GLY:N	3	28.18
(1,41)	1:23:A:LEU:C	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	6	27.96
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	9	27.83
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	2	27.78
(1,70)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	5	27.74
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	10	27.66
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	5	27.28
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	4	27.27
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	3	27.04
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	9	26.78
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	9	26.64
(1,58)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ALA:N	8	26.43
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	2	26.1
(1,76)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:VAL:N	6	25.97
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	2	25.92
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	3	25.89
(1,70)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	10	25.72
(1,201)	1:111:A:GLY:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1	25.55
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	8	25.54
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	8	25.5
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	6	25.42
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	8	25.04
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	10	24.88
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	3	24.82
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	4	24.56
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	4	24.4
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	6	24.39
(1,131)	1:73:A:THR:C	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	9	24.36
(1,70)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	3	24.31
(1,191)	1:105:A:TYR:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	3	24.25
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	10	24.17
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1	24.05
(1,216)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:MET:N	8	23.99
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	4	23.76
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	10	23.67
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	4	23.54
(1,183)	1:101:A:GLY:C	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	5	23.53
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	8	23.37
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	6	23.03
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	2	23.02
(1,40)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:GLY:N	5	22.93
(1,116)	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1:66:A:GLU:N	6	22.78
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	4	22.74
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	7	22.64
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	8	22.63
(1,57)	1:31:A:LYS:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	8	22.59
(1,58)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ALA:N	5	22.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	10	22.44
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	4	22.37
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	7	22.36
(1,80)	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	1:46:A:GLY:N	8	22.26
(1,40)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:GLY:N	6	22.07
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	9	22.0
(1,208)	1:115:A:THR:N	1:115:A:THR:CA	1:115:A:THR:C	1:116:A:MET:N	5	21.87
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	8	21.63
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1	21.54
(1,131)	1:73:A:THR:C	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	8	21.48
(1,1)	1:1:A:MET:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	1	21.35
(1,116)	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1:66:A:GLU:N	8	21.34
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	3	21.32
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	9	21.28
(1,20)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ASN:N	1	21.19
(1,68)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:TYR:N	8	20.89
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	3	20.88
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	5	20.74
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	1	20.51
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	9	20.4
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	2	20.36
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	10	20.15
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	7	20.08
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	1	20.06
(1,126)	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	1:71:A:LEU:N	5	19.95
(1,126)	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	1:71:A:LEU:N	7	19.93
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	6	19.81
(1,197)	1:108:A:CYS:C	1:109:A:ASP:N	1:109:A:ASP:CA	1:109:A:ASP:C	4	19.78
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	8	19.75
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	6	19.75
(1,59)	1:32:A:LYS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	10	19.59
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	2	19.52
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	5	19.37
(1,135)	1:75:A:ASN:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	7	19.29
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	1	19.04
(1,126)	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	1:71:A:LEU:N	8	18.84
(1,194)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:CYS:N	4	18.69
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	3	18.69
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	3	18.51
(1,208)	1:115:A:THR:N	1:115:A:THR:CA	1:115:A:THR:C	1:116:A:MET:N	10	18.49
(1,163)	1:90:A:VAL:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	2	18.45
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	5	18.36
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	8	18.29
(1,177)	1:97:A:ASP:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	10	18.23
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	7	17.85
(1,58)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ALA:N	10	17.73
(1,3)	1:2:A:VAL:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	9	17.72
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	2	17.71
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1	17.6
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	10	17.58
(1,59)	1:32:A:LYS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	8	17.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	8	17.33
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	1	17.22
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	3	17.21
(1,202)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	7	17.2
(1,126)	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	1:71:A:LEU:N	10	17.2
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	2	17.19
(1,98)	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1:55:A:SER:N	2	17.16
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	5	17.05
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	10	16.96
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	10	16.94
(1,8)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:GLY:N	4	16.9
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	2	16.88
(1,218)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:ALA:N	9	16.82
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	9	16.81
(1,179)	1:98:A:GLY:C	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	3	16.61
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	9	16.55
(1,68)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:TYR:N	2	16.53
(1,191)	1:105:A:TYR:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	6	16.41
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	10	16.3
(1,177)	1:97:A:ASP:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	9	16.26
(1,131)	1:73:A:THR:C	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	2	16.25
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	9	16.18
(1,65)	1:37:A:GLY:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	10	16.14
(1,40)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:GLY:N	4	16.05
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	2	15.97
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	4	15.96
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	7	15.89
(1,65)	1:37:A:GLY:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	4	15.79
(1,160)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:90:A:VAL:N	6	15.76
(1,100)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLY:N	4	15.75
(1,59)	1:32:A:LYS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	2	15.69
(1,102)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:MET:N	9	15.64
(1,49)	1:27:A:GLN:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	9	15.52
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	9	15.51
(1,68)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:TYR:N	4	15.5
(1,134)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:MET:N	4	15.41
(1,86)	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1:49:A:PHE:N	10	15.4
(1,206)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:THR:N	8	15.38
(1,3)	1:2:A:VAL:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	7	15.38
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	1	15.35
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	2	15.32
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	3	15.25
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	1	15.12
(1,217)	1:121:A:MET:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	7	15.06
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	10	15.03
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	1	14.98
(1,17)	1:10:A:LEU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	6	14.98
(1,177)	1:97:A:ASP:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1	14.94
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	8	14.9
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	5	14.83
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	9	14.75

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	7	14.73
(1,147)	1:82:A:THR:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	1	14.72
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	6	14.71
(1,135)	1:75:A:ASN:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	4	14.55
(1,70)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	4	14.51
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	7	14.46
(1,221)	1:123:A:ALA:C	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	8	14.45
(1,192)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:PHE:N	10	14.3
(1,80)	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	1:46:A:GLY:N	1	14.22
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	5	14.21
(1,135)	1:75:A:ASN:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	2	14.13
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	4	14.12
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	4	14.01
(1,80)	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	1:46:A:GLY:N	5	13.92
(1,230)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ARG:N	8	13.85
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	5	13.84
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	6	13.76
(1,71)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	9	13.73
(1,184)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:ARG:N	2	13.64
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	5	13.63
(1,79)	1:44:A:VAL:C	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	9	13.61
(1,116)	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1:66:A:GLU:N	9	13.53
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	6	13.39
(1,8)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:GLY:N	6	13.33
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	6	13.3
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	7	13.28
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	6	13.28
(1,219)	1:122:A:VAL:C	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	1	13.25
(1,1)	1:1:A:MET:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	4	13.25
(1,65)	1:37:A:GLY:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	2	13.14
(1,10)	1:7:A:THR:N	1:7:A:THR:CA	1:7:A:THR:C	1:8:A:TYR:N	4	13.12
(1,156)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	3	13.07
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	4	13.06
(1,178)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	2	12.99
(1,109)	1:59:A:SER:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	1	12.98
(1,73)	1:41:A:GLU:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	8	12.98
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	2	12.97
(1,50)	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	1:29:A:SER:N	2	12.8
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	2	12.74
(1,147)	1:82:A:THR:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	7	12.74
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	10	12.71
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	5	12.68
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	9	12.67
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	10	12.65
(1,74)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:ILE:N	6	12.54
(1,119)	1:66:A:GLU:C	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	7	12.52
(1,157)	1:87:A:SER:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	3	12.51
(1,163)	1:90:A:VAL:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	10	12.49
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	9	12.45
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	3	12.31
(1,178)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	1	12.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:32:A:LYS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	7	12.26
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	1	12.23
(1,58)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ALA:N	2	12.23
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	8	12.17
(1,165)	1:91:A:VAL:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	5	12.17
(1,84)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	5	12.12
(1,102)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:MET:N	7	12.1
(1,211)	1:116:A:MET:C	1:117:A:CYS:N	1:117:A:CYS:CA	1:117:A:CYS:C	6	12.03
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	9	12.03
(1,147)	1:82:A:THR:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	5	12.01
(1,100)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLY:N	9	12.01
(1,179)	1:98:A:GLY:C	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	9	11.99
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	6	11.77
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	10	11.72
(1,56)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:LYS:N	3	11.71
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	3	11.69
(1,208)	1:115:A:THR:N	1:115:A:THR:CA	1:115:A:THR:C	1:116:A:MET:N	9	11.67
(1,230)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ARG:N	6	11.56
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	10	11.55
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	8	11.5
(1,201)	1:111:A:GLY:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	2	11.43
(1,166)	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	1:93:A:SER:N	10	11.31
(1,3)	1:2:A:VAL:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	2	11.27
(1,102)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:MET:N	10	11.23
(1,191)	1:105:A:TYR:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	8	11.17
(1,224)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:TYR:N	9	11.14
(1,67)	1:38:A:VAL:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	5	10.99
(1,59)	1:32:A:LYS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	5	10.97
(1,50)	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	1:29:A:SER:N	9	10.97
(1,50)	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	1:29:A:SER:N	10	10.9
(1,1)	1:1:A:MET:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	8	10.87
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	8	10.82
(1,206)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:THR:N	10	10.8
(1,109)	1:59:A:SER:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	6	10.77
(1,165)	1:91:A:VAL:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	8	10.73
(1,192)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:PHE:N	9	10.69
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1	10.61
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	9	10.59
(1,214)	1:118:A:ALA:N	1:118:A:ALA:CA	1:118:A:ALA:C	1:119:A:GLY:N	7	10.5
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	1	10.38
(1,109)	1:59:A:SER:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	3	10.34
(1,163)	1:90:A:VAL:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	9	10.31
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	1	10.29
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	3	10.29
(1,127)	1:71:A:LEU:C	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	6	10.25
(1,128)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:THR:N	7	10.23
(1,56)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:LYS:N	8	10.23
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	7	10.22
(1,184)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:ARG:N	9	10.19
(1,58)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ALA:N	6	10.19
(1,28)	1:17:A:GLU:N	1:17:A:GLU:CA	1:17:A:GLU:C	1:18:A:GLU:N	2	10.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,109)	1:59:A:SER:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	10	10.11
(1,217)	1:121:A:MET:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	2	10.07
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	3	10.07
(1,13)	1:8:A:TYR:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	4	10.06
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	6	10.05
(1,165)	1:91:A:VAL:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	10	10.04
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	8	9.99
(1,208)	1:115:A:THR:N	1:115:A:THR:CA	1:115:A:THR:C	1:116:A:MET:N	7	9.91
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	4	9.89
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	9	9.87
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	4	9.85
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	10	9.84
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	2	9.81
(1,135)	1:75:A:ASN:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	5	9.81
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	9	9.8
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	7	9.79
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	2	9.76
(1,119)	1:66:A:GLU:C	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	6	9.74
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1	9.73
(1,42)	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	1:25:A:VAL:N	2	9.71
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	7	9.66
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	10	9.6
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	8	9.56
(1,206)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:THR:N	7	9.51
(1,56)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:LYS:N	1	9.5
(1,175)	1:96:A:PRO:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	6	9.44
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	7	9.42
(1,163)	1:90:A:VAL:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	4	9.4
(1,71)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	7	9.37
(1,230)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ARG:N	2	9.34
(1,84)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	6	9.28
(1,72)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:ILE:N	7	9.26
(1,1)	1:1:A:MET:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	10	9.22
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	4	9.15
(1,100)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLY:N	10	9.12
(1,134)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:MET:N	7	9.07
(1,184)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:ARG:N	4	9.06
(1,134)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:MET:N	3	9.06
(1,205)	1:113:A:VAL:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	7	8.93
(1,24)	1:14:A:GLU:N	1:14:A:GLU:CA	1:14:A:GLU:C	1:15:A:ASN:N	2	8.89
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	6	8.86
(1,195)	1:107:A:PHE:C	1:108:A:CYS:N	1:108:A:CYS:CA	1:108:A:CYS:C	5	8.85
(1,77)	1:43:A:ILE:C	1:44:A:VAL:N	1:44:A:VAL:CA	1:44:A:VAL:C	2	8.84
(1,192)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:PHE:N	6	8.81
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	2	8.8
(1,65)	1:37:A:GLY:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1	8.76
(1,74)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:ILE:N	7	8.61
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	2	8.6
(1,79)	1:44:A:VAL:C	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	4	8.51
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	4	8.5
(1,101)	1:55:A:SER:C	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	8	8.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:GLY:N	10	8.41
(1,84)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	1	8.39
(1,65)	1:37:A:GLY:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	9	8.39
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	10	8.32
(1,116)	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1:66:A:GLU:N	10	8.32
(1,86)	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1:49:A:PHE:N	5	8.32
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	6	8.25
(1,204)	1:113:A:VAL:N	1:113:A:VAL:CA	1:113:A:VAL:C	1:114:A:LEU:N	4	8.24
(1,134)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:MET:N	2	8.23
(1,109)	1:59:A:SER:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	2	8.22
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	8	8.19
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	4	8.17
(1,35)	1:20:A:LEU:C	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	2	8.16
(1,71)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	10	8.07
(1,81)	1:45:A:ASN:C	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	7	8.06
(1,160)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:90:A:VAL:N	1	8.02
(1,221)	1:123:A:ALA:C	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	10	7.97
(1,79)	1:44:A:VAL:C	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	7	7.97
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	6	7.94
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	8	7.94
(1,106)	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	1:59:A:SER:N	9	7.93
(1,60)	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	1:34:A:ASN:N	6	7.87
(1,216)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:MET:N	5	7.86
(1,130)	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	1:74:A:VAL:N	9	7.85
(1,32)	1:19:A:TYR:N	1:19:A:TYR:CA	1:19:A:TYR:C	1:20:A:LEU:N	3	7.81
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	3	7.71
(1,134)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:MET:N	5	7.71
(1,30)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:TYR:N	7	7.71
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	6	7.71
(1,206)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:THR:N	3	7.65
(1,177)	1:97:A:ASP:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	6	7.63
(1,187)	1:103:A:ARG:C	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	2	7.61
(1,188)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:TYR:N	1	7.54
(1,206)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:THR:N	9	7.48
(1,165)	1:91:A:VAL:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	1	7.46
(1,74)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:ILE:N	3	7.45
(1,3)	1:2:A:VAL:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	6	7.41
(1,208)	1:115:A:THR:N	1:115:A:THR:CA	1:115:A:THR:C	1:116:A:MET:N	8	7.38
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	10	7.37
(1,77)	1:43:A:ILE:C	1:44:A:VAL:N	1:44:A:VAL:CA	1:44:A:VAL:C	4	7.36
(1,119)	1:66:A:GLU:C	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	3	7.3
(1,219)	1:122:A:VAL:C	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	9	7.29
(1,13)	1:8:A:TYR:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	3	7.24
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	2	7.22
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	8	7.2
(1,160)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:90:A:VAL:N	3	7.18
(1,83)	1:46:A:GLY:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	9	7.17
(1,224)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:TYR:N	6	7.11
(1,185)	1:102:A:THR:C	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	9	7.06
(1,60)	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	1:34:A:ASN:N	2	6.99
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	10	6.98

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,51)	1:28:A:ASP:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	2	6.9
(1,103)	1:56:A:GLY:C	1:57:A:MET:N	1:57:A:MET:CA	1:57:A:MET:C	1	6.89
(1,80)	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	1:46:A:GLY:N	3	6.89
(1,51)	1:28:A:ASP:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	4	6.86
(1,219)	1:122:A:VAL:C	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	8	6.78
(1,165)	1:91:A:VAL:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	9	6.76
(1,140)	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1:80:A:SER:N	10	6.76
(1,68)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:TYR:N	9	6.7
(1,34)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:ALA:N	2	6.68
(1,86)	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1:49:A:PHE:N	1	6.67
(1,224)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:TYR:N	8	6.66
(1,171)	1:94:A:GLU:C	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	9	6.6
(1,60)	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	1:34:A:ASN:N	9	6.6
(1,220)	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	1:124:A:LYS:N	1	6.55
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	4	6.55
(1,148)	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	1:84:A:LEU:N	7	6.55
(1,160)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:90:A:VAL:N	8	6.53
(1,94)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:SER:N	4	6.51
(1,41)	1:23:A:LEU:C	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	7	6.48
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	3	6.38
(1,102)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:MET:N	3	6.38
(1,191)	1:105:A:TYR:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	7	6.37
(1,69)	1:39:A:VAL:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	8	6.34
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	3	6.32
(1,177)	1:97:A:ASP:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	4	6.32
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	7	6.3
(1,71)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	3	6.3
(1,117)	1:65:A:GLU:C	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	3	6.28
(1,205)	1:113:A:VAL:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	2	6.22
(1,136)	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	1:77:A:ASN:N	7	6.22
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	2	6.2
(1,141)	1:79:A:LYS:C	1:80:A:SER:N	1:80:A:SER:CA	1:80:A:SER:C	10	6.19
(1,77)	1:43:A:ILE:C	1:44:A:VAL:N	1:44:A:VAL:CA	1:44:A:VAL:C	1	6.17
(1,230)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ARG:N	5	6.15
(1,58)	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1:33:A:ALA:N	7	6.14
(1,12)	1:8:A:TYR:N	1:8:A:TYR:CA	1:8:A:TYR:C	1:9:A:LYS:N	4	6.12
(1,184)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:ARG:N	5	6.05
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	8	6.0
(1,175)	1:96:A:PRO:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	9	5.97
(1,146)	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	1:83:A:LYS:N	1	5.96
(1,80)	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	1:46:A:GLY:N	10	5.96
(1,13)	1:8:A:TYR:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1	5.96
(1,191)	1:105:A:TYR:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	4	5.94
(1,211)	1:116:A:MET:C	1:117:A:CYS:N	1:117:A:CYS:CA	1:117:A:CYS:C	2	5.91
(1,49)	1:27:A:GLN:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	10	5.9
(1,190)	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	1:106:A:GLU:N	5	5.89
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	6	5.86
(1,123)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	9	5.85
(1,230)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ARG:N	9	5.84
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	10	5.83
(1,3)	1:2:A:VAL:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	3	5.82

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,202)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	6	5.78
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	10	5.77
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	4	5.76
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	1	5.73
(1,131)	1:73:A:THR:C	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	3	5.7
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	5	5.69
(1,45)	1:25:A:VAL:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	2	5.67
(1,178)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	6	5.66
(1,116)	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1:66:A:GLU:N	1	5.64
(1,165)	1:91:A:VAL:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	3	5.62
(1,181)	1:99:A:ARG:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	5	5.6
(1,64)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:VAL:N	4	5.6
(1,204)	1:113:A:VAL:N	1:113:A:VAL:CA	1:113:A:VAL:C	1:114:A:LEU:N	2	5.59
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	4	5.59
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	9	5.56
(1,211)	1:116:A:MET:C	1:117:A:CYS:N	1:117:A:CYS:CA	1:117:A:CYS:C	8	5.53
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	3	5.51
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	2	5.51
(1,55)	1:30:A:ILE:C	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	5	5.5
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	6	5.45
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	2	5.43
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	9	5.42
(1,9)	1:6:A:GLY:C	1:7:A:THR:N	1:7:A:THR:CA	1:7:A:THR:C	9	5.42
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	5	5.33
(1,100)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLY:N	2	5.33
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	1	5.31
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	9	5.3
(1,79)	1:44:A:VAL:C	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	3	5.3
(1,16)	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	1:11:A:GLU:N	6	5.3
(1,119)	1:66:A:GLU:C	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1	5.27
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	4	5.26
(1,188)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:TYR:N	5	5.19
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	2	5.16
(1,51)	1:28:A:ASP:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	9	5.11
(1,166)	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	1:93:A:SER:N	3	5.09
(1,12)	1:8:A:TYR:N	1:8:A:TYR:CA	1:8:A:TYR:C	1:9:A:LYS:N	1	5.04
(1,1)	1:1:A:MET:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	6	5.02
(1,171)	1:94:A:GLU:C	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	10	4.99
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	4	4.98
(1,127)	1:71:A:LEU:C	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	9	4.97
(1,168)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:GLU:N	7	4.96
(1,164)	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	1:92:A:ASN:N	10	4.96
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	4	4.96
(1,30)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:TYR:N	2	4.96
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	10	4.94
(1,223)	1:124:A:LYS:C	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	6	4.88
(1,131)	1:73:A:THR:C	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	5	4.88
(1,188)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:TYR:N	3	4.85
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	7	4.84
(1,7)	1:4:A:LEU:C	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	7	4.8
(1,123)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	1	4.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	3	4.71
(1,116)	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1:66:A:GLU:N	5	4.7
(1,210)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:CYS:N	6	4.65
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	4	4.64
(1,1)	1:1:A:MET:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	2	4.64
(1,215)	1:119:A:GLY:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	8	4.63
(1,53)	1:29:A:SER:C	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	5	4.63
(1,191)	1:105:A:TYR:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	9	4.62
(1,122)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	2	4.6
(1,35)	1:20:A:LEU:C	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	8	4.6
(1,79)	1:44:A:VAL:C	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	2	4.5
(1,219)	1:122:A:VAL:C	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	10	4.48
(1,119)	1:66:A:GLU:C	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	4	4.48
(1,84)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	10	4.47
(1,157)	1:87:A:SER:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	7	4.45
(1,184)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:ARG:N	7	4.43
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	6	4.42
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	10	4.4
(1,205)	1:113:A:VAL:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	3	4.39
(1,83)	1:46:A:GLY:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	2	4.33
(1,192)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:PHE:N	5	4.3
(1,191)	1:105:A:TYR:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	10	4.27
(1,166)	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	1:93:A:SER:N	2	4.24
(1,85)	1:47:A:ASN:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	7	4.23
(1,3)	1:2:A:VAL:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	1	4.23
(1,15)	1:9:A:LYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	8	4.22
(1,224)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:TYR:N	5	4.18
(1,142)	1:80:A:SER:N	1:80:A:SER:CA	1:80:A:SER:C	1:81:A:PHE:N	7	4.18
(1,123)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	4	4.17
(1,130)	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	1:74:A:VAL:N	2	4.16
(1,123)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	10	4.16
(1,59)	1:32:A:LYS:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	6	4.15
(1,192)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:PHE:N	2	4.11
(1,222)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:ARG:N	1	4.08
(1,137)	1:77:A:ASN:C	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	7	4.03
(1,206)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:THR:N	5	4.02
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	1	4.01
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	1	4.0
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	5	4.0
(1,60)	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	1:34:A:ASN:N	5	3.97
(1,40)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:GLY:N	2	3.93
(1,56)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:LYS:N	2	3.91
(1,15)	1:9:A:LYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	9	3.91
(1,216)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:MET:N	6	3.9
(1,10)	1:7:A:THR:N	1:7:A:THR:CA	1:7:A:THR:C	1:8:A:TYR:N	6	3.87
(1,52)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:ILE:N	5	3.84
(1,42)	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	1:25:A:VAL:N	4	3.82
(1,134)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:MET:N	6	3.8
(1,152)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLY:N	2	3.74
(1,68)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:TYR:N	3	3.73
(1,100)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLY:N	7	3.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,126)	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	1:71:A:LEU:N	2	3.63
(1,126)	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	1:71:A:LEU:N	4	3.62
(1,147)	1:82:A:THR:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	3	3.61
(1,53)	1:29:A:SER:C	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	1	3.59
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	7	3.58
(1,83)	1:46:A:GLY:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1	3.54
(1,77)	1:43:A:ILE:C	1:44:A:VAL:N	1:44:A:VAL:CA	1:44:A:VAL:C	9	3.52
(1,230)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ARG:N	10	3.51
(1,102)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:MET:N	4	3.46
(1,179)	1:98:A:GLY:C	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	4	3.44
(1,140)	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1:80:A:SER:N	6	3.44
(1,17)	1:10:A:LEU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1	3.44
(1,207)	1:114:A:LEU:C	1:115:A:THR:N	1:115:A:THR:CA	1:115:A:THR:C	8	3.4
(1,94)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:SER:N	1	3.38
(1,224)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:TYR:N	2	3.37
(1,147)	1:82:A:THR:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	6	3.36
(1,121)	1:67:A:VAL:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	9	3.35
(1,180)	1:99:A:ARG:N	1:99:A:ARG:CA	1:99:A:ARG:C	1:100:A:LYS:N	9	3.33
(1,8)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:GLY:N	7	3.33
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	9	3.31
(1,204)	1:113:A:VAL:N	1:113:A:VAL:CA	1:113:A:VAL:C	1:114:A:LEU:N	3	3.26
(1,165)	1:91:A:VAL:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	4	3.26
(1,140)	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1:80:A:SER:N	3	3.24
(1,193)	1:106:A:GLU:C	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	6	3.23
(1,184)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:ARG:N	10	3.11
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	1	3.06
(1,50)	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	1:29:A:SER:N	4	3.04
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	5	3.02
(1,171)	1:94:A:GLU:C	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	6	2.97
(1,13)	1:8:A:TYR:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	5	2.94
(1,102)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:MET:N	6	2.9
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	9	2.87
(1,140)	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1:80:A:SER:N	7	2.82
(1,53)	1:29:A:SER:C	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	7	2.81
(1,83)	1:46:A:GLY:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	3	2.79
(1,201)	1:111:A:GLY:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	3	2.77
(1,154)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:SER:N	7	2.72
(1,74)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:ILE:N	8	2.67
(1,224)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:TYR:N	10	2.65
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	5	2.63
(1,218)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:ALA:N	1	2.6
(1,42)	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	1:25:A:VAL:N	6	2.6
(1,42)	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	1:25:A:VAL:N	9	2.58
(1,41)	1:23:A:LEU:C	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	1	2.57
(1,82)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:ASN:N	10	2.55
(1,145)	1:81:A:PHE:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	8	2.49
(1,211)	1:116:A:MET:C	1:117:A:CYS:N	1:117:A:CYS:CA	1:117:A:CYS:C	7	2.48
(1,216)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:MET:N	2	2.47
(1,175)	1:96:A:PRO:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	4	2.46
(1,17)	1:10:A:LEU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	8	2.45
(1,171)	1:94:A:GLU:C	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	5	2.43

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	1	2.42
(1,3)	1:2:A:VAL:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	5	2.41
(1,86)	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1:49:A:PHE:N	9	2.39
(1,144)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	8	2.35
(1,146)	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	1:83:A:LYS:N	7	2.25
(1,140)	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1:80:A:SER:N	1	2.24
(1,134)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:MET:N	9	2.23
(1,160)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:90:A:VAL:N	4	2.19
(1,176)	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	1:98:A:GLY:N	9	2.16
(1,127)	1:71:A:LEU:C	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	7	2.16
(1,115)	1:64:A:ASN:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1	2.16
(1,81)	1:45:A:ASN:C	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	2	2.15
(1,163)	1:90:A:VAL:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	6	2.14
(1,156)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	9	2.12
(1,161)	1:89:A:LEU:C	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	4	2.08
(1,17)	1:10:A:LEU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	9	2.07
(1,164)	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	1:92:A:ASN:N	5	2.06
(1,14)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	7	2.06
(1,56)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:LYS:N	5	2.03
(1,156)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	1	1.98
(1,102)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:MET:N	5	1.97
(1,230)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ARG:N	7	1.96
(1,162)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:VAL:N	5	1.89
(1,163)	1:90:A:VAL:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	7	1.88
(1,125)	1:69:A:GLU:C	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	3	1.83
(1,216)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:MET:N	3	1.8
(1,93)	1:51:A:PHE:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	10	1.8
(1,132)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:ASN:N	5	1.79
(1,89)	1:49:A:PHE:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	7	1.78
(1,74)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:ILE:N	4	1.77
(1,130)	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	1:74:A:VAL:N	8	1.76
(1,41)	1:23:A:LEU:C	1:24:A:GLY:N	1:24:A:GLY:CA	1:24:A:GLY:C	10	1.75
(1,115)	1:64:A:ASN:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	8	1.73
(1,51)	1:28:A:ASP:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	10	1.73
(1,94)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:SER:N	5	1.68
(1,92)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:LYS:N	8	1.65
(1,211)	1:116:A:MET:C	1:117:A:CYS:N	1:117:A:CYS:CA	1:117:A:CYS:C	4	1.64
(1,80)	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	1:46:A:GLY:N	4	1.62
(1,6)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:ALA:N	1	1.61
(1,122)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	4	1.58
(1,217)	1:121:A:MET:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	6	1.57
(1,119)	1:66:A:GLU:C	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	10	1.46
(1,157)	1:87:A:SER:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	6	1.45
(1,79)	1:44:A:VAL:C	1:45:A:ASN:N	1:45:A:ASN:CA	1:45:A:ASN:C	10	1.43
(1,140)	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1:80:A:SER:N	9	1.39
(1,177)	1:97:A:ASP:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	8	1.37
(1,178)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ARG:N	10	1.33
(1,101)	1:55:A:SER:C	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	5	1.32
(1,217)	1:121:A:MET:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	3	1.29
(1,57)	1:31:A:LYS:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	3	1.28
(1,210)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:CYS:N	2	1.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,71)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	5	1.26
(1,68)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:TYR:N	5	1.26
(1,123)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	5	1.25
(1,217)	1:121:A:MET:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	5	1.23
(1,130)	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	1:74:A:VAL:N	5	1.2
(1,225)	1:125:A:ARG:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	7	1.14
(1,169)	1:93:A:SER:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	5	1.13
(1,164)	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	1:92:A:ASN:N	9	1.13
(1,129)	1:72:A:GLY:C	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	10	1.12
(1,81)	1:45:A:ASN:C	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	9	1.09
(1,160)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:90:A:VAL:N	5	1.06
(1,5)	1:3:A:GLN:C	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	2	1.06
(1,172)	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	1:96:A:PRO:N	9	1.05
(1,167)	1:92:A:ASN:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	8	1.04
(1,109)	1:59:A:SER:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	8	1.0
(1,13)	1:8:A:TYR:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	7	1.0