



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:28 AM UTC

PDB ID : 9CUV / pdb_00009cuv
BMRB ID : 27141
Title : Solution Structure of the N-terminal signalling domain of Pseudomonas cap-
ferrum PupB
Authors : Morgan, D.M.; Sultana, T.; Colbert, C.L.
Deposited on : 2024-07-26

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

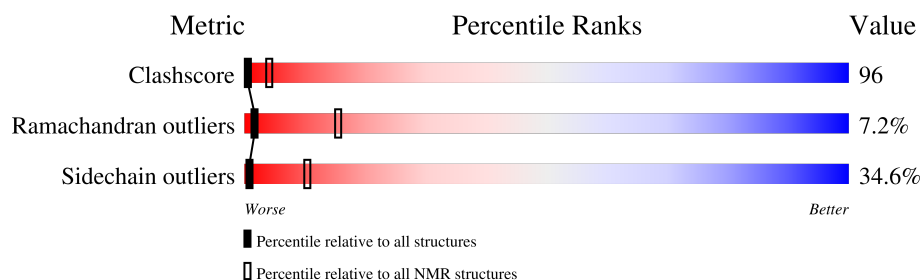
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	82	18% 52% 26% .

2 Ensemble composition and analysis

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

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:4-A:82 (79)	0.69	4

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1131 atoms, of which 559 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PupB N-terminal Signaling Domain.

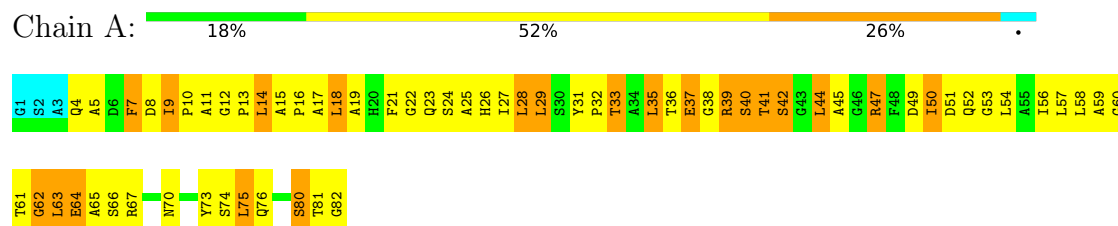
Mol	Chain	Residues	Atoms					Trace
1	A	82	Total	C	H	N	O	0
			1131	355	559	100	117	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: PupB N-terminal Signaling Domain

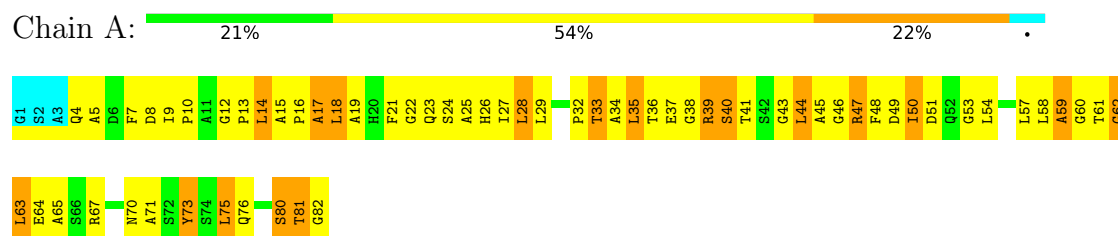


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

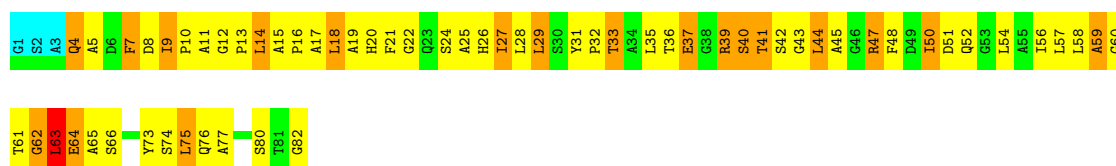
- Molecule 1: PupB N-terminal Signaling Domain



4.2.2 Score per residue for model 2

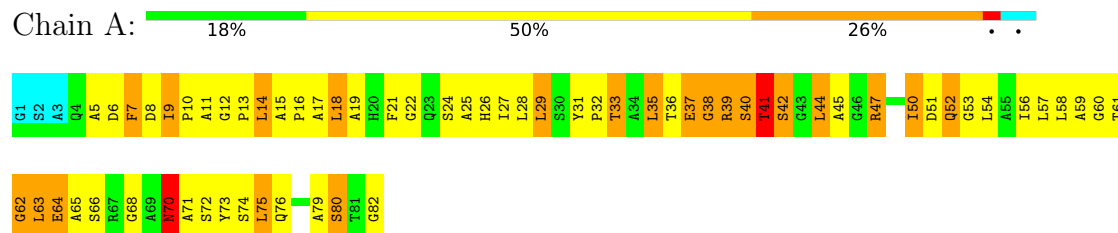
- Molecule 1: PupB N-terminal Signaling Domain





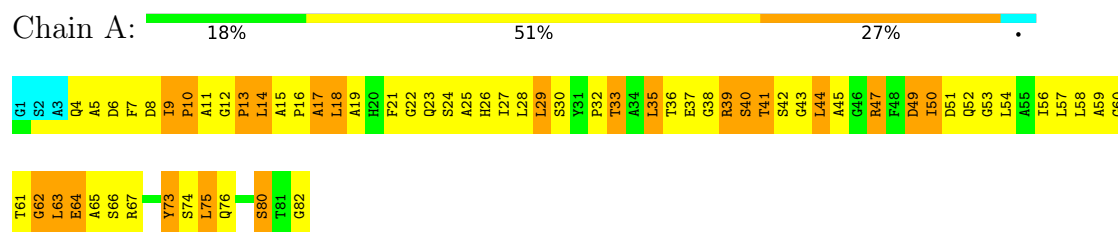
4.2.3 Score per residue for model 3

- Molecule 1: PupB N-terminal Signaling Domain



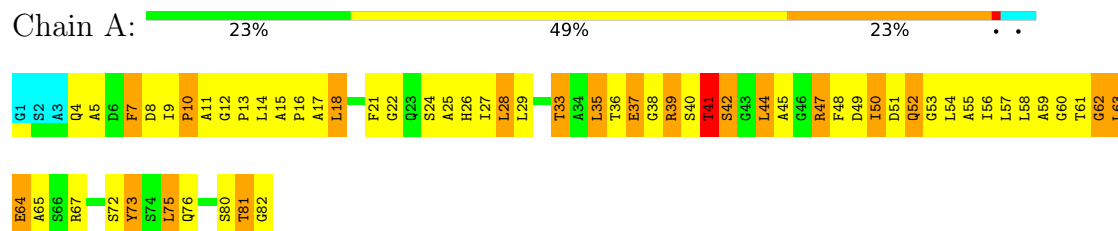
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: PupB N-terminal Signaling Domain



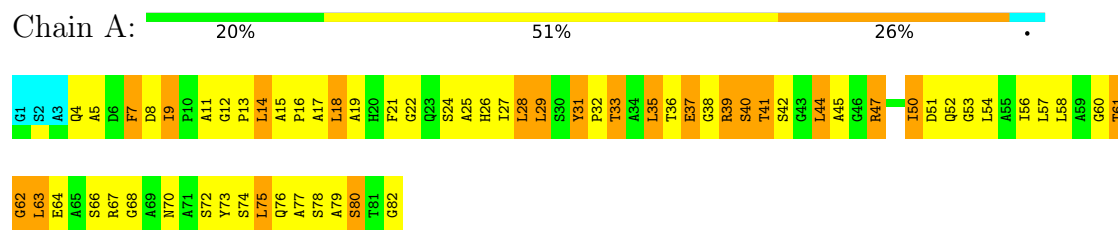
4.2.5 Score per residue for model 5

- Molecule 1: PupB N-terminal Signaling Domain



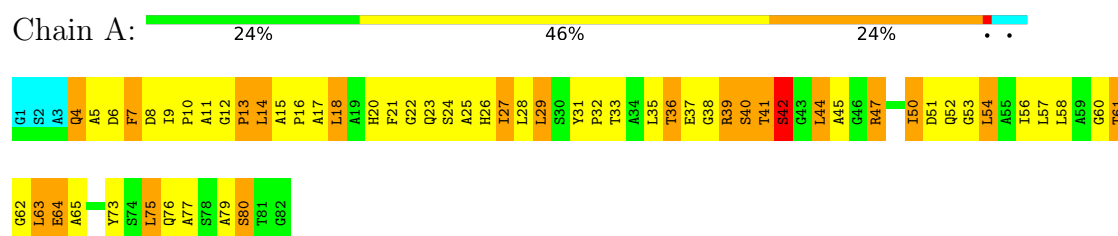
4.2.6 Score per residue for model 6

- Molecule 1: PupB N-terminal Signaling Domain



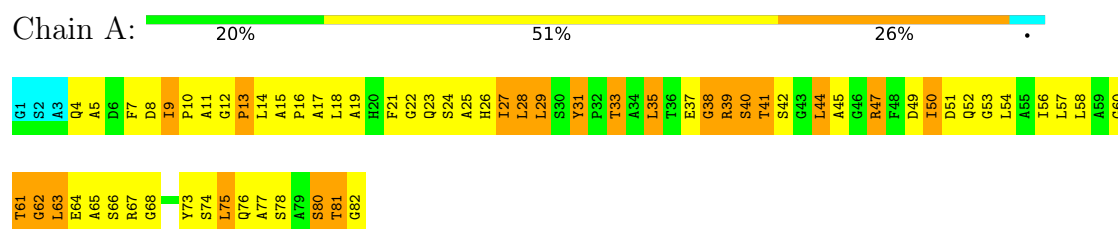
4.2.7 Score per residue for model 7

- Molecule 1: PupB N-terminal Signaling Domain



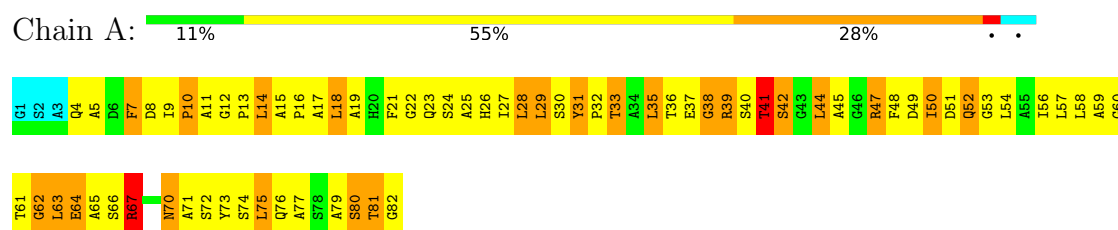
4.2.8 Score per residue for model 8

- Molecule 1: PupB N-terminal Signaling Domain



4.2.9 Score per residue for model 9

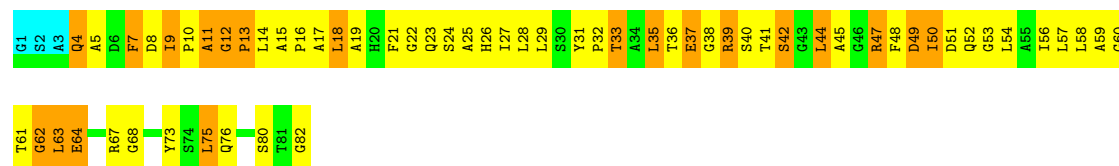
- Molecule 1: PupB N-terminal Signaling Domain



4.2.10 Score per residue for model 10

- Molecule 1: PupB N-terminal Signaling Domain

Chain A: 22% 50% 24% .



5 Refinement protocol and experimental data overview

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

Of the 50 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
CNSSOLVE	refinement	1.2
ARIA	structure calculation	2

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	884
Number of shifts mapped to atoms	884
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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	0.90±0.03	0±0/567 (0.0± 0.1%)	1.08±0.03	2±1/770 (0.3± 0.1%)
All	All	0.90	1/5670 (0.0%)	1.08	22/7700 (0.3%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	42	SER	N-CA	-5.15	1.39	1.46	7	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	33	THR	N-CA-C	-7.97	102.19	112.23	9	10
1	A	17	ALA	N-CA-C	-5.79	105.10	111.82	4	2
1	A	41	THR	CA-C-N	-5.73	115.11	122.79	9	3
1	A	41	THR	C-N-CA	-5.73	115.11	122.79	9	3
1	A	63	LEU	N-CA-C	5.32	117.35	109.69	2	1
1	A	61	THR	N-CA-C	5.16	117.02	107.73	8	3

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	557	544	542	106±10
All	All	5570	5440	5420	1058

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 96.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:HD12	1:A:29:LEU:HD11	1.07	1.23	4	8
1:A:18:LEU:HD13	1:A:29:LEU:HD12	0.89	1.42	8	1
1:A:15:ALA:HB2	1:A:36:THR:HB	0.88	1.46	6	8
1:A:54:LEU:HG	1:A:58:LEU:HD12	0.87	1.47	4	6
1:A:11:ALA:HA	1:A:42:SER:HA	0.86	1.42	10	9
1:A:59:ALA:O	1:A:61:THR:N	0.85	2.10	10	7
1:A:44:LEU:HB2	1:A:57:LEU:HD13	0.84	1.46	1	2
1:A:14:LEU:HD23	1:A:41:THR:HG21	0.84	1.49	1	2
1:A:61:THR:O	1:A:63:LEU:N	0.83	2.12	8	10
1:A:9:ILE:HG21	1:A:57:LEU:HD11	0.79	1.54	10	9
1:A:27:ILE:HG13	1:A:29:LEU:HD21	0.79	1.53	5	8
1:A:18:LEU:CD1	1:A:29:LEU:HD12	0.78	2.08	8	1
1:A:75:LEU:HD13	1:A:76:GLN:H	0.78	1.37	1	1
1:A:29:LEU:HD22	1:A:29:LEU:N	0.78	1.93	9	8
1:A:17:ALA:HB1	1:A:57:LEU:HD11	0.76	1.54	9	10
1:A:32:PRO:O	1:A:36:THR:HG23	0.76	1.79	2	7
1:A:44:LEU:CB	1:A:57:LEU:HD13	0.76	2.11	10	8
1:A:73:TYR:CD2	1:A:73:TYR:C	0.74	2.65	1	1
1:A:11:ALA:C	1:A:41:THR:O	0.73	2.31	10	1
1:A:15:ALA:HB3	1:A:16:PRO:HD3	0.72	1.60	5	10
1:A:73:TYR:CZ	1:A:75:LEU:HD23	0.71	2.20	1	1
1:A:67:ARG:HA	1:A:73:TYR:HB2	0.70	1.61	9	2
1:A:28:LEU:C	1:A:29:LEU:HD22	0.70	2.11	5	7
1:A:21:PHE:CE1	1:A:54:LEU:HD22	0.70	2.20	5	1
1:A:44:LEU:HB2	1:A:57:LEU:CD1	0.70	2.15	1	6
1:A:14:LEU:HD12	1:A:39:ARG:CZ	0.70	2.17	7	2
1:A:39:ARG:HD3	1:A:63:LEU:HD21	0.70	1.63	10	4
1:A:28:LEU:C	1:A:29:LEU:HD13	0.69	2.13	4	7
1:A:54:LEU:O	1:A:58:LEU:HB2	0.68	1.89	2	8
1:A:44:LEU:HB3	1:A:57:LEU:HD13	0.67	1.65	10	8
1:A:29:LEU:HD12	1:A:73:TYR:CD2	0.67	2.25	4	2
1:A:73:TYR:CD1	1:A:73:TYR:C	0.67	2.71	5	2
1:A:29:LEU:HA	1:A:73:TYR:O	0.67	1.90	3	6
1:A:18:LEU:HD13	1:A:57:LEU:HD23	0.67	1.65	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:HD12	1:A:75:LEU:HD22	0.67	1.64	7	1
1:A:28:LEU:O	1:A:29:LEU:HD13	0.67	1.89	1	8
1:A:73:TYR:OH	1:A:75:LEU:HD23	0.66	1.89	1	2
1:A:58:LEU:HD11	1:A:65:ALA:HB3	0.66	1.65	9	1
1:A:54:LEU:CG	1:A:58:LEU:HD12	0.66	2.20	4	1
1:A:38:GLY:HA3	1:A:39:ARG:HH21	0.66	1.50	6	3
1:A:14:LEU:HG	1:A:63:LEU:HD12	0.65	1.68	1	1
1:A:39:ARG:HD2	1:A:63:LEU:HD11	0.65	1.69	7	2
1:A:7:PHE:C	1:A:45:ALA:HA	0.64	2.17	1	10
1:A:39:ARG:CD	1:A:63:LEU:HD21	0.64	2.23	5	6
1:A:27:ILE:CG1	1:A:29:LEU:HD21	0.64	2.23	5	7
1:A:63:LEU:HD13	1:A:75:LEU:CD1	0.64	2.21	1	3
1:A:63:LEU:HD13	1:A:75:LEU:HD12	0.64	1.68	9	8
1:A:9:ILE:HG21	1:A:57:LEU:CD1	0.64	2.21	10	5
1:A:9:ILE:N	1:A:44:LEU:O	0.64	2.31	3	10
1:A:13:PRO:HA	1:A:40:SER:HA	0.64	1.68	1	5
1:A:14:LEU:CD1	1:A:18:LEU:HD22	0.64	2.23	4	6
1:A:41:THR:HG22	1:A:61:THR:OG1	0.63	1.92	1	1
1:A:14:LEU:CD2	1:A:41:THR:HG21	0.63	2.23	1	1
1:A:18:LEU:HD13	1:A:57:LEU:CD2	0.63	2.23	10	4
1:A:58:LEU:HD22	1:A:63:LEU:HB3	0.63	1.71	6	4
1:A:50:ILE:O	1:A:54:LEU:HD23	0.63	1.94	5	1
1:A:14:LEU:HD23	1:A:41:THR:CG2	0.62	2.25	8	4
1:A:58:LEU:HD11	1:A:65:ALA:HB2	0.62	1.71	5	6
1:A:25:ALA:HB1	1:A:27:ILE:HG23	0.62	1.72	1	10
1:A:29:LEU:HD11	1:A:54:LEU:HD11	0.62	1.69	7	2
1:A:25:ALA:CB	1:A:27:ILE:HG23	0.62	2.24	7	9
1:A:29:LEU:HD12	1:A:73:TYR:CE2	0.62	2.29	4	1
1:A:31:TYR:CD2	1:A:35:LEU:HD22	0.62	2.30	9	1
1:A:61:THR:C	1:A:63:LEU:H	0.61	2.03	3	10
1:A:11:ALA:HA	1:A:42:SER:CA	0.61	2.25	6	7
1:A:39:ARG:HG3	1:A:80:SER:HB2	0.61	1.71	7	4
1:A:39:ARG:HD2	1:A:63:LEU:HD21	0.61	1.71	4	5
1:A:13:PRO:HB2	1:A:16:PRO:HD2	0.61	1.72	2	6
1:A:58:LEU:O	1:A:59:ALA:C	0.61	2.43	9	7
1:A:64:GLU:O	1:A:76:GLN:N	0.61	2.34	3	10
1:A:14:LEU:N	1:A:40:SER:HA	0.61	2.11	2	6
1:A:13:PRO:O	1:A:16:PRO:HD2	0.61	1.95	10	2
1:A:50:ILE:O	1:A:54:LEU:HB2	0.61	1.95	7	6
1:A:27:ILE:CD1	1:A:29:LEU:HD21	0.61	2.26	3	6
1:A:73:TYR:C	1:A:73:TYR:HD1	0.61	2.03	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD12	1:A:57:LEU:HB2	0.60	1.70	10	9
1:A:29:LEU:HA	1:A:73:TYR:CD1	0.60	2.30	5	1
1:A:61:THR:O	1:A:63:LEU:HD23	0.60	1.95	7	1
1:A:35:LEU:HD21	1:A:77:ALA:HB2	0.60	1.73	9	1
1:A:58:LEU:CD1	1:A:65:ALA:HB3	0.60	2.27	9	1
1:A:14:LEU:HA	1:A:41:THR:HG22	0.60	1.74	9	5
1:A:18:LEU:HG	1:A:29:LEU:HG	0.60	1.73	4	6
1:A:62:GLY:N	1:A:82:GLY:H	0.60	1.94	8	2
1:A:29:LEU:HD12	1:A:73:TYR:CG	0.59	2.32	1	2
1:A:41:THR:HB	1:A:57:LEU:O	0.59	1.97	2	6
1:A:40:SER:O	1:A:61:THR:HB	0.59	1.97	8	3
1:A:61:THR:C	1:A:63:LEU:N	0.59	2.60	8	10
1:A:27:ILE:HB	1:A:50:ILE:HD11	0.59	1.74	6	9
1:A:27:ILE:CD1	1:A:29:LEU:HD11	0.59	2.21	1	2
1:A:58:LEU:HD21	1:A:75:LEU:HD21	0.59	1.75	7	1
1:A:32:PRO:HG2	1:A:35:LEU:HB2	0.59	1.73	4	1
1:A:15:ALA:HB2	1:A:36:THR:CB	0.58	2.24	1	5
1:A:30:SER:N	1:A:73:TYR:O	0.58	2.36	9	2
1:A:62:GLY:HA3	1:A:82:GLY:H	0.58	1.58	1	7
1:A:14:LEU:HD12	1:A:39:ARG:NH2	0.58	2.13	7	2
1:A:12:GLY:N	1:A:41:THR:O	0.58	2.37	10	7
1:A:54:LEU:HB3	1:A:58:LEU:HD12	0.58	1.74	9	3
1:A:7:PHE:O	1:A:45:ALA:HA	0.58	1.97	1	10
1:A:44:LEU:HD21	1:A:53:GLY:HA2	0.58	1.76	4	8
1:A:50:ILE:HG22	1:A:51:ASP:N	0.58	2.13	5	10
1:A:54:LEU:HD21	1:A:65:ALA:HB3	0.57	1.76	4	1
1:A:65:ALA:HB2	1:A:75:LEU:HD13	0.57	1.76	7	1
1:A:50:ILE:O	1:A:54:LEU:CB	0.57	2.53	4	7
1:A:33:THR:O	1:A:37:GLU:HG3	0.57	2.00	1	4
1:A:73:TYR:CE1	1:A:75:LEU:HD22	0.57	2.34	4	1
1:A:16:PRO:HA	1:A:19:ALA:HB3	0.57	1.74	1	4
1:A:59:ALA:O	1:A:61:THR:HG22	0.57	2.00	1	6
1:A:75:LEU:HD12	1:A:76:GLN:N	0.57	2.15	7	1
1:A:29:LEU:N	1:A:29:LEU:CD2	0.57	2.68	2	7
1:A:15:ALA:HB3	1:A:16:PRO:CD	0.56	2.29	8	3
1:A:29:LEU:HA	1:A:73:TYR:CD2	0.56	2.35	1	1
1:A:8:ASP:HA	1:A:45:ALA:CB	0.56	2.31	5	10
1:A:39:ARG:N	1:A:39:ARG:HE	0.56	1.98	2	2
1:A:14:LEU:HD13	1:A:18:LEU:CD2	0.56	2.31	1	1
1:A:22:GLY:HA2	1:A:27:ILE:HG12	0.55	1.79	9	9
1:A:64:GLU:HG3	1:A:76:GLN:HB2	0.55	1.77	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:THR:HA	1:A:39:ARG:NH2	0.55	2.16	2	2
1:A:41:THR:HG21	1:A:57:LEU:HG	0.55	1.77	9	3
1:A:75:LEU:HD12	1:A:76:GLN:H	0.55	1.60	7	1
1:A:64:GLU:O	1:A:75:LEU:HD13	0.55	2.01	9	4
1:A:18:LEU:HD21	1:A:73:TYR:OH	0.55	2.01	4	1
1:A:4:GLN:N	1:A:4:GLN:CD	0.55	2.64	7	2
1:A:18:LEU:CD1	1:A:57:LEU:HD23	0.55	2.31	10	4
1:A:44:LEU:HD12	1:A:57:LEU:HD22	0.55	1.78	10	2
1:A:18:LEU:HD23	1:A:31:TYR:CE2	0.55	2.37	6	4
1:A:50:ILE:CG2	1:A:51:ASP:N	0.54	2.71	7	10
1:A:14:LEU:CD2	1:A:41:THR:HG22	0.54	2.32	8	4
1:A:22:GLY:HA2	1:A:27:ILE:CG1	0.54	2.33	5	9
1:A:44:LEU:HD11	1:A:53:GLY:CA	0.54	2.32	1	1
1:A:75:LEU:HD13	1:A:76:GLN:N	0.54	2.15	1	1
1:A:7:PHE:N	1:A:7:PHE:CD1	0.54	2.75	6	3
1:A:62:GLY:O	1:A:63:LEU:HD23	0.54	2.03	5	1
1:A:63:LEU:HB3	1:A:75:LEU:HD11	0.54	1.80	1	2
1:A:61:THR:O	1:A:61:THR:HG23	0.54	2.02	9	3
1:A:12:GLY:O	1:A:41:THR:HG23	0.53	2.03	7	5
1:A:35:LEU:O	1:A:39:ARG:NE	0.53	2.41	9	8
1:A:44:LEU:CB	1:A:57:LEU:CD1	0.53	2.86	2	9
1:A:13:PRO:HA	1:A:40:SER:HB3	0.53	1.79	8	2
1:A:13:PRO:HB2	1:A:16:PRO:CD	0.53	2.34	8	8
1:A:14:LEU:HA	1:A:41:THR:CG2	0.53	2.33	3	7
1:A:14:LEU:HD13	1:A:18:LEU:HD22	0.53	1.81	4	5
1:A:12:GLY:O	1:A:41:THR:O	0.53	2.27	9	4
1:A:28:LEU:HB3	1:A:72:SER:HA	0.52	1.81	5	2
1:A:5:ALA:HB3	1:A:25:ALA:HA	0.52	1.80	4	3
1:A:5:ALA:O	1:A:47:ARG:HA	0.52	2.03	5	9
1:A:14:LEU:CB	1:A:39:ARG:HB2	0.52	2.35	4	3
1:A:13:PRO:C	1:A:16:PRO:HD2	0.52	2.30	10	2
1:A:35:LEU:O	1:A:39:ARG:CZ	0.52	2.58	7	2
1:A:62:GLY:CA	1:A:82:GLY:H	0.52	2.18	3	6
1:A:28:LEU:C	1:A:29:LEU:HD23	0.52	2.30	8	1
1:A:14:LEU:HD13	1:A:63:LEU:HD12	0.51	1.82	5	1
1:A:64:GLU:CG	1:A:76:GLN:HB2	0.51	2.35	1	5
1:A:44:LEU:CD1	1:A:57:LEU:HB2	0.51	2.36	10	8
1:A:14:LEU:O	1:A:15:ALA:C	0.51	2.53	8	8
1:A:35:LEU:HA	1:A:39:ARG:CZ	0.51	2.36	6	1
1:A:32:PRO:CG	1:A:35:LEU:HB2	0.51	2.35	4	1
1:A:54:LEU:O	1:A:58:LEU:N	0.51	2.42	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:PHE:CD2	1:A:7:PHE:N	0.51	2.78	7	5
1:A:52:GLN:O	1:A:56:ILE:N	0.51	2.43	8	9
1:A:35:LEU:HD11	1:A:77:ALA:CB	0.50	2.37	2	1
1:A:32:PRO:HG2	1:A:35:LEU:H	0.50	1.67	4	1
1:A:14:LEU:O	1:A:17:ALA:N	0.50	2.45	10	2
1:A:73:TYR:CE1	1:A:75:LEU:HD23	0.50	2.41	1	1
1:A:41:THR:HB	1:A:61:THR:HG21	0.50	1.83	1	1
1:A:31:TYR:HD2	1:A:35:LEU:HD22	0.50	1.64	9	1
1:A:48:PHE:HB3	1:A:52:GLN:HB3	0.50	1.83	5	3
1:A:27:ILE:HD12	1:A:29:LEU:CD2	0.50	2.36	7	2
1:A:17:ALA:C	1:A:57:LEU:HD21	0.50	2.32	1	1
1:A:14:LEU:HD23	1:A:41:THR:HG22	0.50	1.83	8	2
1:A:13:PRO:HD3	1:A:40:SER:HB3	0.49	1.84	10	1
1:A:70:ASN:O	1:A:72:SER:N	0.49	2.46	3	1
1:A:50:ILE:HD13	1:A:54:LEU:CD2	0.49	2.38	5	1
1:A:54:LEU:HG	1:A:65:ALA:HB3	0.49	1.83	7	1
1:A:35:LEU:HD11	1:A:77:ALA:HB3	0.49	1.85	7	1
1:A:70:ASN:H	1:A:70:ASN:HD22	0.49	1.49	9	1
1:A:21:PHE:CE2	1:A:54:LEU:N	0.49	2.80	8	3
1:A:14:LEU:CD1	1:A:63:LEU:HD12	0.49	2.37	5	1
1:A:62:GLY:HA3	1:A:81:THR:N	0.49	2.22	9	3
1:A:14:LEU:H	1:A:40:SER:HA	0.49	1.68	9	5
1:A:29:LEU:HD12	1:A:73:TYR:CZ	0.49	2.43	4	1
1:A:44:LEU:HD11	1:A:53:GLY:C	0.49	2.33	1	1
1:A:29:LEU:HB3	1:A:73:TYR:CE1	0.48	2.42	4	1
1:A:27:ILE:CG2	1:A:50:ILE:HG12	0.48	2.38	9	6
1:A:28:LEU:O	1:A:72:SER:HA	0.48	2.08	3	1
1:A:6:ASP:HA	1:A:47:ARG:HA	0.48	1.84	7	2
1:A:9:ILE:HB	1:A:44:LEU:O	0.48	2.08	9	3
1:A:29:LEU:HD11	1:A:54:LEU:CD1	0.48	2.38	8	1
1:A:35:LEU:O	1:A:38:GLY:N	0.48	2.47	7	1
1:A:15:ALA:HB2	1:A:36:THR:HG21	0.48	1.86	5	1
1:A:73:TYR:C	1:A:73:TYR:HD2	0.48	2.15	1	1
1:A:17:ALA:O	1:A:21:PHE:N	0.48	2.46	8	7
1:A:13:PRO:HB2	1:A:16:PRO:CG	0.48	2.38	4	2
1:A:5:ALA:CB	1:A:25:ALA:HA	0.48	2.37	3	7
1:A:70:ASN:HD22	1:A:70:ASN:N	0.48	2.06	3	2
1:A:21:PHE:O	1:A:25:ALA:HB3	0.48	2.09	7	4
1:A:15:ALA:CB	1:A:36:THR:HB	0.47	2.40	2	2
1:A:14:LEU:HB2	1:A:39:ARG:C	0.47	2.34	4	1
1:A:9:ILE:O	1:A:43:GLY:HA3	0.47	2.10	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:CB	1:A:50:ILE:HD11	0.47	2.38	7	2
1:A:36:THR:C	1:A:38:GLY:H	0.47	2.17	10	3
1:A:44:LEU:C	1:A:44:LEU:CD2	0.47	2.87	10	6
1:A:8:ASP:C	1:A:9:ILE:HG13	0.47	2.33	1	1
1:A:29:LEU:HD12	1:A:73:TYR:CD1	0.47	2.44	1	2
1:A:14:LEU:O	1:A:18:LEU:HD22	0.47	2.10	5	1
1:A:14:LEU:HB3	1:A:18:LEU:CD2	0.47	2.40	10	1
1:A:14:LEU:HB3	1:A:39:ARG:HB2	0.47	1.87	4	2
1:A:65:ALA:HB1	1:A:73:TYR:CD2	0.47	2.45	5	1
1:A:67:ARG:NE	1:A:71:ALA:HA	0.47	2.25	9	1
1:A:35:LEU:O	1:A:39:ARG:HG2	0.46	2.09	9	3
1:A:14:LEU:HB3	1:A:39:ARG:NH2	0.46	2.25	2	1
1:A:10:PRO:O	1:A:12:GLY:N	0.46	2.49	1	4
1:A:15:ALA:O	1:A:19:ALA:N	0.46	2.49	6	4
1:A:5:ALA:HA	1:A:47:ARG:HH21	0.46	1.70	5	1
1:A:27:ILE:HG21	1:A:50:ILE:CD1	0.46	2.40	7	3
1:A:39:ARG:NH1	1:A:80:SER:HB3	0.46	2.26	4	4
1:A:22:GLY:O	1:A:26:HIS:N	0.46	2.48	10	10
1:A:4:GLN:HG3	1:A:49:ASP:CG	0.46	2.36	1	1
1:A:21:PHE:O	1:A:25:ALA:CB	0.46	2.64	7	6
1:A:33:THR:O	1:A:37:GLU:HG2	0.46	2.11	5	5
1:A:64:GLU:N	1:A:76:GLN:O	0.46	2.48	9	5
1:A:40:SER:C	1:A:41:THR:CG2	0.45	2.89	1	1
1:A:67:ARG:HG2	1:A:68:GLY:N	0.45	2.26	6	3
1:A:73:TYR:CG	1:A:74:SER:N	0.45	2.84	9	1
1:A:66:SER:N	1:A:74:SER:O	0.45	2.49	6	4
1:A:38:GLY:HA3	1:A:39:ARG:NH2	0.45	2.22	6	1
1:A:44:LEU:HB3	1:A:57:LEU:CD1	0.45	2.40	2	4
1:A:56:ILE:HG22	1:A:57:LEU:N	0.45	2.26	6	3
1:A:65:ALA:HB2	1:A:75:LEU:CD2	0.45	2.42	1	1
1:A:56:ILE:O	1:A:59:ALA:HB2	0.45	2.10	4	3
1:A:9:ILE:HD13	1:A:17:ALA:O	0.45	2.11	1	1
1:A:65:ALA:HB2	1:A:75:LEU:HD22	0.45	1.88	1	1
1:A:73:TYR:CD1	1:A:74:SER:N	0.45	2.84	4	1
1:A:70:ASN:O	1:A:71:ALA:HB3	0.45	2.12	1	1
1:A:44:LEU:C	1:A:44:LEU:HD22	0.45	2.37	10	5
1:A:9:ILE:HB	1:A:44:LEU:HB3	0.45	1.87	10	1
1:A:12:GLY:O	1:A:41:THR:N	0.45	2.50	6	1
1:A:54:LEU:HD22	1:A:58:LEU:HD11	0.45	1.87	9	1
1:A:9:ILE:O	1:A:44:LEU:N	0.45	2.50	1	1
1:A:21:PHE:CZ	1:A:53:GLY:HA3	0.45	2.46	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ARG:HG2	1:A:63:LEU:HD21	0.45	1.87	7	1
1:A:54:LEU:HG	1:A:58:LEU:CD1	0.45	2.42	7	1
1:A:44:LEU:HB2	1:A:57:LEU:HD12	0.45	1.88	8	4
1:A:9:ILE:HG22	1:A:10:PRO:O	0.45	2.12	4	2
1:A:67:ARG:HA	1:A:73:TYR:CB	0.44	2.37	9	1
1:A:35:LEU:C	1:A:39:ARG:HG2	0.44	2.37	4	3
1:A:75:LEU:CD1	1:A:76:GLN:H	0.44	2.20	1	2
1:A:39:ARG:HB3	1:A:61:THR:OG1	0.44	2.13	7	2
1:A:27:ILE:CG2	1:A:50:ILE:HD11	0.44	2.43	7	1
1:A:12:GLY:O	1:A:13:PRO:C	0.44	2.61	4	6
1:A:66:SER:O	1:A:73:TYR:CE1	0.44	2.71	9	1
1:A:21:PHE:CD2	1:A:25:ALA:HB2	0.44	2.48	1	4
1:A:43:GLY:O	1:A:56:ILE:HG22	0.44	2.13	4	2
1:A:62:GLY:C	1:A:63:LEU:HD23	0.44	2.37	2	3
1:A:14:LEU:O	1:A:18:LEU:N	0.44	2.49	10	1
1:A:62:GLY:HA3	1:A:80:SER:C	0.44	2.37	3	2
1:A:4:GLN:HA	1:A:49:ASP:HA	0.44	1.88	4	3
1:A:49:ASP:O	1:A:50:ILE:C	0.44	2.61	4	5
1:A:9:ILE:H	1:A:45:ALA:HB2	0.44	1.72	7	2
1:A:35:LEU:HG	1:A:39:ARG:HD2	0.44	1.90	8	2
1:A:4:GLN:HB3	1:A:48:PHE:O	0.44	2.13	2	1
1:A:13:PRO:HB2	1:A:16:PRO:HG2	0.44	1.90	7	2
1:A:18:LEU:HD21	1:A:75:LEU:CD2	0.44	2.43	7	1
1:A:25:ALA:HB1	1:A:27:ILE:CG2	0.44	2.42	7	1
1:A:54:LEU:HD22	1:A:58:LEU:CD1	0.44	2.43	9	1
1:A:29:LEU:HB3	1:A:73:TYR:CE2	0.44	2.48	1	1
1:A:54:LEU:CD1	1:A:73:TYR:HE2	0.44	2.26	4	1
1:A:13:PRO:HA	1:A:40:SER:CB	0.44	2.43	8	2
1:A:64:GLU:HG2	1:A:76:GLN:O	0.44	2.13	7	2
1:A:78:SER:C	1:A:80:SER:H	0.44	2.21	8	1
1:A:21:PHE:CE1	1:A:54:LEU:N	0.43	2.86	7	4
1:A:9:ILE:HD13	1:A:57:LEU:HD13	0.43	1.89	3	3
1:A:58:LEU:CD2	1:A:75:LEU:HD11	0.43	2.43	8	1
1:A:54:LEU:O	1:A:58:LEU:CB	0.43	2.63	2	2
1:A:70:ASN:C	1:A:72:SER:N	0.43	2.76	3	1
1:A:35:LEU:HG	1:A:39:ARG:NH1	0.43	2.28	4	1
1:A:66:SER:O	1:A:74:SER:N	0.43	2.50	3	1
1:A:7:PHE:CE2	1:A:21:PHE:HE2	0.43	2.32	1	1
1:A:14:LEU:CG	1:A:63:LEU:HD12	0.43	2.43	1	1
1:A:31:TYR:CD1	1:A:35:LEU:HD22	0.43	2.48	8	1
1:A:62:GLY:HA3	1:A:79:ALA:O	0.43	2.13	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:GLN:HB2	1:A:47:ARG:NH2	0.43	2.29	10	1
1:A:44:LEU:CB	1:A:57:LEU:HD12	0.43	2.44	8	2
1:A:61:THR:O	1:A:62:GLY:C	0.43	2.62	8	1
1:A:27:ILE:O	1:A:28:LEU:HD22	0.43	2.14	3	2
1:A:14:LEU:HD11	1:A:75:LEU:CD2	0.43	2.44	7	1
1:A:32:PRO:HD2	1:A:35:LEU:HB2	0.43	1.91	7	1
1:A:63:LEU:HD12	1:A:75:LEU:CD1	0.43	2.44	10	1
1:A:54:LEU:O	1:A:56:ILE:N	0.42	2.51	5	1
1:A:73:TYR:OH	1:A:75:LEU:CD2	0.42	2.66	5	1
1:A:4:GLN:CD	1:A:4:GLN:H	0.42	2.22	6	1
1:A:22:GLY:HA2	1:A:27:ILE:H	0.42	1.74	7	1
1:A:28:LEU:O	1:A:29:LEU:HD23	0.42	2.13	8	1
1:A:31:TYR:CD2	1:A:32:PRO:HD2	0.42	2.49	9	1
1:A:10:PRO:C	1:A:43:GLY:HA3	0.42	2.40	1	1
1:A:18:LEU:HD21	1:A:75:LEU:HD21	0.42	1.90	9	1
1:A:27:ILE:HD12	1:A:29:LEU:CD1	0.42	2.33	2	2
1:A:18:LEU:HD23	1:A:57:LEU:CD2	0.42	2.44	8	1
1:A:50:ILE:O	1:A:54:LEU:N	0.42	2.52	8	1
1:A:11:ALA:CA	1:A:42:SER:HA	0.42	2.30	10	5
1:A:7:PHE:CD1	1:A:7:PHE:N	0.42	2.86	3	1
1:A:15:ALA:HB2	1:A:36:THR:CG2	0.42	2.44	9	3
1:A:52:GLN:HE21	1:A:52:GLN:HA	0.42	1.73	9	1
1:A:63:LEU:HD22	1:A:77:ALA:HA	0.42	1.92	8	4
1:A:68:GLY:HA3	1:A:72:SER:O	0.42	2.15	3	1
1:A:80:SER:O	1:A:81:THR:C	0.42	2.63	8	1
1:A:79:ALA:O	1:A:80:SER:C	0.42	2.63	3	2
1:A:28:LEU:CA	1:A:29:LEU:HD22	0.42	2.44	9	1
1:A:31:TYR:CD1	1:A:36:THR:HG22	0.42	2.50	7	1
1:A:18:LEU:HB3	1:A:29:LEU:HG	0.41	1.92	1	1
1:A:50:ILE:O	1:A:54:LEU:CD2	0.41	2.66	5	1
1:A:35:LEU:O	1:A:36:THR:C	0.41	2.63	2	2
1:A:64:GLU:HG3	1:A:76:GLN:CB	0.41	2.45	2	1
1:A:73:TYR:CD2	1:A:74:SER:O	0.41	2.74	9	1
1:A:12:GLY:C	1:A:41:THR:H	0.41	2.23	10	1
1:A:4:GLN:CD	1:A:4:GLN:N	0.41	2.78	1	1
1:A:35:LEU:HD11	1:A:77:ALA:HB2	0.41	1.92	6	1
1:A:58:LEU:CD1	1:A:65:ALA:HB2	0.41	2.46	3	1
1:A:64:GLU:HG2	1:A:76:GLN:HB2	0.41	1.92	4	1
1:A:63:LEU:HA	1:A:76:GLN:O	0.41	2.16	9	1
1:A:14:LEU:HA	1:A:17:ALA:HB3	0.41	1.93	10	1
1:A:54:LEU:HD11	1:A:73:TYR:CE1	0.41	2.50	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLY:CA	1:A:27:ILE:CG1	0.41	2.99	10	1
1:A:67:ARG:CD	1:A:71:ALA:HA	0.41	2.45	9	1
1:A:15:ALA:N	1:A:16:PRO:CD	0.41	2.83	10	1
1:A:21:PHE:CD1	1:A:25:ALA:HB2	0.41	2.51	3	1
1:A:63:LEU:CD1	1:A:75:LEU:HG	0.41	2.46	5	1
1:A:46:GLY:HA3	1:A:48:PHE:CE2	0.41	2.50	1	1
1:A:18:LEU:HG	1:A:29:LEU:CG	0.41	2.44	3	1
1:A:9:ILE:HD11	1:A:17:ALA:O	0.41	2.16	5	1
1:A:38:GLY:C	1:A:39:ARG:HG3	0.41	2.41	7	1
1:A:33:THR:O	1:A:34:ALA:C	0.40	2.64	1	1
1:A:54:LEU:O	1:A:55:ALA:C	0.40	2.64	5	1
1:A:21:PHE:CE2	1:A:25:ALA:HB2	0.40	2.51	6	1
1:A:38:GLY:C	1:A:39:ARG:HE	0.40	2.23	6	1
1:A:70:ASN:ND2	1:A:72:SER:OG	0.40	2.54	6	1
1:A:79:ALA:O	1:A:80:SER:O	0.40	2.39	7	1
1:A:8:ASP:HA	1:A:45:ALA:HB2	0.40	1.92	8	1
1:A:66:SER:HB2	1:A:74:SER:OG	0.40	2.16	2	1
1:A:63:LEU:CD1	1:A:75:LEU:HD12	0.40	2.43	9	1
1:A:80:SER:C	1:A:82:GLY:N	0.40	2.78	1	1
1:A:39:ARG:HH11	1:A:63:LEU:HD11	0.40	1.76	2	1
1:A:6:ASP:C	1:A:7:PHE:CD1	0.40	3.00	3	1
1:A:41:THR:OG1	1:A:57:LEU:HG	0.40	2.16	6	1
1:A:56:ILE:O	1:A:57:LEU:C	0.40	2.64	6	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/82 (95%)	52±4 (67±5%)	20±3 (26±4%)	6±1 (7±2%)	2	15
All	All	780/820 (95%)	521 (67%)	203 (26%)	56 (7%)	2	15

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	60	GLY	10
1	A	62	GLY	10
1	A	80	SER	8
1	A	10	PRO	7
1	A	38	GLY	6
1	A	81	THR	4
1	A	13	PRO	4
1	A	59	ALA	2
1	A	70	ASN	1
1	A	71	ALA	1
1	A	67	ARG	1
1	A	11	ALA	1
1	A	12	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	54/55 (98%)	35±2 (65±5%)	19±2 (35±5%)	1	10
All	All	540/550 (98%)	353 (65%)	187 (35%)	1	10

All 32 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	24	SER	10
1	A	39	ARG	10
1	A	44	LEU	10
1	A	47	ARG	10
1	A	50	ILE	10
1	A	63	LEU	10
1	A	75	LEU	10
1	A	18	LEU	9
1	A	35	LEU	8
1	A	41	THR	8
1	A	14	LEU	7
1	A	40	SER	7
1	A	7	PHE	7

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Mol	Chain	Res	Type	Models (Total)
1	A	29	LEU	7
1	A	64	GLU	7
1	A	23	GLN	6
1	A	28	LEU	6
1	A	9	ILE	6
1	A	37	GLU	6
1	A	4	GLN	5
1	A	42	SER	5
1	A	31	TYR	4
1	A	73	TYR	3
1	A	27	ILE	3
1	A	52	GLN	3
1	A	20	HIS	2
1	A	70	ASN	2
1	A	49	ASP	2
1	A	78	SER	1
1	A	36	THR	1
1	A	54	LEU	1
1	A	67	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% 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 [i](#)

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	884
Number of shifts mapped to atoms	884
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	82	-0.05 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	71	0.06 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	76	-0.00 ± 0.22	None needed (< 0.5 ppm)
^{15}N	77	-0.01 ± 0.27	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 863 atoms were assigned a chemical shift out of a possible 961. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	389/397 (98%)	162/164 (99%)	152/158 (96%)	75/75 (100%)
Sidechain	425/500 (85%)	293/333 (88%)	127/153 (83%)	5/14 (36%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	49/64 (77%)	27/31 (87%)	22/29 (76%)	0/4 (0%)
Overall	863/961 (90%)	482/528 (91%)	301/340 (89%)	80/93 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 883 atoms were assigned a chemical shift out of a possible 984. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	403/413 (98%)	168/171 (98%)	158/164 (96%)	77/78 (99%)
Sidechain	431/507 (85%)	297/338 (88%)	129/155 (83%)	5/14 (36%)
Aromatic	49/64 (77%)	27/31 (87%)	22/29 (76%)	0/4 (0%)
Overall	883/984 (90%)	492/540 (91%)	309/348 (89%)	82/96 (85%)

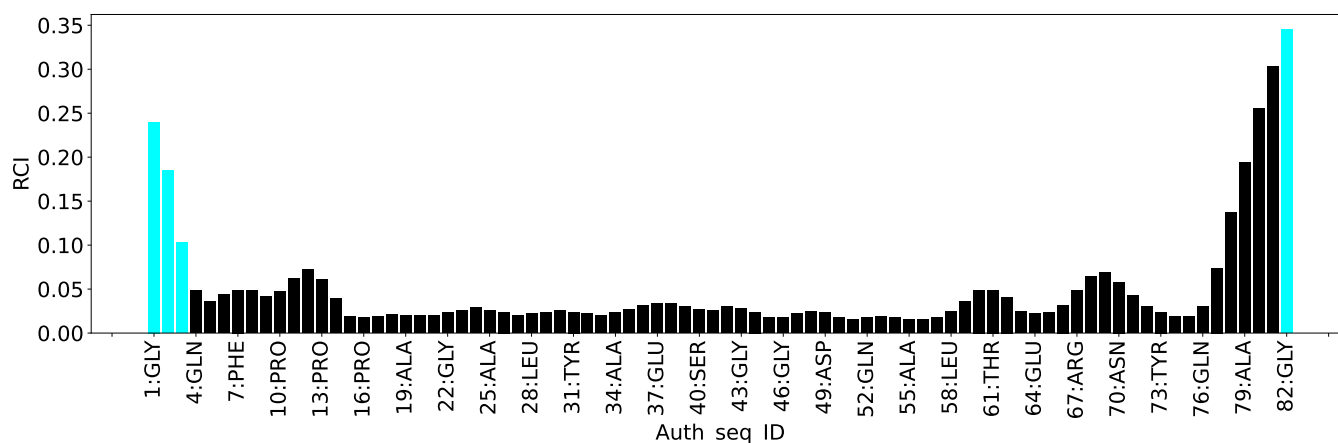
7.1.4 Statistically unusual chemical shifts [i](#)

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	1101
Intra-residue ($ i-j =0$)	491
Sequential ($ i-j =1$)	295
Medium range ($ i-j >1$ and $ i-j <5$)	105
Long range ($ i-j \geq 5$)	160
Inter-chain	0
Hydrogen bond restraints	50
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	13.4
Number of long range restraints per residue ¹	2.2

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)	100.1	0.2
0.2-0.5 (Medium)	294.7	0.5
>0.5 (Large)	227.7	15.71

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

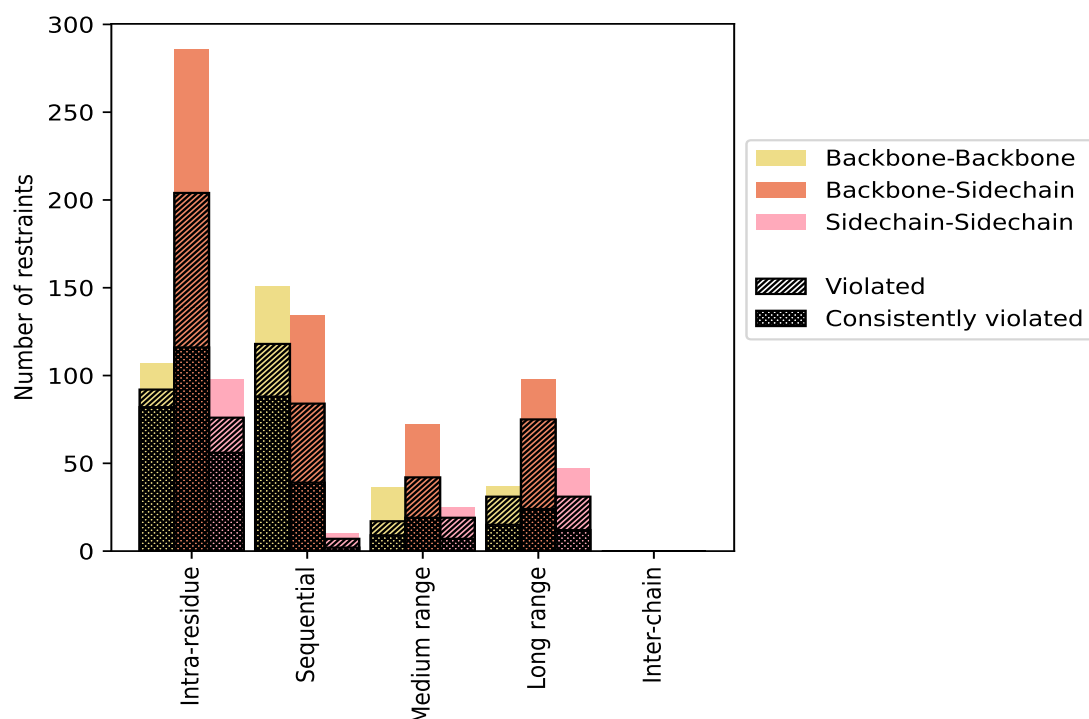
9.1 Summary of distance violations ⓘ

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)	491	44.6	372	75.8	33.8	254	51.7	23.1
Backbone-Backbone	107	9.7	92	86.0	8.4	82	76.6	7.4
Backbone-Sidechain	286	26.0	204	71.3	18.5	116	40.6	10.5
Sidechain-Sidechain	98	8.9	76	77.6	6.9	56	57.1	5.1
Sequential (i-j =1)	295	26.8	209	70.8	19.0	129	43.7	11.7
Backbone-Backbone	151	13.7	118	78.1	10.7	88	58.3	8.0
Backbone-Sidechain	134	12.2	84	62.7	7.6	39	29.1	3.5
Sidechain-Sidechain	10	0.9	7	70.0	0.6	2	20.0	0.2
Medium range (i-j >1 & i-j <5)	105	9.5	57	54.3	5.2	23	21.9	2.1
Backbone-Backbone	36	3.3	17	47.2	1.5	9	25.0	0.8
Backbone-Sidechain	44	4.0	21	47.7	1.9	7	15.9	0.6
Sidechain-Sidechain	25	2.3	19	76.0	1.7	7	28.0	0.6
Long range (i-j ≥5)	160	14.5	119	74.4	10.8	44	27.5	4.0
Backbone-Backbone	37	3.4	31	83.8	2.8	15	40.5	1.4
Backbone-Sidechain	76	6.9	57	75.0	5.2	17	22.4	1.5
Sidechain-Sidechain	47	4.3	31	66.0	2.8	12	25.5	1.1
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	50	4.5	39	78.0	3.5	19	38.0	1.7
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1101	100.0	796	72.3	72.3	469	42.6	42.6
Backbone-Backbone	331	30.1	258	77.9	23.4	194	58.6	17.6
Backbone-Sidechain	590	53.6	405	68.6	36.8	198	33.6	18.0
Sidechain-Sidechain	180	16.3	133	73.9	12.1	77	42.8	7.0

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

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



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

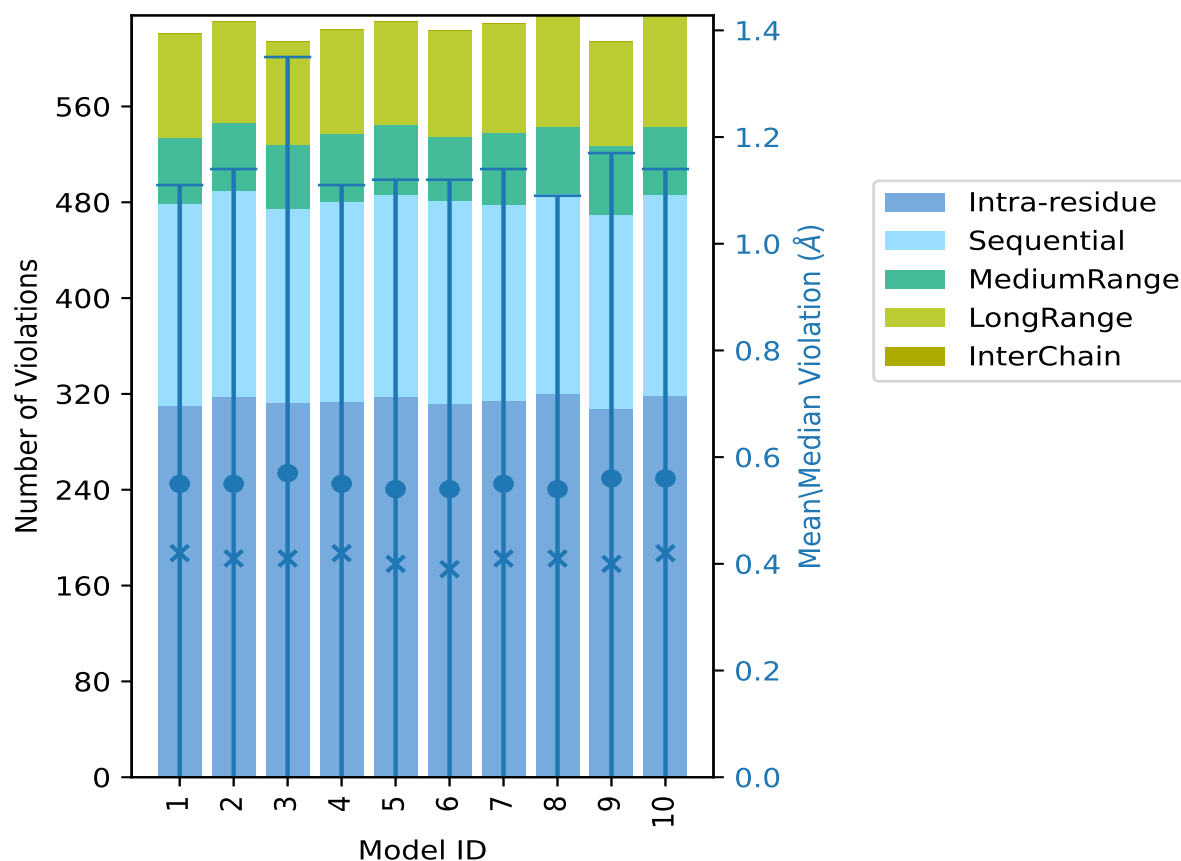
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	310	169	55	87	0	621	0.55	7.4	0.56	0.42
2	318	172	56	85	0	631	0.55	9.86	0.59	0.41
3	313	162	53	86	0	614	0.57	15.71	0.78	0.41
4	314	167	56	87	0	624	0.55	8.25	0.56	0.42
5	318	168	59	86	0	631	0.54	8.4	0.58	0.4
6	312	169	54	88	0	623	0.54	9.25	0.58	0.39
7	314	164	60	91	0	629	0.55	10.42	0.59	0.41
8	320	167	56	92	0	635	0.54	8.84	0.55	0.41
9	308	162	57	87	0	614	0.56	9.01	0.61	0.4
10	319	167	57	93	0	636	0.56	8.51	0.58	0.42

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 294(IR:119, SQ:86, MR:48, LR:41, 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	%
18	16	4	16	0	54	1	10.0
12	9	4	16	0	41	2	20.0
14	11	5	7	0	37	3	30.0

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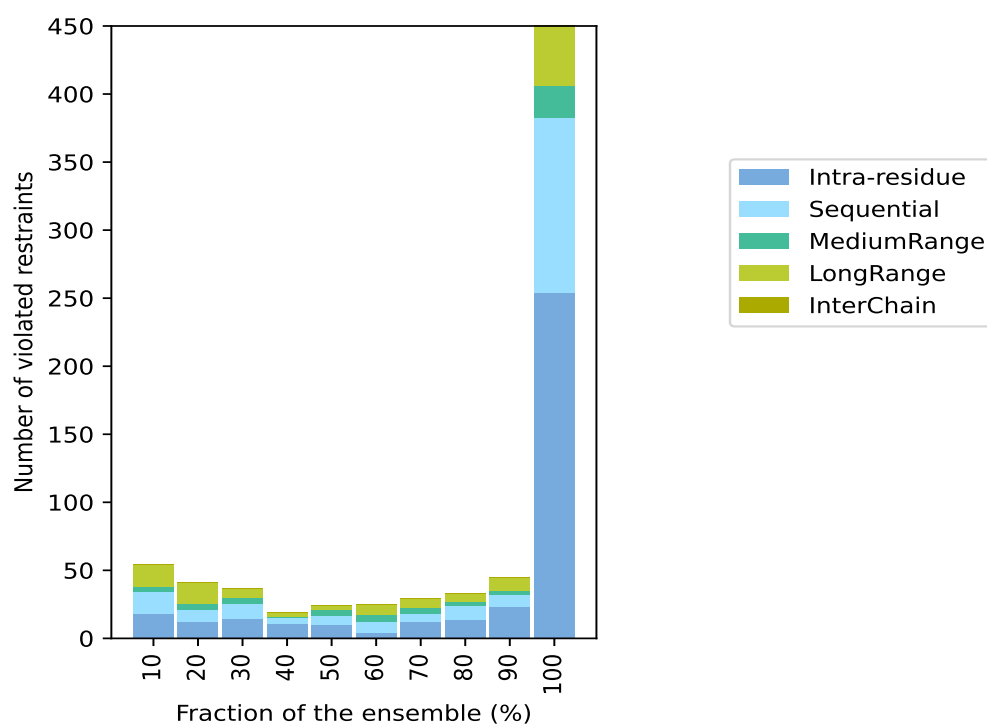
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
11	4	1	3	0	19	4	40.0
10	7	4	3	0	24	5	50.0
4	8	5	8	0	25	6	60.0
12	6	5	6	0	29	7	70.0
14	10	3	6	0	33	8	80.0
23	9	3	10	0	45	9	90.0
254	129	23	44	0	450	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 ⓘ

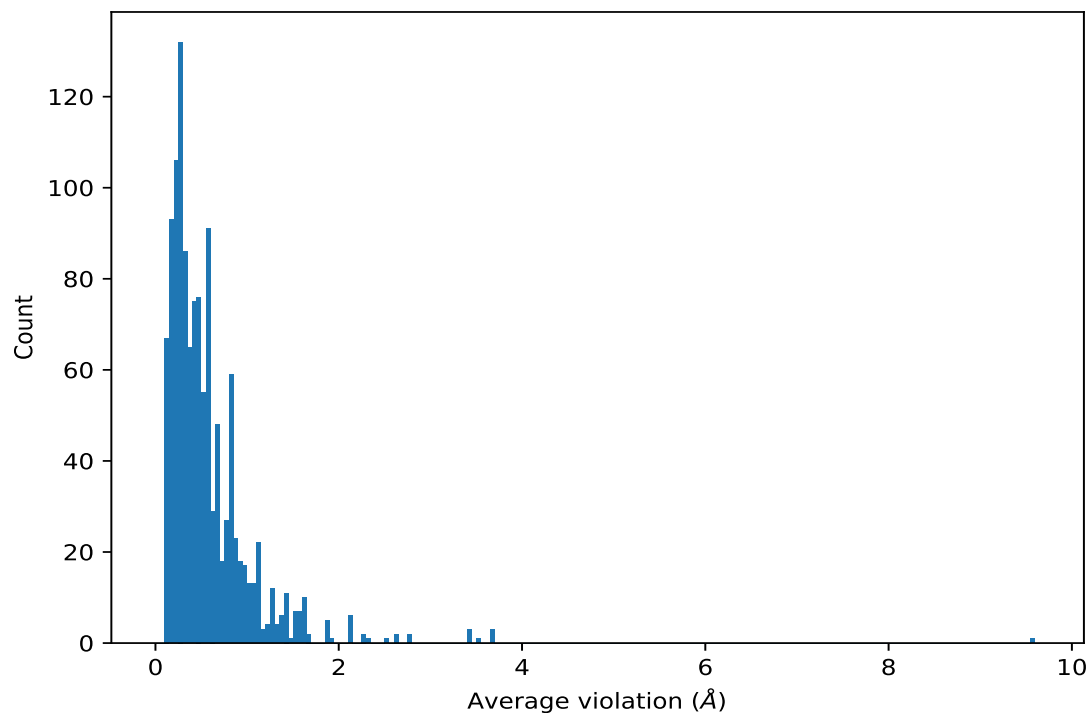


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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)
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	10	9.57	2.2	8.93
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	10	3.68	0.67	3.98
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	10	3.68	0.67	3.98
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	10	3.68	0.67	3.98
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	10	3.55	1.14	4.03
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	10	3.41	0.49	3.36
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	10	3.41	0.49	3.36
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	10	3.41	0.49	3.36
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	10	2.76	0.69	2.8
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	10	2.76	0.69	2.8
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	10	2.65	0.07	2.62
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	10	2.62	0.12	2.69
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	10	2.53	0.44	2.54
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	10	2.32	0.59	2.43
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	10	2.29	0.09	2.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	10	2.26	0.03	2.28
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	10	2.14	0.44	2.19
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	10	2.14	0.44	2.19
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	10	2.14	0.44	2.19
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	10	2.1	0.32	2.19
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	10	2.1	0.32	2.19
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	10	2.1	0.32	2.19
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	10	1.89	0.01	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	10	1.89	0.01	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	10	1.89	0.01	1.89
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	10	1.86	0.13	1.9
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	10	1.86	0.07	1.86
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	10	1.69	0.1	1.65
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	10	1.68	0.03	1.68
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	10	1.65	0.06	1.66
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	10	1.61	0.12	1.61
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	10	1.61	0.12	1.61
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	10	1.61	0.12	1.61
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	10	1.61	0.12	1.61
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	10	1.61	0.12	1.61
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	10	1.61	0.12	1.61
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	10	1.61	0.12	1.61
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	10	1.61	0.12	1.61
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	10	1.61	0.12	1.61
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	10	1.59	0.43	1.76
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	10	1.59	0.43	1.76
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	10	1.59	0.02	1.6
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	10	1.58	0.08	1.54
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	10	1.58	0.08	1.54
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	10	1.58	0.08	1.54
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	10	1.53	0.41	1.66
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	10	1.53	0.41	1.66
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	10	1.53	0.41	1.66
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	10	1.52	0.11	1.58
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	10	1.52	0.51	1.38
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	10	1.52	0.51	1.38
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	10	1.52	0.51	1.38
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	10	1.49	0.05	1.5
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	10	1.45	0.12	1.49
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	10	1.43	0.83	1.02
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	10	1.43	0.83	1.02
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	10	1.43	0.83	1.02

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	10	1.43	0.83	1.02
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	10	1.43	0.83	1.02
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	10	1.43	0.83	1.02
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	10	1.43	0.83	1.02
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	10	1.43	0.83	1.02
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	10	1.43	0.83	1.02
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	10	1.43	0.21	1.54
(5,19)	1:22:A:GLY:H	1:21:A:PHE:HB3	10	1.38	0.15	1.44
(5,19)	1:22:A:GLY:H	1:7:A:PHE:HB3	10	1.38	0.15	1.44
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	10	1.38	0.09	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	10	1.38	0.09	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	10	1.38	0.09	1.34
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	10	1.38	0.34	1.58
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	10	1.32	0.14	1.28
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	10	1.31	0.04	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	10	1.31	0.04	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	10	1.31	0.04	1.29
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	10	1.29	0.05	1.29
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	10	1.29	0.05	1.29
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	10	1.29	0.05	1.29
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	10	1.27	0.06	1.25
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	10	1.26	0.11	1.3
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	10	1.25	0.27	1.31
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	10	1.25	0.27	1.31
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	10	1.25	0.27	1.31
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	10	1.24	0.0	1.24
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	10	1.2	0.04	1.18
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	10	1.19	0.02	1.19
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	10	1.12	0.14	1.08
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	10	1.11	0.09	1.12
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	10	1.11	0.09	1.12
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	10	1.11	0.09	1.12
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	10	1.1	0.29	1.23
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	10	1.1	0.23	1.2
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	10	1.08	0.06	1.1
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	10	1.08	0.06	1.1
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	10	1.08	0.06	1.1
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	10	1.08	0.19	1.15
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	10	1.08	0.19	1.15
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	10	1.08	0.19	1.15
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	10	1.05	0.03	1.06
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	10	1.05	0.03	1.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	10	1.05	0.03	1.06
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	10	1.03	0.11	1.04
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	10	1.03	0.11	1.04
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	10	1.03	0.11	1.04
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	10	1.03	0.05	1.03
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	10	1.03	0.09	1.02
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	10	1.02	0.07	1.03
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	10	1.0	0.23	0.92
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	10	1.0	0.23	0.92
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	10	1.0	0.23	0.92
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	10	1.0	0.22	1.08
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	10	1.0	0.22	1.08
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	10	1.0	0.22	1.08
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	10	0.99	0.23	1.1
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	10	0.99	0.03	0.98
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	10	0.98	0.06	0.99
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	10	0.98	0.06	0.99
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	10	0.98	0.06	0.99
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	10	0.97	0.07	1.0
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	10	0.97	0.12	0.94
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	10	0.95	0.37	1.03
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	10	0.95	0.37	1.03
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	10	0.95	0.37	1.03
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	10	0.93	0.0	0.93
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	10	0.92	0.18	0.98
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	10	0.92	0.18	0.98
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	10	0.92	0.01	0.92
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	10	0.92	0.01	0.92
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	10	0.92	0.01	0.92
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	10	0.91	0.07	0.92
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	10	0.91	0.07	0.92
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	10	0.91	0.07	0.92
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	10	0.91	0.07	0.92
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	10	0.91	0.07	0.92
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	10	0.91	0.07	0.92
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	10	0.88	0.0	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	10	0.88	0.0	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	10	0.88	0.0	0.88
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	10	0.88	0.06	0.89
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	10	0.88	0.06	0.89
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	10	0.88	0.06	0.89
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	10	0.87	0.1	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	10	0.87	0.1	0.86
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	10	0.87	0.1	0.86
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	10	0.87	0.01	0.86
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	10	0.87	0.01	0.86
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	10	0.87	0.01	0.86
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	10	0.86	0.02	0.88
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	10	0.86	0.11	0.83
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	10	0.86	0.11	0.83
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	10	0.86	0.11	0.83
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	10	0.85	0.19	0.75
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	10	0.85	0.19	0.75
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	10	0.85	0.19	0.75
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	10	0.85	0.19	0.75
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	10	0.85	0.19	0.75
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	10	0.85	0.19	0.75
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	10	0.85	0.01	0.85
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	10	0.83	0.29	0.83
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	10	0.83	0.04	0.84
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	10	0.83	0.13	0.85
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	10	0.83	0.13	0.85
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	10	0.83	0.13	0.85
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	10	0.82	0.08	0.86
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	10	0.82	0.08	0.86
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	10	0.82	0.08	0.86
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	10	0.82	0.1	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	10	0.82	0.1	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	10	0.82	0.1	0.79
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	10	0.82	0.3	0.84
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	10	0.82	0.3	0.84
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	10	0.82	0.3	0.84
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	10	0.82	0.3	0.84
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	10	0.82	0.3	0.84
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	10	0.82	0.3	0.84
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	10	0.82	0.3	0.84
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	10	0.82	0.3	0.84
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	10	0.82	0.3	0.84
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	10	0.82	0.33	0.9
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	10	0.82	0.07	0.83
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	10	0.82	0.07	0.83
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	10	0.82	0.03	0.81
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	10	0.81	0.34	0.84
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	10	0.81	0.04	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	10	0.81	0.04	0.8
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	10	0.81	0.03	0.8
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	10	0.81	0.02	0.81
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	10	0.81	0.02	0.81
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	10	0.81	0.02	0.81
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	10	0.8	0.09	0.76
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	10	0.8	0.07	0.8
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	10	0.8	0.07	0.8
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	10	0.8	0.07	0.8
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	10	0.8	0.04	0.8
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	10	0.79	0.2	0.88
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	10	0.79	0.2	0.88
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	10	0.79	0.2	0.88
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	10	0.78	0.2	0.75
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	10	0.78	0.2	0.75
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	10	0.78	0.21	0.85
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	10	0.78	0.21	0.85
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	10	0.78	0.11	0.77
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	10	0.78	0.03	0.78
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	10	0.76	0.2	0.81
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	10	0.76	0.2	0.81
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	10	0.76	0.2	0.81
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	10	0.75	0.31	0.72
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	10	0.75	0.04	0.76
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	10	0.74	0.2	0.73
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	10	0.74	0.25	0.62
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	10	0.74	0.25	0.62
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	10	0.71	0.02	0.7
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	10	0.7	0.26	0.57
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	10	0.7	0.1	0.72
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	10	0.69	0.03	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	10	0.69	0.03	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	10	0.69	0.03	0.7
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	10	0.69	0.11	0.68
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	10	0.69	0.03	0.69
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	10	0.69	0.49	0.48
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	10	0.69	0.49	0.48
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	10	0.68	0.02	0.69
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	10	0.68	0.02	0.69
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	10	0.68	0.19	0.74
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	10	0.68	0.19	0.74
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	10	0.68	0.19	0.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	10	0.68	0.19	0.68
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	10	0.68	0.02	0.67
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	10	0.68	0.02	0.67
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	10	0.67	0.19	0.74
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	10	0.67	0.05	0.69
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	10	0.67	0.05	0.69
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	10	0.67	0.0	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	10	0.67	0.0	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	10	0.67	0.0	0.67
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	10	0.67	0.27	0.8
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	10	0.67	0.27	0.8
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	10	0.66	0.07	0.68
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	10	0.66	0.07	0.68
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	10	0.66	0.03	0.66
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	10	0.66	0.03	0.66
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	10	0.66	0.2	0.74
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	10	0.66	0.0	0.66
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	10	0.66	0.93	0.36
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	10	0.65	0.24	0.64
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	10	0.64	0.01	0.64
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	10	0.64	0.23	0.7
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	10	0.64	0.23	0.7
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	10	0.64	0.23	0.7
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	10	0.64	0.23	0.7
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	10	0.64	0.23	0.7
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	10	0.64	0.23	0.7
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	10	0.63	0.13	0.68
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	10	0.62	0.09	0.65
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	10	0.62	0.06	0.63
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	10	0.62	0.01	0.62
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	10	0.62	0.01	0.62
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	10	0.62	0.04	0.62
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	10	0.61	0.01	0.62
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	10	0.61	0.01	0.62
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	10	0.61	0.02	0.6
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	10	0.61	0.12	0.59
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	10	0.61	0.14	0.66
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	10	0.61	0.14	0.66
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	10	0.61	0.19	0.72
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	10	0.61	0.19	0.72
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	10	0.61	0.12	0.62
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	10	0.61	0.06	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	10	0.6	0.23	0.61
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	10	0.6	0.23	0.61
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	10	0.6	0.23	0.61
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	10	0.6	0.23	0.62
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	10	0.6	0.23	0.62
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	10	0.6	0.23	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	10	0.6	0.01	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	10	0.6	0.01	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	10	0.6	0.01	0.6
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	10	0.6	0.1	0.66
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	10	0.59	0.01	0.59
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	10	0.59	0.14	0.62
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	10	0.57	0.16	0.65
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	10	0.57	0.18	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	10	0.57	0.18	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	10	0.57	0.18	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	10	0.57	0.18	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	10	0.57	0.18	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	10	0.57	0.18	0.53
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	10	0.57	0.02	0.57
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	10	0.57	0.02	0.57
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	10	0.57	0.02	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	10	0.57	0.02	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	10	0.57	0.02	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	10	0.57	0.02	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	10	0.57	0.02	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	10	0.57	0.02	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	10	0.57	0.02	0.57
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	10	0.57	0.06	0.58
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	10	0.57	0.01	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	10	0.56	0.03	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	10	0.56	0.03	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	10	0.56	0.03	0.56
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	10	0.56	0.11	0.56
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	10	0.56	0.24	0.56
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	10	0.56	0.17	0.66
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	10	0.56	0.1	0.52
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	10	0.56	0.1	0.52
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	10	0.56	0.1	0.52
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	10	0.56	0.21	0.54
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	10	0.56	0.21	0.54
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	10	0.56	0.21	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	10	0.56	0.09	0.56
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	10	0.56	0.09	0.56
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	10	0.56	0.09	0.56
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	10	0.55	0.05	0.54
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	10	0.55	0.05	0.54
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	10	0.55	0.07	0.5
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	10	0.55	0.07	0.5
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	10	0.55	0.02	0.55
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	10	0.55	0.02	0.55
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	10	0.55	0.14	0.54
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	10	0.55	0.14	0.54
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	10	0.55	0.14	0.54
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	10	0.55	0.07	0.55
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	10	0.55	0.07	0.55
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	10	0.55	0.09	0.53
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	10	0.54	0.02	0.54
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	10	0.54	0.0	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	10	0.54	0.0	0.54
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	10	0.54	0.3	0.45
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	10	0.54	0.04	0.54
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	10	0.54	0.01	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	10	0.53	0.02	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	10	0.53	0.02	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	10	0.53	0.02	0.54
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	10	0.53	0.04	0.55
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	10	0.53	0.29	0.53
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	10	0.53	0.04	0.52
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	10	0.53	0.01	0.53
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	10	0.53	0.01	0.53
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	10	0.52	0.02	0.52
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	10	0.52	0.28	0.52
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	10	0.52	0.08	0.55
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	10	0.52	0.08	0.55
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	10	0.52	0.01	0.52
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	10	0.52	0.02	0.52
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	10	0.52	0.02	0.52
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	10	0.52	0.01	0.52
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	10	0.51	0.22	0.59
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	10	0.51	0.02	0.52
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	10	0.51	0.07	0.52
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	10	0.51	0.07	0.52
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	10	0.51	0.09	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	10	0.51	0.09	0.52
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	10	0.51	0.13	0.48
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	10	0.51	0.19	0.62
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	10	0.51	0.3	0.47
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	10	0.51	0.3	0.47
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	10	0.51	0.02	0.51
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	10	0.5	0.01	0.5
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	10	0.5	0.1	0.56
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	10	0.5	0.01	0.5
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	10	0.5	0.03	0.5
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	10	0.5	0.02	0.5
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	10	0.5	0.01	0.49
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	10	0.5	0.01	0.49
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	10	0.5	0.01	0.49
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	10	0.49	0.05	0.48
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	10	0.49	0.03	0.49
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	10	0.49	0.01	0.49
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	10	0.49	0.05	0.49
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	10	0.49	0.1	0.5
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	10	0.48	0.01	0.48
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	10	0.48	0.03	0.47
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	10	0.48	0.0	0.48
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	10	0.48	0.02	0.48
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	10	0.48	0.02	0.48
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	10	0.48	0.08	0.46
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	10	0.48	0.08	0.46
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	10	0.48	0.02	0.48
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	10	0.48	0.02	0.48
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	10	0.48	0.02	0.48
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	10	0.48	0.02	0.47
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	10	0.48	0.01	0.48
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	10	0.47	0.0	0.47
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	10	0.47	0.02	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	10	0.47	0.0	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	10	0.47	0.0	0.47
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	10	0.47	0.12	0.52
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	10	0.47	0.12	0.52
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	10	0.46	0.01	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	10	0.46	0.01	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	10	0.46	0.01	0.46
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	10	0.46	0.02	0.47
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	10	0.46	0.02	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	10	0.46	0.01	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	10	0.46	0.0	0.46
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	10	0.46	0.05	0.48
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	10	0.46	0.04	0.44
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	10	0.46	0.04	0.44
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	10	0.46	0.0	0.46
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	10	0.46	0.09	0.48
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	10	0.46	0.09	0.48
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	10	0.46	0.09	0.48
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	10	0.46	0.09	0.48
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	10	0.46	0.09	0.48
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	10	0.46	0.09	0.48
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	10	0.46	0.09	0.48
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	10	0.46	0.09	0.48
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	10	0.46	0.09	0.48
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	10	0.46	0.12	0.53
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	10	0.46	0.16	0.4
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	10	0.46	0.16	0.4
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	10	0.46	0.16	0.4
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	10	0.46	0.16	0.4
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	10	0.46	0.16	0.4
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	10	0.46	0.16	0.4
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	10	0.45	0.11	0.45
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	10	0.45	0.01	0.45
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	10	0.45	0.02	0.45
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	10	0.45	0.01	0.45
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	10	0.45	0.16	0.5
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	10	0.45	0.16	0.5
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	10	0.45	0.01	0.45
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	10	0.45	0.01	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	10	0.45	0.0	0.45
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	10	0.45	0.01	0.45
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	10	0.45	0.08	0.44
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	10	0.45	0.09	0.44
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	10	0.45	0.09	0.44
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	10	0.44	0.01	0.44
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	10	0.44	0.06	0.42
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	10	0.44	0.15	0.5
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	10	0.44	0.03	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	10	0.44	0.03	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	10	0.44	0.03	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	10	0.44	0.03	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	10	0.44	0.03	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	10	0.44	0.03	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	10	0.44	0.03	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	10	0.44	0.03	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	10	0.44	0.03	0.44
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	10	0.44	0.01	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	10	0.44	0.0	0.44
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	10	0.44	0.02	0.45
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	10	0.44	0.02	0.45
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	10	0.44	0.04	0.42
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	10	0.44	0.04	0.42
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	10	0.43	0.14	0.46
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	10	0.43	0.02	0.43
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	10	0.43	0.02	0.44
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	10	0.43	0.07	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	10	0.43	0.07	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	10	0.43	0.07	0.4
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	10	0.43	0.08	0.4
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	10	0.43	0.05	0.43
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	10	0.43	0.05	0.43
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	10	0.42	0.24	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	10	0.42	0.24	0.35
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	10	0.42	0.04	0.43
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	10	0.42	0.01	0.42
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	10	0.42	0.09	0.41
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	10	0.42	0.01	0.42
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	10	0.42	0.02	0.42
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	10	0.42	0.16	0.42
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	10	0.42	0.16	0.42
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	10	0.42	0.12	0.38
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	10	0.42	0.01	0.41
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	10	0.41	0.05	0.42
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	10	0.41	0.01	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	10	0.41	0.01	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	10	0.41	0.01	0.41
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	10	0.41	0.08	0.46
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	10	0.41	0.1	0.44
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	10	0.41	0.1	0.44
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	10	0.41	0.1	0.44
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	10	0.41	0.03	0.4
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	10	0.41	0.03	0.4
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	10	0.41	0.02	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	10	0.41	0.02	0.41
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	10	0.4	0.01	0.41
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	10	0.4	0.05	0.42
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	10	0.4	0.09	0.4
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	10	0.4	0.0	0.4
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	10	0.4	0.02	0.39
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	10	0.39	0.03	0.4
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	10	0.39	0.01	0.4
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	10	0.39	0.03	0.4
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	10	0.39	0.03	0.4
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	10	0.39	0.03	0.4
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	10	0.39	0.01	0.4
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	10	0.39	0.02	0.38
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	10	0.39	0.04	0.38
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	10	0.39	0.03	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	10	0.39	0.03	0.4
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	10	0.39	0.08	0.35
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	10	0.39	0.05	0.39
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	10	0.39	0.03	0.38
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	10	0.38	0.06	0.36
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	10	0.38	0.05	0.4
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	10	0.38	0.1	0.35
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	10	0.38	0.17	0.42
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	10	0.38	0.17	0.42
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	10	0.37	0.01	0.38
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	10	0.37	0.0	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	10	0.37	0.0	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	10	0.37	0.0	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	10	0.37	0.0	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	10	0.37	0.0	0.37
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	10	0.36	0.03	0.36
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	10	0.36	0.03	0.36
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	10	0.36	0.03	0.36
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	10	0.36	0.03	0.37
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	10	0.36	0.09	0.36
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	10	0.36	0.06	0.38
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	10	0.36	0.03	0.36
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	10	0.36	0.18	0.31
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	10	0.36	0.34	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	10	0.36	0.34	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	10	0.36	0.34	0.26
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	10	0.36	0.1	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	10	0.36	0.1	0.32
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	10	0.36	0.1	0.32
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	10	0.36	0.12	0.32
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	10	0.35	0.1	0.36
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	10	0.35	0.1	0.36
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	10	0.35	0.1	0.36
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	10	0.35	0.02	0.36
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	10	0.35	0.05	0.34
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	10	0.35	0.16	0.4
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	10	0.35	0.16	0.4
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	10	0.35	0.08	0.36
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	10	0.35	0.02	0.34
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	10	0.35	0.02	0.34
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	10	0.35	0.08	0.36
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	10	0.35	0.0	0.35
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	10	0.35	0.01	0.36
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	10	0.35	0.06	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	10	0.35	0.02	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	10	0.35	0.02	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	10	0.35	0.02	0.34
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	10	0.35	0.06	0.36
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	10	0.35	0.05	0.36
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	10	0.35	0.05	0.36
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	10	0.35	0.05	0.36
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	10	0.34	0.04	0.35
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	10	0.34	0.09	0.33
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	10	0.34	0.02	0.34
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	10	0.34	0.19	0.26
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	10	0.34	0.0	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	10	0.34	0.0	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	10	0.34	0.0	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	10	0.34	0.0	0.34
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	10	0.34	0.01	0.34
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	10	0.34	0.0	0.34
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	10	0.34	0.01	0.34
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	10	0.33	0.02	0.33
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	10	0.33	0.11	0.3
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	10	0.33	0.03	0.33
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	10	0.32	0.09	0.29
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	10	0.32	0.01	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	10	0.32	0.01	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	10	0.32	0.01	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	10	0.32	0.06	0.34
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	10	0.32	0.01	0.32
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	10	0.32	0.03	0.31
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	10	0.32	0.02	0.32
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	10	0.31	0.04	0.3
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	10	0.31	0.05	0.32
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	10	0.31	0.06	0.32
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	10	0.31	0.06	0.3
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	10	0.31	0.06	0.3
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	10	0.31	0.06	0.3
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	10	0.31	0.11	0.3
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	10	0.31	0.02	0.3
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	10	0.31	0.04	0.32
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	10	0.3	0.01	0.31
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	10	0.3	0.01	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	10	0.3	0.01	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	10	0.3	0.01	0.3
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	10	0.3	0.01	0.3
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	10	0.3	0.01	0.3
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	10	0.3	0.01	0.3
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	10	0.3	0.15	0.2
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	10	0.3	0.02	0.3
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	10	0.3	0.02	0.3
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	10	0.3	0.02	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	10	0.3	0.02	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	10	0.3	0.02	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	10	0.3	0.02	0.3
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	10	0.3	0.1	0.3
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	10	0.3	0.01	0.3
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	10	0.3	0.09	0.27
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	10	0.3	0.09	0.27
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	10	0.3	0.09	0.27
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	10	0.3	0.06	0.28
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	10	0.3	0.01	0.3
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	10	0.3	0.02	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	10	0.3	0.01	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	10	0.3	0.01	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	10	0.3	0.01	0.3
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	10	0.3	0.08	0.26
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	10	0.3	0.01	0.29
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	10	0.3	0.01	0.29
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	10	0.3	0.01	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	10	0.29	0.05	0.28
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	10	0.29	0.05	0.29
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	10	0.29	0.05	0.29
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	10	0.29	0.08	0.26
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	10	0.29	0.08	0.26
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	10	0.29	0.0	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	10	0.29	0.0	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	10	0.29	0.0	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	10	0.29	0.0	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	10	0.29	0.0	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	10	0.29	0.0	0.29
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	10	0.29	0.01	0.29
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	10	0.29	0.03	0.29
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	10	0.29	0.02	0.29
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	10	0.29	0.1	0.24
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	10	0.29	0.03	0.29
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	10	0.29	0.03	0.29
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	10	0.29	0.03	0.29
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	10	0.29	0.01	0.29
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	10	0.29	0.03	0.29
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	10	0.29	0.03	0.28
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	10	0.29	0.02	0.28
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	10	0.29	0.02	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	10	0.29	0.02	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	10	0.29	0.02	0.3
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	10	0.29	0.02	0.27
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	10	0.28	0.04	0.29
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	10	0.28	0.02	0.29
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	10	0.28	0.02	0.29
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	10	0.28	0.01	0.28
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	10	0.28	0.01	0.28
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	10	0.28	0.02	0.28
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	10	0.28	0.02	0.29
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	10	0.28	0.02	0.26
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	10	0.28	0.01	0.28
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	10	0.28	0.01	0.28
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	10	0.28	0.01	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	10	0.28	0.01	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	10	0.28	0.01	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	10	0.28	0.01	0.28
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	10	0.28	0.1	0.28
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	10	0.27	0.04	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	10	0.27	0.04	0.29
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	10	0.27	0.04	0.26
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	10	0.27	0.12	0.22
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	10	0.27	0.02	0.26
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	10	0.26	0.02	0.27
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	10	0.26	0.02	0.26
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	10	0.26	0.03	0.25
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	10	0.26	0.01	0.26
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	10	0.26	0.04	0.27
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	10	0.26	0.15	0.18
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	10	0.26	0.07	0.24
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	10	0.25	0.05	0.26
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	10	0.25	0.05	0.26
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	10	0.25	0.05	0.26
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	10	0.25	0.04	0.26
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	10	0.25	0.06	0.24
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	10	0.24	0.05	0.24
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	10	0.24	0.05	0.24
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	10	0.24	0.03	0.24
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	10	0.24	0.02	0.25
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	10	0.24	0.02	0.25
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	10	0.24	0.06	0.22
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	10	0.24	0.02	0.23
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	10	0.23	0.05	0.22
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	10	0.23	0.05	0.22
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	10	0.23	0.0	0.23
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	10	0.23	0.0	0.23
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	10	0.23	0.05	0.26
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	10	0.23	0.05	0.26
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	10	0.23	0.01	0.23
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	10	0.23	0.01	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	10	0.23	0.0	0.23
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	10	0.23	0.01	0.23
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	10	0.23	0.0	0.23
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	10	0.23	0.11	0.2
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	10	0.23	0.0	0.23
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	10	0.23	0.02	0.22
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	10	0.23	0.02	0.22
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	10	0.22	0.06	0.2
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	10	0.22	0.01	0.22
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	10	0.22	0.06	0.22
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	10	0.22	0.01	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	10	0.22	0.02	0.22
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	10	0.22	0.02	0.22
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	10	0.22	0.06	0.2
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	10	0.22	0.06	0.2
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	10	0.22	0.02	0.22
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	10	0.22	0.06	0.2
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	10	0.22	0.06	0.2
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	10	0.21	0.06	0.22
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	10	0.21	0.1	0.18
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	10	0.21	0.01	0.22
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	10	0.21	0.01	0.21
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	10	0.21	0.01	0.21
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	10	0.21	0.01	0.21
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	10	0.21	0.04	0.21
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	10	0.21	0.01	0.21
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	10	0.21	0.05	0.2
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	10	0.21	0.06	0.2
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	10	0.21	0.06	0.2
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	10	0.2	0.02	0.2
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	10	0.2	0.04	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	10	0.2	0.04	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	10	0.2	0.04	0.18
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	10	0.2	0.05	0.19
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	10	0.2	0.03	0.2
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	10	0.2	0.03	0.2
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	10	0.2	0.03	0.2
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	10	0.2	0.01	0.2
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	10	0.2	0.03	0.2
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	10	0.19	0.04	0.18
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	10	0.19	0.02	0.19
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	10	0.19	0.03	0.18
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	10	0.19	0.01	0.18
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	10	0.19	0.01	0.18
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	10	0.19	0.01	0.18
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	10	0.18	0.13	0.15
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	10	0.18	0.02	0.18
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	10	0.18	0.02	0.18
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	10	0.18	0.03	0.17
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	10	0.18	0.0	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	10	0.18	0.0	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	10	0.18	0.0	0.18
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	10	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	10	0.18	0.06	0.16
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	10	0.17	0.01	0.18
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	10	0.17	0.0	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	10	0.17	0.0	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	10	0.17	0.0	0.17
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	10	0.17	0.04	0.15
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	10	0.17	0.02	0.18
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	10	0.17	0.02	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	10	0.17	0.02	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	10	0.17	0.02	0.16
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	10	0.17	0.03	0.15
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	10	0.16	0.01	0.16
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	10	0.16	0.01	0.16
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	10	0.16	0.01	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	10	0.16	0.01	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	10	0.16	0.01	0.16
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	10	0.16	0.03	0.15
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	10	0.16	0.03	0.16
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	10	0.16	0.03	0.16
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	10	0.16	0.03	0.16
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	10	0.16	0.0	0.16
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	10	0.16	0.0	0.16
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	10	0.16	0.0	0.16
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	10	0.15	0.02	0.15
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	10	0.15	0.02	0.15
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	10	0.15	0.02	0.15
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	10	0.15	0.02	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	10	0.15	0.02	0.16
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	10	0.15	0.03	0.14
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	10	0.15	0.03	0.13
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	10	0.14	0.0	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	10	0.14	0.02	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	10	0.14	0.02	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	10	0.14	0.02	0.14
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	10	0.13	0.01	0.13
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	10	0.13	0.01	0.12
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	9	1.56	0.2	1.58
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	9	1.23	0.56	1.5
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	9	1.23	0.56	1.5
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	9	1.23	0.56	1.5
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	9	1.2	0.04	1.19
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	9	1.1	0.39	1.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	9	1.1	0.39	1.27
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	9	1.1	0.39	1.27
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	9	0.99	0.25	1.11
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	9	0.85	0.58	0.53
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	9	0.83	0.51	1.23
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	9	0.83	0.51	1.23
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	9	0.83	0.51	1.23
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	9	0.81	0.33	0.96
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	9	0.8	0.12	0.85
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	9	0.8	0.12	0.85
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	9	0.8	0.12	0.85
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	9	0.76	0.29	0.73
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	9	0.76	0.29	0.73
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	9	0.73	0.23	0.73
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	9	0.73	0.23	0.73
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	9	0.73	0.23	0.73
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	9	0.71	0.25	0.82
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	9	0.63	0.06	0.63
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	9	0.63	0.06	0.63
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	9	0.6	0.06	0.6
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	9	0.6	0.22	0.62
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	9	0.6	0.22	0.62
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	9	0.6	0.22	0.62
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	9	0.58	0.27	0.46
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	9	0.55	0.04	0.58
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	9	0.55	0.04	0.58
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	9	0.55	0.2	0.55
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	9	0.51	0.19	0.56
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	9	0.51	0.19	0.56
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	9	0.51	0.19	0.56
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	9	0.5	0.13	0.47
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	9	0.45	0.2	0.56
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	9	0.45	0.24	0.4
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	9	0.42	0.45	0.28
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	9	0.42	0.3	0.32
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	9	0.41	0.21	0.36
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	9	0.41	0.21	0.36
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	9	0.41	0.13	0.35
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	9	0.37	0.17	0.29
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	9	0.37	0.17	0.29
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	9	0.37	0.17	0.29
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	9	0.37	0.06	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	9	0.34	0.02	0.34
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	9	0.33	0.07	0.32
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	9	0.32	0.1	0.28
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	9	0.31	0.13	0.38
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	9	0.31	0.13	0.38
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	9	0.31	0.13	0.38
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	9	0.3	0.15	0.2
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	9	0.3	0.15	0.2
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	9	0.3	0.15	0.2
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	9	0.28	0.01	0.28
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	9	0.26	0.07	0.31
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	9	0.26	0.07	0.31
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	9	0.26	0.04	0.26
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	9	0.25	0.03	0.26
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	9	0.25	0.03	0.26
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	9	0.25	0.03	0.26
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	9	0.25	0.1	0.22
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	9	0.25	0.1	0.22
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	9	0.21	0.05	0.2
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	9	0.21	0.07	0.2
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	9	0.21	0.07	0.2
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	9	0.21	0.07	0.2
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	9	0.2	0.05	0.18
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	9	0.2	0.01	0.2
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	9	0.19	0.07	0.17
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	9	0.19	0.05	0.2
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	9	0.19	0.03	0.18
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	9	0.18	0.05	0.17
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	9	0.16	0.04	0.14
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	9	0.14	0.01	0.14
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	9	0.14	0.02	0.14
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	9	0.11	0.01	0.11
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	9	0.11	0.01	0.11
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	9	0.11	0.01	0.11
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	8	1.29	0.3	1.23
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	8	0.88	0.28	0.94
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	8	0.88	0.28	0.94
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	8	0.88	0.28	0.94
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	8	0.78	0.42	0.8
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	8	0.78	0.42	0.8
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	8	0.78	0.42	0.8
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	8	0.78	0.22	0.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	8	0.78	0.22	0.88
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	8	0.78	0.22	0.88
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	8	0.77	0.02	0.76
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	8	0.7	0.08	0.7
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	8	0.67	0.06	0.66
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	8	0.67	0.06	0.66
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	8	0.67	0.06	0.66
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	8	0.57	0.18	0.64
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	8	0.57	0.18	0.64
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	8	0.56	0.0	0.56
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	8	0.54	0.24	0.57
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	8	0.52	0.22	0.42
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	8	0.5	0.21	0.47
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	8	0.5	0.21	0.47
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	8	0.5	0.21	0.47
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	8	0.47	0.02	0.48
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	8	0.46	0.27	0.4
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	8	0.46	0.27	0.4
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	8	0.46	0.27	0.4
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	8	0.42	0.12	0.45
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	8	0.42	0.12	0.45
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	8	0.42	0.12	0.45
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	8	0.39	0.09	0.42
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	8	0.38	0.12	0.37
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	8	0.38	0.12	0.37
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	8	0.32	0.23	0.24
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	8	0.3	0.13	0.28
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	8	0.3	0.13	0.28
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	8	0.3	0.13	0.28
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	8	0.28	0.23	0.16
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	8	0.27	0.08	0.25
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	8	0.26	0.04	0.26
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	8	0.25	0.02	0.25
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	8	0.24	0.05	0.24
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	8	0.24	0.05	0.24
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	8	0.2	0.01	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	8	0.2	0.01	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	8	0.2	0.01	0.2
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	8	0.19	0.13	0.12
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	8	0.18	0.04	0.18
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	8	0.18	0.06	0.17
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	8	0.17	0.04	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	8	0.16	0.03	0.17
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	8	0.16	0.03	0.17
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	8	0.16	0.03	0.17
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	8	0.15	0.03	0.16
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	8	0.14	0.02	0.15
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	8	0.11	0.01	0.11
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	8	0.11	0.01	0.11
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG21	7	1.11	0.15	1.19
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG22	7	1.11	0.15	1.19
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG23	7	1.11	0.15	1.19
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG21	7	1.11	0.15	1.19
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG22	7	1.11	0.15	1.19
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG23	7	1.11	0.15	1.19
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG21	7	1.11	0.15	1.19
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG22	7	1.11	0.15	1.19
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG23	7	1.11	0.15	1.19
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HE1	7	0.87	0.73	0.67
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HD2	7	0.87	0.73	0.67
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HE2	7	0.87	0.73	0.67
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HD1	7	0.87	0.73	0.67
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD11	7	0.82	0.08	0.83
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD12	7	0.82	0.08	0.83
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD13	7	0.82	0.08	0.83
(2,198)	1:74:A:SER:H	1:73:A:TYR:HB3	7	0.69	0.09	0.68
(1,112)	1:67:A:ARG:HG3	1:67:A:ARG:HD3	7	0.68	0.05	0.67
(1,448)	1:14:A:LEU:HD11	1:18:A:LEU:HG	7	0.6	0.59	0.17
(1,448)	1:14:A:LEU:HD12	1:18:A:LEU:HG	7	0.6	0.59	0.17
(1,448)	1:14:A:LEU:HD13	1:18:A:LEU:HG	7	0.6	0.59	0.17
(1,170)	1:67:A:ARG:HG2	1:67:A:ARG:HD3	7	0.55	0.03	0.54
(1,32)	1:67:A:ARG:HA	1:67:A:ARG:HB2	7	0.53	0.16	0.58
(2,34)	1:50:A:ILE:H	1:4:A:GLN:HA	7	0.5	0.15	0.54
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB1	7	0.48	0.09	0.49
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB2	7	0.48	0.09	0.49
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB3	7	0.48	0.09	0.49
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD11	7	0.38	0.17	0.39
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD12	7	0.38	0.17	0.39
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD13	7	0.38	0.17	0.39
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD11	7	0.37	0.31	0.14
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD12	7	0.37	0.31	0.14
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD13	7	0.37	0.31	0.14
(1,283)	1:39:A:ARG:HD3	1:39:A:ARG:HB3	7	0.37	0.15	0.41
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD11	7	0.36	0.15	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD12	7	0.36	0.15	0.42
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD13	7	0.36	0.15	0.42
(1,122)	1:26:A:HIS:HB3	1:26:A:HIS:HA	7	0.34	0.02	0.34
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD21	7	0.34	0.07	0.34
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD22	7	0.34	0.07	0.34
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD23	7	0.34	0.07	0.34
(2,284)	1:76:A:GLN:H	1:64:A:GLU:H	7	0.33	0.18	0.25
(2,47)	1:61:A:THR:H	1:60:A:GLY:HA2	7	0.31	0.03	0.32
(2,51)	1:80:A:SER:H	1:80:A:SER:HB3	7	0.31	0.05	0.32
(2,419)	1:72:A:SER:H	1:70:A:ASN:HA	7	0.23	0.09	0.2
(1,329)	1:72:A:SER:HB3	1:72:A:SER:HA	7	0.22	0.06	0.21
(2,325)	1:70:A:ASN:HD22	1:70:A:ASN:HB3	7	0.21	0.02	0.21
(2,382)	1:43:A:GLY:H	1:57:A:LEU:HA	7	0.2	0.05	0.2
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE1	7	0.19	0.03	0.19
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE2	7	0.19	0.03	0.19
(1,181)	1:75:A:LEU:HA	1:76:A:GLN:H	7	0.18	0.07	0.17
(2,422)	1:76:A:GLN:H	1:75:A:LEU:HA	7	0.18	0.07	0.17
(2,228)	1:60:A:GLY:H	1:60:A:GLY:HA2	7	0.17	0.01	0.17
(1,22)	1:55:A:ALA:HA	1:55:A:ALA:H	7	0.15	0.04	0.17
(1,452)	1:66:A:SER:HA	1:66:A:SER:HB2	7	0.15	0.01	0.15
(4,38)	1:14:A:LEU:N	1:39:A:ARG:O	7	0.15	0.02	0.15
(1,482)	1:73:A:TYR:HB2	1:73:A:TYR:H	6	0.84	0.04	0.85
(1,11)	1:76:A:GLN:HA	1:64:A:GLU:HG3	6	0.66	0.12	0.68
(2,152)	1:12:A:GLY:H	1:40:A:SER:HB2	6	0.65	0.31	0.69
(2,176)	1:68:A:GLY:H	1:67:A:ARG:HG3	6	0.62	0.12	0.64
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD11	6	0.58	0.44	0.52
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD12	6	0.58	0.44	0.52
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD13	6	0.58	0.44	0.52
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD11	6	0.58	0.44	0.52
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD12	6	0.58	0.44	0.52
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD13	6	0.58	0.44	0.52
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD11	6	0.58	0.44	0.52
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD12	6	0.58	0.44	0.52
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD13	6	0.58	0.44	0.52
(2,66)	1:17:A:ALA:H	1:16:A:PRO:HB2	6	0.52	0.04	0.52
(2,59)	1:66:A:SER:H	1:66:A:SER:HB3	6	0.52	0.02	0.52
(2,224)	1:19:A:ALA:H	1:18:A:LEU:HB2	6	0.46	0.24	0.54
(1,228)	1:39:A:ARG:HD3	1:38:A:GLY:HA3	6	0.41	0.22	0.36
(1,410)	1:55:A:ALA:HB1	1:52:A:GLN:HA	6	0.35	0.07	0.38
(1,410)	1:55:A:ALA:HB2	1:52:A:GLN:HA	6	0.35	0.07	0.38
(1,410)	1:55:A:ALA:HB3	1:52:A:GLN:HA	6	0.35	0.07	0.38
(2,189)	1:68:A:GLY:H	1:73:A:TYR:HA	6	0.35	0.14	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,468)	1:77:A:ALA:H	1:64:A:GLU:HG3	6	0.35	0.26	0.26
(1,393)	1:72:A:SER:HA	1:28:A:LEU:HB2	6	0.35	0.19	0.31
(2,227)	1:19:A:ALA:H	1:16:A:PRO:HB2	6	0.28	0.14	0.23
(2,466)	1:39:A:ARG:HE	1:39:A:ARG:HD2	6	0.28	0.17	0.19
(1,241)	1:39:A:ARG:HD3	1:35:A:LEU:HG	6	0.27	0.05	0.27
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG21	6	0.26	0.09	0.29
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG22	6	0.26	0.09	0.29
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG23	6	0.26	0.09	0.29
(2,211)	1:58:A:LEU:H	1:59:A:ALA:H	6	0.25	0.11	0.2
(1,46)	1:73:A:TYR:HA	1:68:A:GLY:H	6	0.25	0.14	0.18
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB1	6	0.2	0.05	0.2
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB2	6	0.2	0.05	0.2
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB3	6	0.2	0.05	0.2
(1,253)	1:40:A:SER:HA	1:41:A:THR:H	6	0.19	0.06	0.18
(1,418)	1:29:A:LEU:HB3	1:29:A:LEU:HA	6	0.17	0.01	0.18
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD21	6	0.17	0.04	0.16
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD22	6	0.17	0.04	0.16
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD23	6	0.17	0.04	0.16
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD21	6	0.17	0.04	0.16
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD22	6	0.17	0.04	0.16
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD23	6	0.17	0.04	0.16
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD21	6	0.17	0.04	0.16
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD22	6	0.17	0.04	0.16
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD23	6	0.17	0.04	0.16
(1,1)	1:15:A:ALA:HB1	1:16:A:PRO:HB2	6	0.16	0.04	0.16
(1,1)	1:15:A:ALA:HB2	1:16:A:PRO:HB2	6	0.16	0.04	0.16
(1,1)	1:15:A:ALA:HB3	1:16:A:PRO:HB2	6	0.16	0.04	0.16
(1,111)	1:64:A:GLU:HA	1:65:A:ALA:H	6	0.14	0.03	0.14
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD11	5	1.14	0.32	1.29
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD12	5	1.14	0.32	1.29
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD13	5	1.14	0.32	1.29
(2,350)	1:41:A:THR:H	1:40:A:SER:HB2	5	0.78	0.42	0.8
(1,218)	1:40:A:SER:HB2	1:41:A:THR:H	5	0.68	0.42	0.7
(1,485)	1:37:A:GLU:HB2	1:37:A:GLU:HA	5	0.65	0.02	0.66
(1,96)	1:37:A:GLU:HB3	1:37:A:GLU:H	5	0.45	0.06	0.48
(1,286)	1:47:A:ARG:HD2	1:47:A:ARG:HE	5	0.42	0.12	0.46
(3,18)	1:12:A:GLY:HA3	1:13:A:PRO:HD3	5	0.41	0.04	0.41
(2,313)	1:58:A:LEU:H	1:54:A:LEU:HA	5	0.4	0.19	0.47
(1,420)	1:37:A:GLU:HB2	1:37:A:GLU:HG3	5	0.36	0.02	0.36
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB1	5	0.34	0.2	0.32
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB2	5	0.34	0.2	0.32
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB3	5	0.34	0.2	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB2	5	0.34	0.08	0.32
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB3	5	0.34	0.08	0.32
(2,103)	1:43:A:GLY:H	1:11:A:ALA:HA	5	0.29	0.19	0.22
(1,365)	1:37:A:GLU:HA	1:37:A:GLU:HG2	5	0.26	0.04	0.27
(2,53)	1:38:A:GLY:H	1:37:A:GLU:HG3	5	0.26	0.09	0.26
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD11	5	0.25	0.14	0.21
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD12	5	0.25	0.14	0.21
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD13	5	0.25	0.14	0.21
(1,354)	1:75:A:LEU:HD11	1:75:A:LEU:HB3	5	0.22	0.09	0.2
(1,354)	1:75:A:LEU:HD12	1:75:A:LEU:HB3	5	0.22	0.09	0.2
(1,354)	1:75:A:LEU:HD13	1:75:A:LEU:HB3	5	0.22	0.09	0.2
(2,409)	1:21:A:PHE:H	1:18:A:LEU:HA	5	0.21	0.1	0.15
(1,103)	1:37:A:GLU:HB2	1:37:A:GLU:H	5	0.2	0.07	0.25
(2,489)	1:69:A:ALA:H	1:68:A:GLY:HA2	5	0.2	0.04	0.21
(1,214)	1:66:A:SER:HA	1:67:A:ARG:H	5	0.19	0.03	0.2
(1,78)	1:57:A:LEU:HD21	1:57:A:LEU:HB3	5	0.18	0.05	0.21
(1,78)	1:57:A:LEU:HD22	1:57:A:LEU:HB3	5	0.18	0.05	0.21
(1,78)	1:57:A:LEU:HD23	1:57:A:LEU:HB3	5	0.18	0.05	0.21
(1,303)	1:78:A:SER:HA	1:78:A:SER:HB2	5	0.17	0.08	0.12
(1,87)	1:63:A:LEU:HD21	1:64:A:GLU:H	5	0.16	0.05	0.14
(1,87)	1:63:A:LEU:HD22	1:64:A:GLU:H	5	0.16	0.05	0.14
(1,87)	1:63:A:LEU:HD23	1:64:A:GLU:H	5	0.16	0.05	0.14
(1,483)	1:64:A:GLU:HB3	1:64:A:GLU:HA	5	0.16	0.03	0.17
(4,1)	1:18:A:LEU:H	1:14:A:LEU:O	5	0.12	0.02	0.11
(4,16)	1:46:A:GLY:N	1:7:A:PHE:O	5	0.12	0.02	0.11
(4,15)	1:46:A:GLY:H	1:7:A:PHE:O	5	0.11	0.0	0.11
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD11	4	1.27	0.42	1.48
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD12	4	1.27	0.42	1.48
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD13	4	1.27	0.42	1.48
(2,410)	1:4:A:GLN:H	1:4:A:GLN:HG2	4	1.05	0.57	0.9
(2,69)	1:39:A:ARG:HE	1:39:A:ARG:HB2	4	1.0	0.44	1.17
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD11	4	0.64	0.1	0.6
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD12	4	0.64	0.1	0.6
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD13	4	0.64	0.1	0.6
(1,13)	1:73:A:TYR:HA	1:73:A:TYR:HB2	4	0.48	0.15	0.56
(1,436)	1:67:A:ARG:HA	1:67:A:ARG:HG2	4	0.4	0.03	0.41
(2,250)	1:55:A:ALA:H	1:54:A:LEU:HG	4	0.35	0.22	0.26
(2,185)	1:74:A:SER:H	1:67:A:ARG:HA	4	0.31	0.17	0.3
(1,304)	1:14:A:LEU:HD11	1:36:A:THR:HA	4	0.22	0.06	0.22
(1,304)	1:14:A:LEU:HD12	1:36:A:THR:HA	4	0.22	0.06	0.22
(1,304)	1:14:A:LEU:HD13	1:36:A:THR:HA	4	0.22	0.06	0.22
(1,36)	1:52:A:GLN:HB3	1:52:A:GLN:H	4	0.21	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,380)	1:52:A:GLN:H	1:52:A:GLN:HB3	4	0.21	0.05	0.2
(2,16)	1:36:A:THR:H	1:35:A:LEU:H	4	0.2	0.03	0.21
(1,145)	1:11:A:ALA:HA	1:12:A:GLY:H	4	0.19	0.05	0.21
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.17	0.03	0.16
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.17	0.03	0.16
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.17	0.03	0.16
(1,412)	1:42:A:SER:HA	1:42:A:SER:H	4	0.14	0.07	0.11
(1,231)	1:14:A:LEU:HB3	1:14:A:LEU:H	4	0.14	0.04	0.12
(1,340)	1:38:A:GLY:HA2	1:38:A:GLY:H	4	0.14	0.02	0.13
(3,12)	1:32:A:PRO:HG2	1:32:A:PRO:HD2	4	0.12	0.01	0.12
(3,12)	1:32:A:PRO:HG3	1:32:A:PRO:HD2	4	0.12	0.01	0.12
(1,484)	1:29:A:LEU:HA	1:30:A:SER:H	4	0.12	0.02	0.12
(2,387)	1:61:A:THR:H	1:60:A:GLY:H	3	1.91	0.05	1.92
(1,353)	1:39:A:ARG:HB3	1:40:A:SER:H	3	0.95	0.09	0.9
(1,162)	1:73:A:TYR:HB3	1:73:A:TYR:H	3	0.91	0.01	0.9
(2,386)	1:61:A:THR:H	1:60:A:GLY:HA3	3	0.85	0.02	0.86
(5,11)	1:34:A:ALA:H	1:32:A:PRO:HG2	3	0.8	0.45	0.88
(5,11)	1:34:A:ALA:H	1:32:A:PRO:HG3	3	0.8	0.45	0.88
(1,53)	1:11:A:ALA:HA	1:43:A:GLY:HA3	3	0.77	0.18	0.65
(2,77)	1:40:A:SER:H	1:39:A:ARG:HB3	3	0.75	0.09	0.7
(2,48)	1:72:A:SER:H	1:70:A:ASN:HB3	3	0.71	0.82	0.14
(1,324)	1:73:A:TYR:HA	1:67:A:ARG:HA	3	0.68	0.22	0.67
(3,21)	1:14:A:LEU:HD13	1:14:A:LEU:HA	3	0.66	0.04	0.64
(3,21)	1:14:A:LEU:HD11	1:14:A:LEU:HA	3	0.66	0.04	0.64
(3,21)	1:14:A:LEU:HD12	1:14:A:LEU:HA	3	0.66	0.04	0.64
(2,115)	1:26:A:HIS:H	1:26:A:HIS:HB2	3	0.44	0.01	0.44
(1,330)	1:13:A:PRO:HA	1:40:A:SER:HB2	3	0.42	0.14	0.4
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD21	3	0.38	0.31	0.21
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD22	3	0.38	0.31	0.21
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD23	3	0.38	0.31	0.21
(1,38)	1:26:A:HIS:HB2	1:26:A:HIS:HA	3	0.38	0.01	0.38
(2,113)	1:41:A:THR:H	1:40:A:SER:HB3	3	0.38	0.12	0.34
(1,254)	1:9:A:ILE:HA	1:10:A:PRO:HD3	3	0.38	0.12	0.31
(2,355)	1:20:A:HIS:H	1:20:A:HIS:HB3	3	0.36	0.02	0.37
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD11	3	0.34	0.06	0.3
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD12	3	0.34	0.06	0.3
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD13	3	0.34	0.06	0.3
(1,296)	1:27:A:ILE:HG13	1:27:A:ILE:H	3	0.28	0.14	0.23
(1,424)	1:40:A:SER:HB3	1:41:A:THR:H	3	0.28	0.12	0.24
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD11	3	0.28	0.1	0.34
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD12	3	0.28	0.1	0.34
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD13	3	0.28	0.1	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,17)	1:20:A:HIS:HB3	1:20:A:HIS:H	3	0.26	0.02	0.27
(3,36)	1:73:A:TYR:HB2	1:29:A:LEU:HA	3	0.25	0.04	0.22
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD11	3	0.24	0.13	0.16
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD12	3	0.24	0.13	0.16
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD13	3	0.24	0.13	0.16
(1,438)	1:74:A:SER:HA	1:75:A:LEU:H	3	0.24	0.02	0.25
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD11	3	0.23	0.13	0.18
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD12	3	0.23	0.13	0.18
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD13	3	0.23	0.13	0.18
(2,142)	1:59:A:ALA:H	1:56:A:ILE:HA	3	0.23	0.02	0.22
(1,167)	1:54:A:LEU:HB3	1:51:A:ASP:HA	3	0.22	0.07	0.21
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD11	3	0.22	0.08	0.21
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD12	3	0.22	0.08	0.21
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD13	3	0.22	0.08	0.21
(3,10)	1:30:A:SER:HB2	1:30:A:SER:H	3	0.2	0.06	0.24
(2,97)	1:55:A:ALA:H	1:52:A:GLN:HA	3	0.2	0.07	0.23
(2,29)	1:14:A:LEU:H	1:13:A:PRO:HB2	3	0.16	0.0	0.16
(4,37)	1:14:A:LEU:H	1:39:A:ARG:O	3	0.16	0.05	0.15
(2,46)	1:55:A:ALA:H	1:54:A:LEU:H	3	0.14	0.04	0.12
(1,447)	1:61:A:THR:HA	1:61:A:THR:HB	3	0.14	0.0	0.14
(1,240)	1:44:A:LEU:HD21	1:56:A:ILE:HB	3	0.13	0.02	0.11
(1,240)	1:44:A:LEU:HD22	1:56:A:ILE:HB	3	0.13	0.02	0.11
(1,240)	1:44:A:LEU:HD23	1:56:A:ILE:HB	3	0.13	0.02	0.11
(1,3)	1:79:A:ALA:HB1	1:79:A:ALA:H	3	0.12	0.01	0.12
(1,3)	1:79:A:ALA:HB2	1:79:A:ALA:H	3	0.12	0.01	0.12
(1,3)	1:79:A:ALA:HB3	1:79:A:ALA:H	3	0.12	0.01	0.12
(1,493)	1:7:A:PHE:HB2	1:7:A:PHE:H	3	0.12	0.0	0.12
(2,328)	1:37:A:GLU:H	1:33:A:THR:HB	2	1.12	0.48	1.12
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD21	2	1.09	0.02	1.09
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD22	2	1.09	0.02	1.09
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD23	2	1.09	0.02	1.09
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD11	2	0.96	0.03	0.96
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD12	2	0.96	0.03	0.96
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD13	2	0.96	0.03	0.96
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD11	2	0.96	0.03	0.96
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD12	2	0.96	0.03	0.96
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD13	2	0.96	0.03	0.96
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD11	2	0.96	0.03	0.96
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD12	2	0.96	0.03	0.96
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD13	2	0.96	0.03	0.96
(2,75)	1:75:A:LEU:H	1:31:A:TYR:HB2	2	0.94	0.03	0.94
(2,393)	1:24:A:SER:H	1:24:A:SER:HB2	2	0.84	0.02	0.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,317)	1:47:A:ARG:HB2	1:47:A:ARG:HD2	2	0.77	0.03	0.77
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD11	2	0.74	0.0	0.74
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD12	2	0.74	0.0	0.74
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD13	2	0.74	0.0	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD11	2	0.74	0.0	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD12	2	0.74	0.0	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD13	2	0.74	0.0	0.74
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD11	2	0.74	0.0	0.74
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD12	2	0.74	0.0	0.74
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD13	2	0.74	0.0	0.74
(2,332)	1:42:A:SER:H	1:41:A:THR:HG1	2	0.66	0.54	0.66
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD11	2	0.6	0.25	0.6
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD12	2	0.6	0.25	0.6
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD13	2	0.6	0.25	0.6
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD11	2	0.6	0.25	0.6
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD12	2	0.6	0.25	0.6
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD13	2	0.6	0.25	0.6
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD11	2	0.6	0.25	0.6
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD12	2	0.6	0.25	0.6
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD13	2	0.6	0.25	0.6
(1,280)	1:31:A:TYR:HB3	1:32:A:PRO:HD2	2	0.55	0.06	0.55
(2,251)	1:12:A:GLY:H	1:43:A:GLY:HA2	2	0.54	0.19	0.54
(1,265)	1:49:A:ASP:HA	1:4:A:GLN:HG2	2	0.48	0.3	0.48
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB1	2	0.43	0.13	0.43
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB2	2	0.43	0.13	0.43
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB3	2	0.43	0.13	0.43
(1,371)	1:49:A:ASP:HA	1:49:A:ASP:HB3	2	0.41	0.01	0.41
(2,7)	1:30:A:SER:H	1:29:A:LEU:HB3	2	0.41	0.08	0.41
(2,43)	1:54:A:LEU:H	1:54:A:LEU:HG	2	0.39	0.02	0.39
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD11	2	0.32	0.2	0.32
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD12	2	0.32	0.2	0.32
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD13	2	0.32	0.2	0.32
(1,27)	1:67:A:ARG:HA	1:67:A:ARG:HG3	2	0.31	0.04	0.31
(1,200)	1:14:A:LEU:HD11	1:36:A:THR:HB	2	0.29	0.02	0.29
(1,200)	1:14:A:LEU:HD12	1:36:A:THR:HB	2	0.29	0.02	0.29
(1,200)	1:14:A:LEU:HD13	1:36:A:THR:HB	2	0.29	0.02	0.29
(2,323)	1:68:A:GLY:H	1:67:A:ARG:HB2	2	0.29	0.01	0.29
(4,39)	1:12:A:GLY:H	1:41:A:THR:O	2	0.28	0.17	0.28
(2,333)	1:37:A:GLU:H	1:37:A:GLU:HG2	2	0.24	0.01	0.24
(1,95)	1:63:A:LEU:HA	1:78:A:SER:H	2	0.24	0.08	0.24
(2,473)	1:78:A:SER:H	1:63:A:LEU:HA	2	0.24	0.08	0.24
(2,38)	1:50:A:ILE:H	1:49:A:ASP:HB2	2	0.23	0.06	0.23

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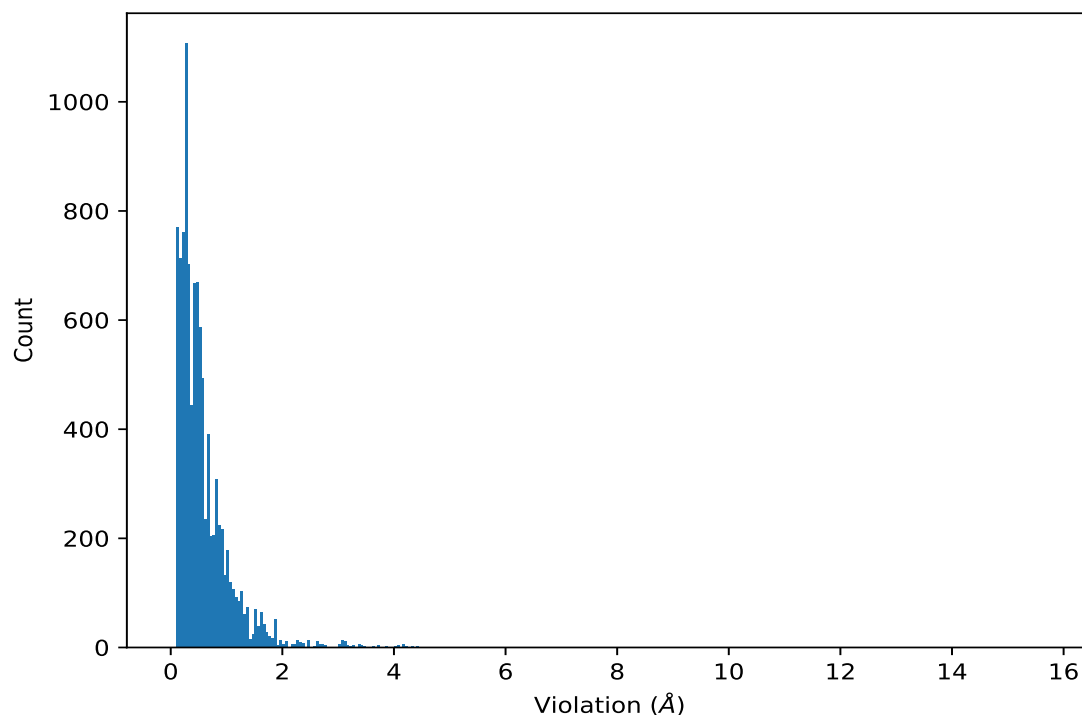
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,425)	1:71:A:ALA:HB1	1:71:A:ALA:H	2	0.22	0.11	0.22
(1,425)	1:71:A:ALA:HB2	1:71:A:ALA:H	2	0.22	0.11	0.22
(1,425)	1:71:A:ALA:HB3	1:71:A:ALA:H	2	0.22	0.11	0.22
(1,237)	1:75:A:LEU:HB3	1:75:A:LEU:H	2	0.22	0.08	0.22
(1,440)	1:18:A:LEU:HA	1:21:A:PHE:HB2	2	0.19	0.07	0.19
(1,146)	1:63:A:LEU:HB3	1:63:A:LEU:HG	2	0.18	0.01	0.18
(1,73)	1:76:A:GLN:HA	1:77:A:ALA:H	2	0.18	0.03	0.18
(2,157)	1:53:A:GLY:H	1:48:A:PHE:HB3	2	0.18	0.06	0.18
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD21	2	0.17	0.01	0.17
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD22	2	0.17	0.01	0.17
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD23	2	0.17	0.01	0.17
(2,459)	1:66:A:SER:H	1:73:A:TYR:HB2	2	0.16	0.04	0.16
(2,54)	1:38:A:GLY:H	1:39:A:ARG:HA	2	0.16	0.02	0.16
(1,268)	1:13:A:PRO:HD3	1:13:A:PRO:HA	2	0.16	0.01	0.16
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD11	2	0.14	0.01	0.14
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD12	2	0.14	0.01	0.14
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD13	2	0.14	0.01	0.14
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB1	2	0.14	0.02	0.14
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB2	2	0.14	0.02	0.14
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB3	2	0.14	0.02	0.14
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB1	2	0.14	0.02	0.14
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB2	2	0.14	0.02	0.14
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB3	2	0.14	0.02	0.14
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB1	2	0.14	0.02	0.14
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB2	2	0.14	0.02	0.14
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB3	2	0.14	0.02	0.14
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD21	2	0.14	0.02	0.14
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD22	2	0.14	0.02	0.14
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD23	2	0.14	0.02	0.14
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD21	2	0.12	0.02	0.12
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD22	2	0.12	0.02	0.12
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD23	2	0.12	0.02	0.12
(1,455)	1:19:A:ALA:HB1	1:20:A:HIS:H	2	0.12	0.01	0.12
(1,455)	1:19:A:ALA:HB2	1:20:A:HIS:H	2	0.12	0.01	0.12
(1,455)	1:19:A:ALA:HB3	1:20:A:HIS:H	2	0.12	0.01	0.12
(1,372)	1:40:A:SER:HA	1:40:A:SER:HB2	2	0.12	0.0	0.12
(2,371)	1:74:A:SER:H	1:73:A:TYR:HB2	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	3	15.71
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	7	10.42
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	2	9.86
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	6	9.25
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	9	9.01
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	8	8.84
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	10	8.51
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	5	8.4
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	4	8.25
(1,5)	1:21:A:PHE:HB2	1:1:A:GLY:HA3	1	7.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	10	5.08
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	9	4.63
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	5	4.44
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	5	4.44
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	5	4.44
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	3	4.36
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	6	4.3
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	6	4.3
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	6	4.3
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	1	4.26
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	2	4.21
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	2	4.21
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	2	4.21
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	4	4.18
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	4	4.18
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	4	4.18
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	1	4.16
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	1	4.16
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	1	4.16
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	3	4.1
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	3	4.1
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	3	4.1
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	4	4.07
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	1	4.04
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	1	4.04
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	1	4.04
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	5	3.98
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	7	3.86
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	7	3.86
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	7	3.86
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	9	3.73
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	9	3.73
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	9	3.7
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	9	3.7
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	9	3.7
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	10	3.65
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	10	3.65
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	6	3.49
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	6	3.49
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	6	3.49
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	1	3.44
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	4	3.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	4	3.42
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	4	3.42
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	5	3.38
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	3	3.36
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	3	3.36
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	3	3.36
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	10	3.36
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	10	3.36
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	10	3.36
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	6	3.29
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	6	3.29
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	5	3.27
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	5	3.27
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	8	3.22
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	8	3.22
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	8	3.22
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	9	3.18
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	2	3.16
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	2	3.16
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	2	3.16
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	9	3.13
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	9	3.13
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	9	3.13
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	10	3.11
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	10	3.11
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	10	3.11
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	10	3.11
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	10	3.11
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	10	3.11
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	10	3.11
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	10	3.11
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	10	3.11
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	3	3.09
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	7	3.06
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	7	3.06
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	7	3.06
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	9	3.06
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	9	3.06
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	9	3.06
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	9	3.06
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	9	3.06
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	9	3.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	9	3.06
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	9	3.06
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	9	3.06
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	5	3.05
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	5	3.05
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	5	3.05
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	8	3.0
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	8	3.0
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	2	3.0
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	10	2.89
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	9	2.8
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	9	2.8
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	9	2.8
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	8	2.79
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	6	2.75
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	5	2.74
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	2	2.72
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	4	2.72
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	10	2.72
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	2	2.72
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	6	2.72
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	1	2.71
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	4	2.69
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	5	2.69
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	9	2.69
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	10	2.68
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	10	2.68
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	10	2.68
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	8	2.68
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	7	2.65
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	2	2.65
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	7	2.65
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	9	2.62
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD11	8	2.62
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD12	8	2.62
(1,491)	1:63:A:LEU:HG	1:18:A:LEU:HD13	8	2.62
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	1	2.61
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	1	2.61
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	1	2.6
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	9	2.6
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	5	2.59
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	3	2.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,7)	1:7:A:PHE:H	1:45:A:ALA:O	8	2.57
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	6	2.49
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	1	2.49
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	1	2.49
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	1	2.49
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	10	2.49
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	8	2.46
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	7	2.45
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	5	2.45
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	5	2.45
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	5	2.45
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	10	2.45
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	10	2.45
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	10	2.45
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	3	2.45
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	1	2.42
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	7	2.4
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	3	2.4
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	3	2.4
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	3	2.4
(1,57)	1:10:A:PRO:HG3	1:11:A:ALA:HA	8	2.39
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	8	2.38
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	10	2.37
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	7	2.36
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	3	2.35
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	4	2.33
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	6	2.33
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	6	2.33
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	6	2.33
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	4	2.32
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	4	2.32
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	4	2.32
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	2	2.32
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	4	2.32
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	6	2.31
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	6	2.3
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	4	2.29
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	4	2.29
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	4	2.29
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	2	2.28
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	4	2.28
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	9	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	10	2.28
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	2	2.28
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	2	2.28
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	2	2.28
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	1	2.27
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	3	2.26
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	5	2.25
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	7	2.24
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	1	2.22
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	5	2.21
(4,8)	1:7:A:PHE:N	1:45:A:ALA:O	8	2.21
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	3	2.2
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	3	2.2
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	3	2.2
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	2	2.18
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	2	2.18
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	5	2.18
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	5	2.18
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	5	2.18
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	7	2.15
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	7	2.15
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	10	2.13
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	8	2.08
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	8	2.08
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	8	2.08
(1,102)	1:57:A:LEU:HD11	1:14:A:LEU:HB3	10	2.07
(1,102)	1:57:A:LEU:HD12	1:14:A:LEU:HB3	10	2.07
(1,102)	1:57:A:LEU:HD13	1:14:A:LEU:HB3	10	2.07
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	2	2.06
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HD2	8	2.06
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	3	2.06
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	2	2.06
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	2	2.06
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	2	2.06
(1,190)	1:28:A:LEU:HB3	1:27:A:ILE:H	9	2.05
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	3	2.01
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	3	2.01
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	3	2.01
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	7	2.0
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	7	2.0
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	7	2.0
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	9	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	3	1.99
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	9	1.99
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	9	1.99
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	9	1.99
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	10	1.98
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	10	1.98
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	10	1.98
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	1	1.97
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	3	1.96
(2,410)	1:4:A:GLN:H	1:4:A:GLN:HG2	9	1.96
(2,387)	1:61:A:THR:H	1:60:A:GLY:H	7	1.96
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	6	1.96
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	4	1.94
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	7	1.94
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	7	1.94
(2,387)	1:61:A:THR:H	1:60:A:GLY:H	8	1.92
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	8	1.91
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	5	1.9
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	4	1.9
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	4	1.9
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	9	1.9
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	9	1.9
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	10	1.9
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	10	1.9
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	7	1.9
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	7	1.9
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	7	1.9
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	10	1.89
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HD1	9	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	1	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	1	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	1	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	2	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	2	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	2	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	6	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	6	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	6	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	8	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	8	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	8	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	9	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	9	1.89
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	9	1.89
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	10	1.89
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	1	1.88
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	1	1.88
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	1	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	3	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	3	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	3	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	4	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	4	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	4	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	10	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	10	1.88
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	10	1.88
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	4	1.87
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	4	1.87
(2,48)	1:72:A:SER:H	1:70:A:ASN:HB3	1	1.87
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG21	5	1.87
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG22	5	1.87
(1,115)	1:27:A:ILE:HB	1:27:A:ILE:HG23	5	1.87
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	5	1.87
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	1	1.86
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	2	1.85
(2,387)	1:61:A:THR:H	1:60:A:GLY:H	6	1.85
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	3	1.85
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	4	1.85
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	7	1.83
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	7	1.82
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	7	1.82
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	7	1.82
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	4	1.82
(3,9)	1:30:A:SER:HB2	1:66:A:SER:H	3	1.81
(3,9)	1:30:A:SER:HB3	1:66:A:SER:H	3	1.81
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	3	1.81
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	7	1.8
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	7	1.8
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	7	1.8
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	7	1.8
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	7	1.8
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	7	1.8
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	7	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	7	1.8
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	7	1.8
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	9	1.79
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	6	1.78
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	6	1.77
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	6	1.77
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	7	1.76
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	9	1.76
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	5	1.76
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	5	1.76
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	1	1.76
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	4	1.76
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	4	1.76
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	4	1.76
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	2	1.75
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	2	1.75
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	6	1.75
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	6	1.75
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	6	1.75
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	2	1.75
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	2	1.75
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	2	1.75
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	2	1.75
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	6	1.74
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	6	1.74
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	6	1.74
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	6	1.74
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	6	1.74
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	6	1.74
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	6	1.74
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	6	1.74
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	6	1.74
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	8	1.74
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	8	1.74
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	8	1.74
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	8	1.74
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	8	1.74
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	8	1.74
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	8	1.74
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	8	1.74
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	8	1.74
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	6	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	7	1.72
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	3	1.72
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	3	1.72
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	7	1.71
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	7	1.71
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	7	1.71
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	9	1.71
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	9	1.71
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	9	1.71
(1,75)	1:76:A:GLN:HA	1:78:A:SER:H	2	1.71
(2,301)	1:2:A:SER:H	1:4:A:GLN:HA	6	1.7
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	2	1.7
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	6	1.7
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	8	1.7
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	10	1.7
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	6	1.7
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	6	1.7
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	6	1.7
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	1	1.69
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	10	1.69
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	10	1.69
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	7	1.69
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	7	1.69
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	7	1.69
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	1	1.68
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	3	1.68
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	10	1.68
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	2	1.68
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	7	1.68
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	9	1.68
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	1	1.68
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	1	1.68
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	8	1.68
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	8	1.68
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	8	1.68
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	1	1.68
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	1	1.68
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	1	1.68
(1,9)	1:39:A:ARG:HD2	1:61:A:THR:HB	7	1.68
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	9	1.67
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	10	1.67
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	10	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	10	1.67
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	1	1.67
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	3	1.67
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	9	1.67
(1,448)	1:14:A:LEU:HD11	1:18:A:LEU:HG	5	1.67
(1,448)	1:14:A:LEU:HD12	1:18:A:LEU:HG	5	1.67
(1,448)	1:14:A:LEU:HD13	1:18:A:LEU:HG	5	1.67
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	5	1.66
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	6	1.66
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	8	1.66
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	4	1.66
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	8	1.65
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	2	1.65
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	1	1.65
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	5	1.65
(4,23)	1:63:A:LEU:H	1:61:A:THR:OG1	6	1.64
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	8	1.64
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	6	1.64
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	5	1.64
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	9	1.64
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	9	1.64
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	9	1.64
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	8	1.63
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	1	1.63
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	2	1.63
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	4	1.63
(2,174)	1:70:A:ASN:H	1:69:A:ALA:H	6	1.63
(2,80)	1:27:A:ILE:H	1:22:A:GLY:HA2	5	1.63
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	3	1.63
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	3	1.63
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	3	1.63
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	9	1.63
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	9	1.63
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	9	1.63
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	9	1.63
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	9	1.63
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	9	1.63
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	9	1.63
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	9	1.63
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	9	1.63
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	6	1.62
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	5	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	5	1.62
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	5	1.62
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	5	1.62
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	5	1.62
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	5	1.62
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	5	1.62
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	5	1.62
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	5	1.62
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	5	1.62
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	5	1.62
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	5	1.62
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	3	1.61
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	10	1.61
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	7	1.61
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	9	1.61
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	5	1.61
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	5	1.61
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	5	1.61
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	7	1.6
(2,328)	1:37:A:GLU:H	1:33:A:THR:HB	4	1.6
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	4	1.6
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	2	1.6
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	3	1.6
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	10	1.6
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	5	1.6
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	4	1.6
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	4	1.6
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	4	1.6
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	4	1.6
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	4	1.6
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	4	1.6
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	4	1.6
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	4	1.6
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	4	1.6
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	10	1.59
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	1	1.59
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	3	1.59
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	4	1.59
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	10	1.59
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD11	9	1.59
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD12	9	1.59
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD13	9	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	10	1.59
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	10	1.59
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	10	1.59
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	10	1.59
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	10	1.59
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	10	1.59
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	10	1.59
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	10	1.59
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	10	1.59
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	3	1.58
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	4	1.58
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	10	1.58
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	2	1.57
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	5	1.57
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	8	1.57
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	9	1.57
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	5	1.57
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	9	1.57
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	10	1.57
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	10	1.57
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	10	1.57
(5,19)	1:22:A:GLY:H	1:21:A:PHE:HB3	3	1.56
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	1	1.56
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	2	1.56
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	10	1.55
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	2	1.55
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	2	1.55
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	2	1.55
(2,158)	1:49:A:ASP:H	1:48:A:PHE:HB3	5	1.55
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	7	1.55
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	7	1.55
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	7	1.55
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	4	1.54
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	5	1.54
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	3	1.54
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	3	1.54
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	3	1.54
(5,19)	1:22:A:GLY:H	1:7:A:PHE:HB3	2	1.53
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	1	1.53
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	1	1.53
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	1	1.53
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	4	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	4	1.53
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	4	1.53
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	6	1.53
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	6	1.53
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	6	1.53
(5,19)	1:22:A:GLY:H	1:21:A:PHE:HB3	6	1.52
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	9	1.52
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	9	1.52
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	9	1.52
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	5	1.52
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	8	1.52
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	3	1.52
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	9	1.52
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	9	1.51
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	6	1.51
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	6	1.51
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	6	1.51
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	7	1.51
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	7	1.51
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	7	1.51
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	6	1.51
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD11	10	1.51
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD12	10	1.51
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD13	10	1.51
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	3	1.51
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	3	1.51
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	3	1.51
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	3	1.51
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	3	1.51
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	3	1.51
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	3	1.51
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	3	1.51
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	3	1.51
(2,415)	1:33:A:THR:H	1:34:A:ALA:H	4	1.5
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	8	1.5
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	8	1.5
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	8	1.5
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	7	1.5
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	3	1.5
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	3	1.5
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	3	1.5
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	8	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	8	1.5
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	8	1.5
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	4	1.5
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	2	1.5
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	2	1.5
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	2	1.5
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	2	1.5
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	2	1.5
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	2	1.5
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	2	1.5
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	2	1.5
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	2	1.5
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	4	1.5
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	4	1.5
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	4	1.5
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	9	1.5
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	9	1.5
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	9	1.5
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	3	1.49
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	3	1.49
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	3	1.49
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	3	1.49
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	10	1.49
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	1	1.49
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	8	1.49
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	4	1.48
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	9	1.48
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB1	8	1.48
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB2	8	1.48
(2,168)	1:9:A:ILE:H	1:45:A:ALA:HB3	8	1.48
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	10	1.48
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	1	1.47
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	8	1.47
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	2	1.47
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	2	1.47
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	2	1.47
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	6	1.47
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	6	1.47
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	6	1.47
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	3	1.46
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	2	1.46
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	6	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,19)	1:22:A:GLY:H	1:21:A:PHE:HB3	1	1.44
(5,19)	1:22:A:GLY:H	1:7:A:PHE:HB3	4	1.44
(5,19)	1:22:A:GLY:H	1:7:A:PHE:HB3	7	1.44
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	4	1.44
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD11	5	1.44
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD12	5	1.44
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD13	5	1.44
(5,19)	1:22:A:GLY:H	1:7:A:PHE:HB3	8	1.43
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	1	1.43
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	1	1.43
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	1	1.43
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	10	1.42
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	10	1.42
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	10	1.42
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	10	1.41
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	6	1.4
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	6	1.4
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	6	1.4
(2,69)	1:39:A:ARG:HE	1:39:A:ARG:HB2	7	1.4
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	7	1.4
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	4	1.4
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	4	1.4
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	4	1.4
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB1	1	1.4
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB2	1	1.4
(1,135)	1:56:A:ILE:HD11	1:59:A:ALA:HB3	1	1.4
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB1	1	1.4
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB2	1	1.4
(1,135)	1:56:A:ILE:HD12	1:59:A:ALA:HB3	1	1.4
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB1	1	1.4
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB2	1	1.4
(1,135)	1:56:A:ILE:HD13	1:59:A:ALA:HB3	1	1.4
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	1	1.39
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	1	1.39
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	1	1.39
(2,52)	1:38:A:GLY:H	1:39:A:ARG:H	2	1.39
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	7	1.39
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	7	1.39
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	7	1.39
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	9	1.38
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	2	1.38
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	2	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	2	1.38
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	7	1.38
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	4	1.38
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	4	1.38
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	4	1.38
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	2	1.38
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	2	1.38
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	2	1.38
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	9	1.38
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	9	1.38
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	9	1.38
(2,413)	1:4:A:GLN:H	1:50:A:ILE:HG13	1	1.37
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	3	1.37
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	6	1.37
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	6	1.37
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	6	1.37
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	6	1.37
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	1	1.37
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	1	1.37
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	1	1.37
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	10	1.37
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	10	1.37
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	10	1.37
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	7	1.37
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	7	1.37
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	7	1.37
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	1	1.36
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	8	1.36
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	2	1.36
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	1	1.36
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	1	1.36
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	1	1.36
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	7	1.36
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	7	1.36
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	7	1.36
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	9	1.36
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	9	1.36
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	9	1.36
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	2	1.36
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	6	1.36
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	7	1.36
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	7	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	7	1.36
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	10	1.35
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	3	1.35
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	2	1.35
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	2	1.35
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	2	1.35
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	2	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	2	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	2	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	4	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	4	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	4	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	9	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	9	1.34
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	9	1.34
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	7	1.34
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	7	1.34
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	7	1.34
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	3	1.34
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	5	1.34
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	5	1.34
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	5	1.34
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	8	1.33
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	8	1.33
(2,114)	1:62:A:GLY:H	1:61:A:THR:HA	8	1.33
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	3	1.33
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	3	1.33
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	3	1.33
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	7	1.33
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	7	1.32
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	1	1.32
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	5	1.32
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	7	1.32
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD11	2	1.32
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD12	2	1.32
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD13	2	1.32
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	10	1.32
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	10	1.32
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	10	1.32
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	6	1.32
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	6	1.32
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	6	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	5	1.32
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	5	1.32
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	5	1.32
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	8	1.32
(5,11)	1:34:A:ALA:H	1:32:A:PRO:HG2	4	1.31
(5,11)	1:34:A:ALA:H	1:32:A:PRO:HG3	4	1.31
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	7	1.31
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	3	1.31
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	3	1.31
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	3	1.31
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD11	6	1.31
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD12	6	1.31
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD13	6	1.31
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	5	1.31
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	5	1.31
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	5	1.31
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	10	1.31
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	10	1.31
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	10	1.31
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	1	1.3
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	1	1.3
(2,350)	1:41:A:THR:H	1:40:A:SER:HB2	5	1.3
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	2	1.3
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	4	1.3
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	10	1.3
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	10	1.3
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	5	1.29
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	8	1.29
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	8	1.29
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	8	1.29
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	9	1.29
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	5	1.29
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	5	1.29
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	5	1.29
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG21	10	1.29
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG22	10	1.29
(2,134)	1:57:A:LEU:H	1:56:A:ILE:HG23	10	1.29
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD11	3	1.29
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD12	3	1.29
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD13	3	1.29
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD11	8	1.29
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD12	8	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:61:A:THR:HB	1:63:A:LEU:HD13	8	1.29
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	2	1.29
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	2	1.29
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	2	1.29
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	8	1.29
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	8	1.29
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	8	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	4	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	4	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	4	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	6	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	6	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	6	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	8	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	8	1.29
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	8	1.29
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	2	1.29
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	2	1.29
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	2	1.29
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	7	1.29
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	4	1.29
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	4	1.29
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	4	1.29
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	4	1.28
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	4	1.28
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	4	1.28
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	4	1.28
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	5	1.28
(2,69)	1:39:A:ARG:HE	1:39:A:ARG:HB2	2	1.28
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	2	1.28
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	2	1.28
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	2	1.28
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	6	1.28
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	6	1.28
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	6	1.28
(1,147)	1:9:A:ILE:HD11	1:18:A:LEU:HG	8	1.28
(1,147)	1:9:A:ILE:HD12	1:18:A:LEU:HG	8	1.28
(1,147)	1:9:A:ILE:HD13	1:18:A:LEU:HG	8	1.28
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	3	1.27
(2,253)	1:44:A:LEU:H	1:9:A:ILE:HB	1	1.27
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	8	1.27
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	8	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	8	1.27
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	9	1.27
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	9	1.27
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	9	1.27
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	1	1.27
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	9	1.27
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD11	10	1.27
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD12	10	1.27
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD13	10	1.27
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG21	4	1.27
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG22	4	1.27
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG23	4	1.27
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG21	4	1.27
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG22	4	1.27
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG23	4	1.27
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG21	4	1.27
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG22	4	1.27
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG23	4	1.27
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	6	1.27
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	6	1.27
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	6	1.27
(1,417)	1:9:A:ILE:HB	1:44:A:LEU:H	1	1.27
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	7	1.27
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	7	1.27
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	7	1.27
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	3	1.27
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	3	1.27
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	3	1.27
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	8	1.27
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	4	1.27
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	4	1.27
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	4	1.27
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	2	1.27
(1,185)	1:41:A:THR:HB	1:42:A:SER:HG	3	1.27
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	3	1.26
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	2	1.26
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	9	1.26
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	3	1.26
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	3	1.26
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	3	1.26
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	3	1.26
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	5	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	3	1.26
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	3	1.25
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	4	1.25
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	9	1.24
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	3	1.24
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	3	1.24
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	3	1.24
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	4	1.24
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	4	1.24
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	4	1.24
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	7	1.24
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	2	1.24
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	4	1.24
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	9	1.24
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	9	1.24
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	9	1.24
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	6	1.24
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	7	1.24
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	10	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	1	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	2	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	3	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	4	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	5	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	6	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	7	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	8	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	9	1.24
(1,123)	1:47:A:ARG:HD3	1:47:A:ARG:HD2	10	1.24
(5,19)	1:22:A:GLY:H	1:7:A:PHE:HB3	5	1.23
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	4	1.23
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	2	1.23
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	2	1.23
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	2	1.23
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	1	1.23
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	1	1.23
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	1	1.23
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	6	1.23
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	7	1.23
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	4	1.23
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG21	3	1.23
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG22	3	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG23	3	1.23
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG21	3	1.23
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG22	3	1.23
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG23	3	1.23
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG21	3	1.23
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG22	3	1.23
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG23	3	1.23
(1,448)	1:14:A:LEU:HD11	1:18:A:LEU:HG	10	1.23
(1,448)	1:14:A:LEU:HD12	1:18:A:LEU:HG	10	1.23
(1,448)	1:14:A:LEU:HD13	1:18:A:LEU:HG	10	1.23
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB1	1	1.23
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB2	1	1.23
(1,359)	1:8:A:ASP:HA	1:45:A:ALA:HB3	1	1.23
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	2	1.23
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	2	1.23
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	2	1.23
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	2	1.22
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	4	1.22
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	4	1.22
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	4	1.22
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	3	1.22
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	5	1.22
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	6	1.21
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	3	1.21
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	6	1.21
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG21	9	1.21
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG22	9	1.21
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG23	9	1.21
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG21	9	1.21
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG22	9	1.21
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG23	9	1.21
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG21	9	1.21
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG22	9	1.21
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG23	9	1.21
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	7	1.21
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	9	1.21
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	9	1.21
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	9	1.21
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	9	1.21
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	9	1.21
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	9	1.21
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	9	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	9	1.21
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	9	1.21
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	9	1.21
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	9	1.21
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	6	1.21
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	10	1.2
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	10	1.2
(2,332)	1:42:A:SER:H	1:41:A:THR:HG1	10	1.2
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	8	1.2
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	2	1.2
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	7	1.2
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	7	1.2
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	7	1.2
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	5	1.2
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	5	1.2
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	5	1.2
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	2	1.2
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	3	1.2
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	10	1.2
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	1	1.2
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	1	1.2
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	1	1.2
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	5	1.2
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	7	1.2
(1,218)	1:40:A:SER:HB2	1:41:A:THR:H	5	1.2
(2,58)	1:76:A:GLN:H	1:66:A:SER:H	9	1.19
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG21	2	1.19
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG22	2	1.19
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG23	2	1.19
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG21	2	1.19
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG22	2	1.19
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG23	2	1.19
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG21	2	1.19
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG22	2	1.19
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG23	2	1.19
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	6	1.19
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	6	1.19
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	6	1.19
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	1	1.19
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	10	1.19
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	4	1.19
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	2	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	7	1.19
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	1	1.18
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	1	1.18
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	7	1.18
(2,396)	1:22:A:GLY:H	1:27:A:ILE:HG13	7	1.18
(2,350)	1:41:A:THR:H	1:40:A:SER:HB2	10	1.18
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	7	1.18
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	10	1.18
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	10	1.18
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	10	1.18
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	6	1.18
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	6	1.18
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	6	1.18
(2,148)	1:12:A:GLY:H	1:41:A:THR:HG1	10	1.18
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	5	1.18
(1,454)	1:5:A:ALA:HB1	1:25:A:ALA:HA	7	1.18
(1,454)	1:5:A:ALA:HB2	1:25:A:ALA:HA	7	1.18
(1,454)	1:5:A:ALA:HB3	1:25:A:ALA:HA	7	1.18
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	9	1.18
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	9	1.18
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	9	1.18
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	4	1.18
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	3	1.18
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	8	1.18
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	3	1.18
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	8	1.18
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	8	1.17
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	8	1.17
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	8	1.17
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	1	1.17
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	1	1.17
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	1	1.17
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	8	1.17
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	9	1.17
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	9	1.17
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	1	1.17
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	6	1.17
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	4	1.17
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	5	1.17
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	9	1.17
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	2	1.17
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	2	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	2	1.17
(5,19)	1:22:A:GLY:H	1:7:A:PHE:HB3	9	1.16
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	8	1.16
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	8	1.16
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	2	1.16
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	2	1.16
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	2	1.16
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	3	1.16
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	3	1.16
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	3	1.16
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	3	1.16
(1,257)	1:9:A:ILE:HB	1:44:A:LEU:HB3	2	1.16
(1,198)	1:38:A:GLY:HA2	1:37:A:GLU:HA	1	1.16
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	7	1.15
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	7	1.15
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	7	1.15
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	7	1.15
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	7	1.15
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	7	1.15
(1,380)	1:48:A:PHE:HB3	1:49:A:ASP:H	5	1.15
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	6	1.15
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	6	1.15
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	6	1.15
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	8	1.15
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	8	1.15
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	8	1.15
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	10	1.15
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	8	1.14
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	8	1.14
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	8	1.14
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	6	1.14
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	7	1.14
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	8	1.14
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	8	1.14
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	8	1.14
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	2	1.14
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	4	1.14
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	6	1.14
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	6	1.14
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	6	1.14
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	1	1.13
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	1	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	2	1.13
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	2	1.13
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	2	1.13
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	4	1.13
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	4	1.13
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	4	1.13
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	7	1.13
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	5	1.13
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	5	1.13
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	5	1.13
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	5	1.13
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	5	1.13
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	5	1.13
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	5	1.13
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	5	1.13
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	5	1.13
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD11	5	1.13
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD12	5	1.13
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD13	5	1.13
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD11	5	1.13
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD12	5	1.13
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD13	5	1.13
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD11	5	1.13
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD12	5	1.13
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD13	5	1.13
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	3	1.13
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	3	1.13
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	3	1.13
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	1	1.13
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	1	1.13
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	1	1.13
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	6	1.12
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	6	1.12
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	6	1.12
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	6	1.12
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	2	1.12
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	2	1.12
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	6	1.12
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	6	1.12
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	6	1.12
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	3	1.12
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	3	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	3	1.12
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	3	1.12
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	3	1.12
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	3	1.12
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	8	1.12
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	7	1.12
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	2	1.12
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	2	1.12
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	2	1.12
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	6	1.11
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	7	1.11
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	7	1.11
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	7	1.11
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	7	1.11
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	2	1.11
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	2	1.11
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	2	1.11
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	5	1.11
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	5	1.11
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	5	1.11
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	3	1.11
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	3	1.11
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	3	1.11
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD21	8	1.11
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD22	8	1.11
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD23	8	1.11
(5,19)	1:22:A:GLY:H	1:7:A:PHE:HB3	10	1.1
(2,249)	1:42:A:SER:H	1:42:A:SER:HG	1	1.1
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	4	1.1
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	4	1.1
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	4	1.1
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	7	1.1
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	7	1.1
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	7	1.1
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	3	1.1
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	3	1.1
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	3	1.1
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	4	1.09
(2,410)	1:4:A:GLN:H	1:4:A:GLN:HG2	5	1.09
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	1	1.09
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	1	1.09
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	1	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,259)	1:11:A:ALA:H	1:10:A:PRO:HB2	1	1.09
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	2	1.09
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	7	1.09
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	9	1.09
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	7	1.08
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	7	1.08
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	7	1.08
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	6	1.08
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	5	1.08
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	8	1.08
(1,218)	1:40:A:SER:HB2	1:41:A:THR:H	10	1.08
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	4	1.08
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	5	1.08
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	1	1.08
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	1	1.08
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	1	1.08
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	1	1.08
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	1	1.08
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	1	1.08
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	1	1.08
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	1	1.08
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	1	1.08
(4,24)	1:63:A:LEU:N	1:61:A:THR:OG1	8	1.07
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	6	1.07
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	3	1.07
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	3	1.07
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	3	1.07
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	10	1.07
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	4	1.07
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	8	1.07
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	8	1.07
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	8	1.07
(1,353)	1:39:A:ARG:HB3	1:40:A:SER:H	6	1.07
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	8	1.07
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	8	1.07
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	8	1.07
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	1	1.07
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	1	1.07
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	1	1.07
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	6	1.07
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	6	1.07
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	6	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	3	1.07
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	3	1.07
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	3	1.07
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	3	1.07
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	3	1.07
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	3	1.07
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	3	1.07
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	3	1.07
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	3	1.07
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	5	1.07
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	5	1.07
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	5	1.07
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD21	7	1.07
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD22	7	1.07
(1,29)	1:29:A:LEU:HA	1:29:A:LEU:HD23	7	1.07
(2,348)	1:81:A:THR:H	1:80:A:SER:HA	8	1.06
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	2	1.06
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	2	1.06
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	2	1.06
(2,69)	1:39:A:ARG:HE	1:39:A:ARG:HB2	5	1.06
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	2	1.06
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	10	1.06
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	1	1.06
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	1	1.06
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	1	1.06
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	4	1.06
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	4	1.06
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	4	1.06
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	5	1.06
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	5	1.06
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	5	1.06
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD11	8	1.06
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD12	8	1.06
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD13	8	1.06
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD11	8	1.06
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD12	8	1.06
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD13	8	1.06
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD11	8	1.06
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD12	8	1.06
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD13	8	1.06
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	5	1.06
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	5	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	5	1.06
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	5	1.05
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	5	1.05
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	5	1.05
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	9	1.05
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	3	1.05
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	1	1.05
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	4	1.05
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	4	1.05
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	4	1.05
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	2	1.05
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	2	1.05
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	2	1.05
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	8	1.05
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	8	1.05
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	8	1.05
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	5	1.05
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	5	1.05
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	5	1.05
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	3	1.05
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	3	1.05
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	3	1.05
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	3	1.05
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	3	1.05
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	3	1.05
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	3	1.05
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	3	1.05
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	3	1.05
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	8	1.05
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	8	1.05
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	8	1.05
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	4	1.04
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	4	1.04
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	8	1.04
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	1	1.04
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	1	1.04
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	1	1.04
(2,152)	1:12:A:GLY:H	1:40:A:SER:HB2	1	1.04
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	1	1.04
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	5	1.04
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	10	1.04
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	7	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	1	1.04
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	6	1.04
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	8	1.04
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	8	1.04
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	8	1.04
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	4	1.03
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	4	1.03
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	4	1.03
(2,151)	1:12:A:GLY:H	1:11:A:ALA:HB1	10	1.03
(2,151)	1:12:A:GLY:H	1:11:A:ALA:HB2	10	1.03
(2,151)	1:12:A:GLY:H	1:11:A:ALA:HB3	10	1.03
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	8	1.03
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	3	1.03
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	6	1.03
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	5	1.03
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	5	1.03
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	5	1.03
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	5	1.03
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	5	1.03
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	5	1.03
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	5	1.03
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	5	1.03
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	5	1.03
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	6	1.03
(1,53)	1:11:A:ALA:HA	1:43:A:GLY:HA3	8	1.03
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	6	1.03
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	6	1.03
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	6	1.03
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	1	1.02
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	1	1.02
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	5	1.02
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	5	1.02
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	7	1.02
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	9	1.02
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	9	1.02
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	9	1.02
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	8	1.02
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	8	1.02
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	8	1.02
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	10	1.02
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	10	1.02
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	10	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	9	1.02
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	1	1.02
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	1	1.02
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	1	1.02
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	5	1.02
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	5	1.02
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	5	1.02
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	5	1.02
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	5	1.02
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	5	1.02
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	5	1.02
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	5	1.02
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	5	1.02
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	10	1.02
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	10	1.02
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	10	1.02
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	4	1.02
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	4	1.02
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	4	1.02
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	4	1.02
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	4	1.02
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	4	1.02
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	4	1.02
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	4	1.02
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	4	1.02
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	9	1.02
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	9	1.02
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	9	1.02
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	9	1.02
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	9	1.02
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	9	1.02
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	10	1.02
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	10	1.02
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	10	1.02
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	8	1.02
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	8	1.02
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	8	1.02
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	8	1.02
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	8	1.02
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	8	1.02
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	8	1.02
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	8	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	8	1.02
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	7	1.02
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	2	1.01
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	9	1.01
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	4	1.01
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	4	1.01
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	4	1.01
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	2	1.01
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	2	1.01
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	2	1.01
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	2	1.01
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	3	1.01
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	3	1.01
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	8	1.01
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	8	1.01
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	8	1.01
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	1	1.01
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	2	1.01
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG21	1	1.01
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG22	1	1.01
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG23	1	1.01
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG21	1	1.01
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG22	1	1.01
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG23	1	1.01
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG21	1	1.01
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG22	1	1.01
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG23	1	1.01
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	1	1.01
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	1	1.01
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	1	1.01
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	1	1.01
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	10	1.01
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	10	1.01
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	10	1.01
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	7	1.01
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	7	1.01
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	7	1.01
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	6	1.01
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	2	1.01
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	2	1.01
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	2	1.01
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	2	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	2	1.01
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	2	1.01
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	2	1.01
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	2	1.01
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	2	1.01
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	7	1.01
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	7	1.01
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	7	1.01
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	7	1.01
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	7	1.01
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	7	1.01
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	7	1.01
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	7	1.01
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	7	1.01
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	9	1.01
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	9	1.01
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	9	1.01
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	9	1.01
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	9	1.01
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	9	1.01
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	8	1.0
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	8	1.0
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	8	1.0
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	8	1.0
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	8	1.0
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	8	1.0
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	5	1.0
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	4	1.0
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	9	1.0
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	4	1.0
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	4	1.0
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	4	1.0
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	8	1.0
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	4	1.0
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB1	9	1.0
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB2	9	1.0
(1,262)	1:22:A:GLY:HA2	1:25:A:ALA:HB3	9	1.0
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	2	1.0
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	8	1.0
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	8	1.0
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	8	1.0
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	6	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	6	0.99
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	10	0.99
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	10	0.99
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	10	0.99
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	4	0.99
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD11	9	0.99
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD12	9	0.99
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD13	9	0.99
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD11	9	0.99
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD12	9	0.99
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD13	9	0.99
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD11	9	0.99
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD12	9	0.99
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD13	9	0.99
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	2	0.98
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	2	0.98
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	3	0.98
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	4	0.98
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	8	0.98
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	8	0.98
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	8	0.98
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	9	0.98
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	4	0.98
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	3	0.98
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	3	0.98
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	1	0.98
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	1	0.98
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	4	0.98
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	4	0.98
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG21	6	0.98
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG22	6	0.98
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG23	6	0.98
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG21	6	0.98
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG22	6	0.98
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG23	6	0.98
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG21	6	0.98
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG22	6	0.98
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG23	6	0.98
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	10	0.98
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	8	0.98
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	6	0.98
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	6	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	6	0.98
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	6	0.98
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	6	0.98
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	6	0.98
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	6	0.98
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	6	0.98
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	6	0.98
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	8	0.98
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	10	0.98
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	10	0.98
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	10	0.98
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	7	0.97
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	7	0.97
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	1	0.97
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	8	0.97
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	5	0.97
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	5	0.97
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	5	0.97
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	7	0.97
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	7	0.97
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	10	0.97
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	10	0.97
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	10	0.97
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	7	0.97
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	7	0.97
(2,75)	1:75:A:LEU:H	1:31:A:TYR:HB2	9	0.97
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	6	0.97
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	6	0.97
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	6	0.97
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	5	0.97
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	9	0.97
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	10	0.97
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	10	0.97
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	10	0.97
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	10	0.97
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	10	0.97
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	10	0.97
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	9	0.97
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	9	0.97
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	9	0.97
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	10	0.97
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	10	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	10	0.97
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	4	0.97
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD11	4	0.97
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD12	4	0.97
(1,182)	1:57:A:LEU:HD11	1:54:A:LEU:HD13	4	0.97
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD11	4	0.97
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD12	4	0.97
(1,182)	1:57:A:LEU:HD12	1:54:A:LEU:HD13	4	0.97
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD11	4	0.97
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD12	4	0.97
(1,182)	1:57:A:LEU:HD13	1:54:A:LEU:HD13	4	0.97
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	3	0.96
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	3	0.96
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	6	0.96
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	6	0.96
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	6	0.96
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	4	0.96
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	9	0.96
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	9	0.96
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	10	0.96
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	2	0.96
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	8	0.96
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	4	0.96
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	4	0.96
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	2	0.96
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	2	0.96
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	2	0.96
(1,471)	1:51:A:ASP:HB2	1:51:A:ASP:H	4	0.96
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	9	0.96
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	9	0.96
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	9	0.96
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	9	0.96
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	1	0.96
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	1	0.96
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	1	0.96
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	1	0.96
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	1	0.96
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	1	0.96
(1,189)	1:45:A:ALA:HB1	1:44:A:LEU:HG	1	0.96
(1,189)	1:45:A:ALA:HB2	1:44:A:LEU:HG	1	0.96
(1,189)	1:45:A:ALA:HB3	1:44:A:LEU:HG	1	0.96
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	10	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	1	0.96
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	1	0.96
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	1	0.96
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	5	0.96
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	5	0.96
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	5	0.96
(2,434)	1:21:A:PHE:H	1:20:A:HIS:H	6	0.95
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	7	0.95
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	7	0.95
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	7	0.95
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	9	0.95
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	9	0.95
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	9	0.95
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	7	0.95
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	7	0.95
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	7	0.95
(2,152)	1:12:A:GLY:H	1:40:A:SER:HB2	9	0.95
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	6	0.95
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	5	0.95
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	8	0.95
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	8	0.95
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	8	0.95
(1,324)	1:73:A:TYR:HA	1:67:A:ARG:HA	5	0.95
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	1	0.95
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	2	0.95
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	2	0.95
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	2	0.95
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	2	0.94
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	1	0.94
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	9	0.94
(2,100)	1:43:A:GLY:H	1:42:A:SER:HA	10	0.94
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	10	0.94
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	1	0.94
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	1	0.94
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	1	0.94
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	3	0.94
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	3	0.94
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	3	0.94
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	3	0.94
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	3	0.94
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	3	0.94
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	9	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	9	0.94
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	9	0.94
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	9	0.94
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	9	0.94
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	9	0.94
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	5	0.94
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	8	0.94
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	9	0.94
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	1	0.94
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	1	0.94
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	1	0.94
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	10	0.94
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	10	0.94
(2,468)	1:77:A:ALA:H	1:64:A:GLU:HG3	7	0.93
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	1	0.93
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	1	0.93
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	5	0.93
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	5	0.93
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	5	0.93
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	1	0.93
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	1	0.93
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	1	0.93
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	6	0.93
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	6	0.93
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	6	0.93
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	9	0.93
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	9	0.93
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	9	0.93
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	4	0.93
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	4	0.93
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	4	0.93
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	9	0.93
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	9	0.93
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	9	0.93
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	9	0.93
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	9	0.93
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	9	0.93
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	1	0.93
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	2	0.93
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	3	0.93
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	4	0.93
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	6	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	7	0.93
(1,370)	1:50:A:ILE:HG13	1:50:A:ILE:HG12	10	0.93
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	3	0.93
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	3	0.93
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	3	0.93
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD11	10	0.93
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD12	10	0.93
(1,179)	1:50:A:ILE:HD11	1:54:A:LEU:HD13	10	0.93
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD11	10	0.93
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD12	10	0.93
(1,179)	1:50:A:ILE:HD12	1:54:A:LEU:HD13	10	0.93
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD11	10	0.93
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD12	10	0.93
(1,179)	1:50:A:ILE:HD13	1:54:A:LEU:HD13	10	0.93
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	6	0.93
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	6	0.93
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	6	0.93
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	4	0.93
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	4	0.93
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	4	0.93
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	4	0.93
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	8	0.92
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	8	0.92
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	6	0.92
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	9	0.92
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	9	0.92
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	9	0.92
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	8	0.92
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	8	0.92
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	8	0.92
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	10	0.92
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	10	0.92
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	10	0.92
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	2	0.92
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	2	0.92
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	2	0.92
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	6	0.92
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	6	0.92
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	6	0.92
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	6	0.92
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	6	0.92
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	4	0.92
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	4	0.92
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	4	0.92
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	5	0.92
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	5	0.92
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	5	0.92
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	6	0.92
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	6	0.92
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	6	0.92
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	8	0.92
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	8	0.92
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	8	0.92
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	6	0.92
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	6	0.92
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	6	0.92
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	9	0.92
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	9	0.92
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	9	0.92
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	7	0.92
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	7	0.92
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	7	0.92
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	7	0.92
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	7	0.92
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	7	0.92
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	7	0.92
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	7	0.92
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	7	0.92
(1,162)	1:73:A:TYR:HB3	1:73:A:TYR:H	4	0.92
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	3	0.92
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	4	0.92
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	4	0.92
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	4	0.92
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	3	0.91
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	3	0.91
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	6	0.91
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	6	0.91
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	6	0.91
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	5	0.91
(2,75)	1:75:A:LEU:H	1:31:A:TYR:HB2	8	0.91
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD11	7	0.91
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD12	7	0.91
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD13	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	2	0.91
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	2	0.91
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	2	0.91
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	4	0.91
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	4	0.91
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	4	0.91
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	3	0.91
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	3	0.91
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	3	0.91
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	7	0.91
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	7	0.91
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	7	0.91
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	10	0.91
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	10	0.91
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	10	0.91
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	3	0.91
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	3	0.91
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	10	0.91
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	10	0.91
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	10	0.91
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	6	0.9
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	10	0.9
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	10	0.9
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	3	0.9
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	3	0.9
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	10	0.9
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	10	0.9
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	10	0.9
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	7	0.9
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD21	10	0.9
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD22	10	0.9
(1,406)	1:63:A:LEU:HA	1:63:A:LEU:HD23	10	0.9
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	4	0.9
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	4	0.9
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	4	0.9
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	4	0.9
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	4	0.9
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	4	0.9
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	1	0.9
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	1	0.9
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	1	0.9
(1,397)	1:50:A:ILE:HD11	1:50:A:ILE:HG13	2	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:50:A:ILE:HD12	1:50:A:ILE:HG13	2	0.9
(1,397)	1:50:A:ILE:HD13	1:50:A:ILE:HG13	2	0.9
(1,353)	1:39:A:ARG:HB3	1:40:A:SER:H	2	0.9
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	2	0.9
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	9	0.9
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	6	0.9
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	6	0.9
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	6	0.9
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	9	0.9
(1,162)	1:73:A:TYR:HB3	1:73:A:TYR:H	1	0.9
(1,162)	1:73:A:TYR:HB3	1:73:A:TYR:H	5	0.9
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	8	0.9
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	8	0.9
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	8	0.9
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	4	0.89
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	4	0.89
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	10	0.89
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	10	0.89
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	6	0.89
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	4	0.89
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	4	0.89
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	4	0.89
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	7	0.89
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	4	0.89
(1,463)	1:47:A:ARG:HA	1:6:A:ASP:HA	8	0.89
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	4	0.89
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	4	0.89
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	4	0.89
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	7	0.89
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	7	0.89
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	7	0.89
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	4	0.89
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	7	0.89
(1,215)	1:10:A:PRO:HB2	1:11:A:ALA:H	1	0.89
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	6	0.89
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	10	0.89
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	5	0.89
(5,11)	1:34:A:ALA:H	1:32:A:PRO:HG2	8	0.88
(5,11)	1:34:A:ALA:H	1:32:A:PRO:HG3	8	0.88
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	6	0.88
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	6	0.88
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	10	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	10	0.88
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	6	0.88
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	5	0.88
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	3	0.88
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	3	0.88
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	3	0.88
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	8	0.88
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD11	6	0.88
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD12	6	0.88
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD13	6	0.88
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	9	0.88
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	9	0.88
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	9	0.88
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	3	0.88
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	3	0.88
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	3	0.88
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	2	0.88
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	2	0.88
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	2	0.88
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	7	0.88
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	7	0.88
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	7	0.88
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	2	0.88
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	2	0.88
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	2	0.88
(1,353)	1:39:A:ARG:HB3	1:40:A:SER:H	7	0.88
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	5	0.88
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	5	0.88
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	5	0.88
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	1	0.88
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	5	0.88
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	7	0.88
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	9	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	2	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	2	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	2	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	3	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	3	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	3	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	4	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	4	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	4	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	5	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	5	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	5	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	6	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	6	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	6	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	7	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	7	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	7	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	8	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	8	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	8	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	9	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	9	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	9	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	10	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	10	0.88
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	10	0.88
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	8	0.88
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	8	0.88
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	8	0.88
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	1	0.87
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	1	0.87
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	1	0.87
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	4	0.87
(2,386)	1:61:A:THR:H	1:60:A:GLY:HA3	6	0.87
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	3	0.87
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	9	0.87
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	9	0.87
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	9	0.87
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	6	0.87
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	8	0.87
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	8	0.87
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	8	0.87
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	5	0.87
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	5	0.87
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	5	0.87
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	7	0.87
(2,77)	1:40:A:SER:H	1:39:A:ARG:HB3	6	0.87
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	4	0.87
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	4	0.87
(1,482)	1:73:A:TYR:HB2	1:73:A:TYR:H	6	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:73:A:TYR:HB2	1:73:A:TYR:H	10	0.87
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	9	0.87
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	9	0.87
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	9	0.87
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	5	0.87
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	5	0.87
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	5	0.87
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	6	0.87
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	6	0.87
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	6	0.87
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	3	0.87
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	3	0.87
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	3	0.87
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	8	0.87
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	8	0.87
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	8	0.87
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	10	0.87
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	10	0.87
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	10	0.87
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD11	10	0.87
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD12	10	0.87
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD13	10	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	1	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	1	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	1	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	3	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	3	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	3	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	8	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	8	0.87
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	8	0.87
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	3	0.87
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	4	0.87
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	4	0.87
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	4	0.87
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	10	0.87
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	8	0.87
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG21	1	0.87
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG22	1	0.87
(1,137)	1:56:A:ILE:HB	1:56:A:ILE:HG23	1	0.87
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	4	0.87
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	4	0.87
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	10	0.87
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	10	0.87
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	10	0.87
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	1	0.86
(2,393)	1:24:A:SER:H	1:24:A:SER:HB2	6	0.86
(2,386)	1:61:A:THR:H	1:60:A:GLY:HA3	7	0.86
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	8	0.86
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	9	0.86
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	8	0.86
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	5	0.86
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	5	0.86
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	5	0.86
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	5	0.86
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	5	0.86
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	3	0.86
(2,191)	1:68:A:GLY:H	1:67:A:ARG:HG2	1	0.86
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	7	0.86
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	6	0.86
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	2	0.86
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	2	0.86
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	2	0.86
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	3	0.86
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	3	0.86
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	3	0.86
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	6	0.86
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	6	0.86
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	6	0.86
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	6	0.86
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	6	0.86
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	6	0.86
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	7	0.86
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	7	0.86
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	7	0.86
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	1	0.86
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	1	0.86
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	1	0.86
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	4	0.86
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	4	0.86
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	4	0.86
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	5	0.86
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	5	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	5	0.86
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	6	0.86
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	6	0.86
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	6	0.86
(1,411)	1:35:A:LEU:HD11	1:35:A:LEU:HG	9	0.86
(1,411)	1:35:A:LEU:HD12	1:35:A:LEU:HG	9	0.86
(1,411)	1:35:A:LEU:HD13	1:35:A:LEU:HG	9	0.86
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	2	0.86
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	2	0.86
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	2	0.86
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	2	0.86
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	2	0.86
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	2	0.86
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	8	0.86
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	10	0.86
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	10	0.86
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	10	0.86
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	2	0.86
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	6	0.86
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	8	0.86
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	7	0.86
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	7	0.86
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	4	0.86
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	10	0.86
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	3	0.86
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	3	0.86
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	3	0.86
(1,11)	1:76:A:GLN:HA	1:64:A:GLU:HG3	7	0.86
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB1	3	0.85
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB2	3	0.85
(2,340)	1:6:A:ASP:H	1:5:A:ALA:HB3	3	0.85
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	4	0.85
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	4	0.85
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	6	0.85
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	6	0.85
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	8	0.85
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	8	0.85
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	7	0.85
(2,265)	1:59:A:ALA:H	1:60:A:GLY:HA2	8	0.85
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	2	0.85
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD11	9	0.85
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD12	9	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD13	9	0.85
(1,482)	1:73:A:TYR:HB2	1:73:A:TYR:H	2	0.85
(1,482)	1:73:A:TYR:HB2	1:73:A:TYR:H	7	0.85
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	7	0.85
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	7	0.85
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	7	0.85
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	7	0.85
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	7	0.85
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	7	0.85
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG21	7	0.85
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG22	7	0.85
(1,457)	1:14:A:LEU:HD11	1:61:A:THR:HG23	7	0.85
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG21	7	0.85
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG22	7	0.85
(1,457)	1:14:A:LEU:HD12	1:61:A:THR:HG23	7	0.85
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG21	7	0.85
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG22	7	0.85
(1,457)	1:14:A:LEU:HD13	1:61:A:THR:HG23	7	0.85
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD11	5	0.85
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD12	5	0.85
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD13	5	0.85
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD11	5	0.85
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD12	5	0.85
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD13	5	0.85
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD11	5	0.85
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD12	5	0.85
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD13	5	0.85
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	1	0.85
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	4	0.85
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	5	0.85
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	7	0.85
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	2	0.85
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	5	0.85
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	2	0.85
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	2	0.85
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	2	0.85
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	10	0.85
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	10	0.85
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	10	0.85
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	2	0.84
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	2	0.84
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	4	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	4	0.84
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	9	0.84
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	9	0.84
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	5	0.84
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	10	0.84
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	10	0.84
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	3	0.84
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	2	0.84
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	2	0.84
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	4	0.84
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	4	0.84
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	6	0.84
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	6	0.84
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	9	0.84
(2,198)	1:74:A:SER:H	1:73:A:TYR:HB3	9	0.84
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	10	0.84
(2,145)	1:56:A:ILE:H	1:56:A:ILE:HG13	8	0.84
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	4	0.84
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	4	0.84
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	4	0.84
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	4	0.84
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	10	0.84
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	7	0.84
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	7	0.84
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	7	0.84
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	9	0.84
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	7	0.84
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	7	0.84
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	7	0.84
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD21	7	0.84
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD22	7	0.84
(1,305)	1:7:A:PHE:HB2	1:44:A:LEU:HD23	7	0.84
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	9	0.84
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	9	0.84
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	9	0.84
(1,228)	1:39:A:ARG:HD3	1:38:A:GLY:HA3	5	0.84
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	2	0.84
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	1	0.84
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	1	0.84
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	1	0.84
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	1	0.84
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	1	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	1	0.84
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	7	0.84
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	7	0.84
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	7	0.84
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	8	0.84
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	3	0.84
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	7	0.84
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	7	0.84
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	7	0.84
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	1	0.83
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	1	0.83
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	1	0.83
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	3	0.83
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	9	0.83
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	7	0.83
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	7	0.83
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	7	0.83
(2,386)	1:61:A:THR:H	1:60:A:GLY:HA3	8	0.83
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	4	0.83
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	4	0.83
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	4	0.83
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	4	0.83
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	7	0.83
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	2	0.83
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	2	0.83
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	2	0.83
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	9	0.83
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	6	0.83
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD11	2	0.83
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD12	2	0.83
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD13	2	0.83
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD11	3	0.83
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD12	3	0.83
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD13	3	0.83
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	3	0.83
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	3	0.83
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	3	0.83
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	1	0.83
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	1	0.83
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	1	0.83
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	2	0.83
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	2	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	2	0.83
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	4	0.83
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	8	0.83
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	8	0.83
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	8	0.83
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	8	0.83
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	8	0.83
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	8	0.83
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	5	0.83
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	5	0.83
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	5	0.83
(1,361)	1:13:A:PRO:HB2	1:13:A:PRO:HB3	10	0.83
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	10	0.83
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	6	0.83
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD11	10	0.83
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD12	10	0.83
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD13	10	0.83
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD11	10	0.83
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD12	10	0.83
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD13	10	0.83
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD11	10	0.83
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD12	10	0.83
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD13	10	0.83
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	1	0.83
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	3	0.83
(1,156)	1:56:A:ILE:HB	1:57:A:LEU:H	4	0.83
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	5	0.83
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	7	0.82
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	7	0.82
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	7	0.82
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	7	0.82
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	7	0.82
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	7	0.82
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	10	0.82
(2,393)	1:24:A:SER:H	1:24:A:SER:HB2	3	0.82
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	1	0.82
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	7	0.82
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	10	0.82
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	8	0.82
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	8	0.82
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	8	0.82
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	1	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	6	0.82
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD21	1	0.82
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD22	1	0.82
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD23	1	0.82
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	7	0.82
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	8	0.82
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	1	0.82
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	3	0.82
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	8	0.82
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD11	4	0.82
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD12	4	0.82
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD13	4	0.82
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	9	0.82
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	7	0.82
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	7	0.82
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	7	0.82
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	9	0.82
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	9	0.82
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	9	0.82
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	3	0.82
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	2	0.82
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	2	0.82
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	2	0.82
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	3	0.82
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	3	0.82
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	3	0.82
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	6	0.82
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	6	0.82
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	6	0.82
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	10	0.82
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	10	0.82
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	10	0.82
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	10	0.82
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	3	0.82
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	3	0.82
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	3	0.82
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	8	0.82
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	1	0.82
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	3	0.82
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	2	0.82
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	2	0.82
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	4	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	1	0.82
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	1	0.81
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	2	0.81
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	2	0.81
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	2	0.81
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	2	0.81
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	4	0.81
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	7	0.81
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	10	0.81
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	3	0.81
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	8	0.81
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	2	0.81
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	5	0.81
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	5	0.81
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	5	0.81
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	4	0.81
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	4	0.81
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	4	0.81
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	5	0.81
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	5	0.81
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	5	0.81
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	7	0.81
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	7	0.81
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	7	0.81
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	8	0.81
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	3	0.81
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	4	0.81
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	6	0.81
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	7	0.81
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	7	0.81
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	7	0.81
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	7	0.8
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	7	0.8
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	7	0.8
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	7	0.8
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	7	0.8
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	7	0.8
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	3	0.8
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	4	0.8
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	4	0.8
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	5	0.8
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	3	0.8
(2,350)	1:41:A:THR:H	1:40:A:SER:HB2	8	0.8
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	5	0.8
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	9	0.8
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	1	0.8
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	1	0.8
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	1	0.8
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	4	0.8
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	4	0.8
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	4	0.8
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	10	0.8
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	10	0.8
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	10	0.8
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	7	0.8
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	7	0.8
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	7	0.8
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	9	0.8
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	9	0.8
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	9	0.8
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD11	9	0.8
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD12	9	0.8
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD13	9	0.8
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	8	0.8
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	8	0.8
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	8	0.8
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	1	0.8
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	1	0.8
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	1	0.8
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	7	0.8
(1,317)	1:47:A:ARG:HB2	1:47:A:ARG:HD2	8	0.8
(1,315)	1:27:A:ILE:HG13	1:22:A:GLY:HA2	6	0.8
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	2	0.8
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	2	0.8
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	2	0.8
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	8	0.8
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	8	0.8
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	8	0.8
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	1	0.8
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	5	0.8
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	2	0.8
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	2	0.8
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	2	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	6	0.79
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	6	0.79
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	6	0.79
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	1	0.79
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	7	0.79
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	2	0.79
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	2	0.79
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	2	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	2	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	2	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	2	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	4	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	4	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	4	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	10	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	10	0.79
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	10	0.79
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	10	0.79
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	10	0.79
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	4	0.79
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	6	0.79
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	8	0.79
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	10	0.79
(1,482)	1:73:A:TYR:HB2	1:73:A:TYR:H	8	0.79
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	5	0.79
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	5	0.79
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	5	0.79
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	7	0.79
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	3	0.79
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	3	0.79
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	3	0.79
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	1	0.79
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	3	0.79
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	8	0.79
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	10	0.79
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	6	0.79
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	9	0.79
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD11	5	0.79
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD12	5	0.79
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD13	5	0.79
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	4	0.78
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	10	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	10	0.78
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	10	0.78
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	7	0.78
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	7	0.78
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	7	0.78
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	7	0.78
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	7	0.78
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	1	0.78
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	10	0.78
(2,209)	1:44:A:LEU:H	1:43:A:GLY:HA2	5	0.78
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	10	0.78
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	10	0.78
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	10	0.78
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	7	0.78
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	6	0.78
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	7	0.78
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	7	0.78
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	9	0.78
(1,482)	1:73:A:TYR:HB2	1:73:A:TYR:H	3	0.78
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	6	0.78
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	6	0.78
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	6	0.78
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	8	0.78
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	8	0.78
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	8	0.78
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	9	0.78
(1,265)	1:49:A:ASP:HA	1:4:A:GLN:HG2	9	0.78
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	5	0.78
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	9	0.78
(1,112)	1:67:A:ARG:HG3	1:67:A:ARG:HD3	9	0.78
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	5	0.78
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	5	0.78
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	5	0.78
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	6	0.78
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	6	0.78
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	6	0.78
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	8	0.77
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	8	0.77
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	2	0.77
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	2	0.77
(2,383)	1:52:A:GLN:H	1:51:A:ASP:HB3	7	0.77
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	5	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	5	0.77
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	9	0.77
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	9	0.77
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	9	0.77
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	9	0.77
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	3	0.77
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	8	0.77
(2,176)	1:68:A:GLY:H	1:67:A:ARG:HG3	2	0.77
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	5	0.77
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	9	0.77
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	5	0.77
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	4	0.77
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	4	0.77
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	1	0.77
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	1	0.77
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	1	0.77
(1,375)	1:58:A:LEU:HD21	1:58:A:LEU:HG	9	0.77
(1,375)	1:58:A:LEU:HD22	1:58:A:LEU:HG	9	0.77
(1,375)	1:58:A:LEU:HD23	1:58:A:LEU:HG	9	0.77
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	2	0.77
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	4	0.77
(1,247)	1:17:A:ALA:HA	1:9:A:ILE:HG21	1	0.77
(1,247)	1:17:A:ALA:HA	1:9:A:ILE:HG22	1	0.77
(1,247)	1:17:A:ALA:HA	1:9:A:ILE:HG23	1	0.77
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	7	0.77
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	8	0.77
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	10	0.77
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	10	0.77
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	10	0.77
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	4	0.77
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	7	0.77
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	7	0.77
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	7	0.77
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	4	0.76
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	4	0.76
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	4	0.76
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	2	0.76
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	8	0.76
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	5	0.76
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	5	0.76
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	5	0.76
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	3	0.76
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	3	0.76
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	3	0.76
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	2	0.76
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	6	0.76
(2,152)	1:12:A:GLY:H	1:40:A:SER:HB2	3	0.76
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	5	0.76
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	4	0.76
(2,33)	1:50:A:ILE:H	1:50:A:ILE:HB	5	0.76
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	1	0.76
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	7	0.76
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	6	0.76
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	10	0.76
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	4	0.76
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	4	0.76
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	4	0.76
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	10	0.76
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	10	0.76
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	10	0.76
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	7	0.76
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	1	0.76
(1,282)	1:50:A:ILE:HB	1:50:A:ILE:H	5	0.76
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	1	0.76
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	1	0.76
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	1	0.76
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	8	0.76
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	8	0.76
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	8	0.76
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	8	0.76
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	8	0.76
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	8	0.76
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	8	0.76
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	8	0.76
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	8	0.76
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	1	0.76
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	2	0.76
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	6	0.76
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	1	0.76
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	7	0.76
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	3	0.76
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	3	0.76
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	6	0.75
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	8	0.75
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	6	0.75
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	3	0.75
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	3	0.75
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	3	0.75
(2,198)	1:74:A:SER:H	1:73:A:TYR:HB3	2	0.75
(2,198)	1:74:A:SER:H	1:73:A:TYR:HB3	10	0.75
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	7	0.75
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	7	0.75
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	10	0.75
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	10	0.75
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	2	0.75
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	4	0.75
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	9	0.75
(1,472)	1:5:A:ALA:HB1	1:6:A:ASP:H	3	0.75
(1,472)	1:5:A:ALA:HB2	1:6:A:ASP:H	3	0.75
(1,472)	1:5:A:ALA:HB3	1:6:A:ASP:H	3	0.75
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE1	7	0.75
(1,398)	1:25:A:ALA:HB1	1:21:A:PHE:HE2	7	0.75
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE1	7	0.75
(1,398)	1:25:A:ALA:HB2	1:21:A:PHE:HE2	7	0.75
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE1	7	0.75
(1,398)	1:25:A:ALA:HB3	1:21:A:PHE:HE2	7	0.75
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	2	0.75
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	2	0.75
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	2	0.75
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	6	0.75
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	6	0.75
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	6	0.75
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	5	0.75
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	5	0.75
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	5	0.75
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	7	0.75
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	7	0.75
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	7	0.75
(1,158)	1:57:A:LEU:HB2	1:57:A:LEU:H	7	0.75
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	2	0.75
(1,31)	1:31:A:TYR:HB3	1:75:A:LEU:HB3	7	0.75
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HE1	1	0.74
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	5	0.74
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	5	0.74
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	2	0.74
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	2	0.74
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	2	0.74
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	7	0.74
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	2	0.74
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	2	0.74
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	2	0.74
(2,222)	1:23:A:GLN:H	1:22:A:GLY:HA3	7	0.74
(2,176)	1:68:A:GLY:H	1:67:A:ARG:HG3	7	0.74
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	6	0.74
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	5	0.74
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	5	0.74
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	5	0.74
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	4	0.74
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	4	0.74
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	4	0.74
(1,448)	1:14:A:LEU:HD11	1:18:A:LEU:HG	8	0.74
(1,448)	1:14:A:LEU:HD12	1:18:A:LEU:HG	8	0.74
(1,448)	1:14:A:LEU:HD13	1:18:A:LEU:HG	8	0.74
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	10	0.74
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	6	0.74
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	6	0.74
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	2	0.74
(1,317)	1:47:A:ARG:HB2	1:47:A:ARG:HD2	5	0.74
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD11	9	0.74
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD12	9	0.74
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD13	9	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD11	9	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD12	9	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD13	9	0.74
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD11	9	0.74
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD12	9	0.74
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD13	9	0.74
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD11	10	0.74
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD12	10	0.74
(1,301)	1:65:A:ALA:HB1	1:54:A:LEU:HD13	10	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD11	10	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD12	10	0.74
(1,301)	1:65:A:ALA:HB2	1:54:A:LEU:HD13	10	0.74
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD11	10	0.74
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD12	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:65:A:ALA:HB3	1:54:A:LEU:HD13	10	0.74
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	2	0.74
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	2	0.74
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	6	0.74
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	6	0.74
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	8	0.74
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	8	0.74
(1,206)	1:49:A:ASP:HB2	1:51:A:ASP:HB2	3	0.74
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	3	0.74
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	8	0.74
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	2	0.73
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	9	0.73
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	9	0.73
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	9	0.73
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	6	0.73
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	6	0.73
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	10	0.73
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	10	0.73
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	8	0.73
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	8	0.73
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	3	0.73
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	9	0.73
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	9	0.73
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	9	0.73
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	9	0.73
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	6	0.73
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	6	0.73
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	6	0.73
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	6	0.73
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	6	0.73
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	5	0.73
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	5	0.73
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	5	0.73
(2,251)	1:12:A:GLY:H	1:43:A:GLY:HA2	1	0.73
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	4	0.73
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	8	0.73
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	8	0.73
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	8	0.73
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	5	0.73
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	5	0.73
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	5	0.73
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	3	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	8	0.73
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	1	0.73
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	1	0.73
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	3	0.73
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	3	0.73
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	5	0.73
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	5	0.73
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	5	0.73
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	9	0.73
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	9	0.73
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	9	0.73
(1,393)	1:72:A:SER:HA	1:28:A:LEU:HB2	10	0.73
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	1	0.73
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	5	0.73
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	6	0.73
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	1	0.73
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	2	0.73
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	6	0.73
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	2	0.73
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	2	0.73
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	2	0.73
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	2	0.73
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	2	0.73
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	2	0.73
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	3	0.73
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	3	0.73
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	3	0.73
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	9	0.73
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	8	0.72
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	8	0.72
(3,21)	1:14:A:LEU:HD11	1:14:A:LEU:HA	10	0.72
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	8	0.72
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	8	0.72
(2,407)	1:24:A:SER:H	1:23:A:GLN:HB3	5	0.72
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	2	0.72
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	4	0.72
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	4	0.72
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	6	0.72
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	6	0.72
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	5	0.72
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	1	0.72
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	1	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	1	0.72
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	8	0.72
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	8	0.72
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	8	0.72
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	5	0.72
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	5	0.72
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD21	7	0.72
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD22	7	0.72
(2,298)	1:45:A:ALA:H	1:44:A:LEU:HD23	7	0.72
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	5	0.72
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	10	0.72
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	10	0.72
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	2	0.72
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	2	0.72
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	9	0.72
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	2	0.72
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	8	0.72
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	9	0.72
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	10	0.72
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	7	0.72
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	7	0.72
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	7	0.72
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	10	0.72
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	10	0.72
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	1	0.72
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	1	0.72
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	1	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	5	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	5	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	5	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	5	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	5	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	5	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	10	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	10	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	10	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	10	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	10	0.72
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	10	0.72
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	6	0.72
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB1	3	0.71
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB2	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,416)	1:35:A:LEU:H	1:34:A:ALA:HB3	3	0.71
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	9	0.71
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	7	0.71
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	2	0.71
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	8	0.71
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	8	0.71
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	8	0.71
(2,224)	1:19:A:ALA:H	1:18:A:LEU:HB2	8	0.71
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD21	1	0.71
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD22	1	0.71
(2,125)	1:63:A:LEU:H	1:63:A:LEU:HD23	1	0.71
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	1	0.71
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	5	0.71
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	5	0.71
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	1	0.71
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	9	0.71
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB1	10	0.71
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB2	10	0.71
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB3	10	0.71
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	9	0.71
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	9	0.71
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	9	0.71
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	9	0.71
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	9	0.71
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	7	0.71
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	10	0.71
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	3	0.71
(1,72)	1:21:A:PHE:HB3	1:18:A:LEU:HA	4	0.71
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	5	0.71
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	3	0.71
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	3	0.71
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	3	0.71
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	9	0.71
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	7	0.7
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	7	0.7
(2,410)	1:4:A:GLN:H	1:4:A:GLN:HG2	10	0.7
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	3	0.7
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	5	0.7
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	10	0.7
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	7	0.7
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	7	0.7
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	9	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	6	0.7
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	2	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	3	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	3	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	3	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	5	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	5	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	5	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	10	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	10	0.7
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	10	0.7
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	1	0.7
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	1	0.7
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	1	0.7
(2,250)	1:55:A:ALA:H	1:54:A:LEU:HG	4	0.7
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	4	0.7
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	3	0.7
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	3	0.7
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	3	0.7
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	5	0.7
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	5	0.7
(2,84)	1:33:A:THR:H	1:33:A:THR:HB	4	0.7
(2,77)	1:40:A:SER:H	1:39:A:ARG:HB3	2	0.7
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	6	0.7
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	6	0.7
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	5	0.7
(2,34)	1:50:A:ILE:H	1:4:A:GLN:HA	4	0.7
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	9	0.7
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	5	0.7
(1,475)	1:9:A:ILE:HD11	1:57:A:LEU:HB3	10	0.7
(1,475)	1:9:A:ILE:HD12	1:57:A:LEU:HB3	10	0.7
(1,475)	1:9:A:ILE:HD13	1:57:A:LEU:HB3	10	0.7
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	6	0.7
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	8	0.7
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	8	0.7
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	8	0.7
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	10	0.7
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	9	0.7
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	1	0.7
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	1	0.7
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	1	0.7
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	1	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	1	0.7
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	1	0.7
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	1	0.7
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	1	0.7
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	1	0.7
(1,218)	1:40:A:SER:HB2	1:41:A:THR:H	8	0.7
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	8	0.7
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	9	0.7
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	4	0.7
(1,112)	1:67:A:ARG:HG3	1:67:A:ARG:HD3	5	0.7
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	2	0.7
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	2	0.7
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	2	0.7
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	3	0.7
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	5	0.7
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	10	0.7
(1,11)	1:76:A:GLN:HA	1:64:A:GLU:HG3	4	0.7
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	3	0.69
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	3	0.69
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	2	0.69
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	2	0.69
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	2	0.69
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	3	0.69
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	3	0.69
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	3	0.69
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	7	0.69
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	7	0.69
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	1	0.69
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	4	0.69
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	1	0.69
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	3	0.69
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	5	0.69
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	5	0.69
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	10	0.69
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	10	0.69
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	2	0.69
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	2	0.69
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	2	0.69
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	6	0.69
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	6	0.69
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	6	0.69
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,224)	1:19:A:ALA:H	1:18:A:LEU:HB2	1	0.69
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD11	1	0.69
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD12	1	0.69
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD13	1	0.69
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	1	0.69
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	5	0.69
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	5	0.69
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	8	0.69
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	8	0.69
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	6	0.69
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	9	0.69
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	10	0.69
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	2	0.69
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	2	0.69
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	2	0.69
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	3	0.69
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	3	0.69
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	3	0.69
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD21	1	0.69
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD22	1	0.69
(1,458)	1:44:A:LEU:HA	1:44:A:LEU:HD23	1	0.69
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	2	0.69
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	7	0.69
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	9	0.69
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	3	0.69
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	4	0.69
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	1	0.69
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	1	0.69
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	1	0.69
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	4	0.69
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	5	0.69
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	4	0.69
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	4	0.69
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	4	0.69
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	9	0.69
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	9	0.69
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	9	0.69
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	1	0.69
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	4	0.69
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	4	0.68
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	4	0.68
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	8	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	8	0.68
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	10	0.68
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	10	0.68
(2,471)	1:61:A:THR:H	1:61:A:THR:HG21	10	0.68
(2,471)	1:61:A:THR:H	1:61:A:THR:HG22	10	0.68
(2,471)	1:61:A:THR:H	1:61:A:THR:HG23	10	0.68
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	5	0.68
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	2	0.68
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	4	0.68
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	6	0.68
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	8	0.68
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	5	0.68
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	7	0.68
(2,198)	1:74:A:SER:H	1:73:A:TYR:HB3	6	0.68
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	2	0.68
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	2	0.68
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	2	0.68
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	7	0.68
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	5	0.68
(2,77)	1:40:A:SER:H	1:39:A:ARG:HB3	7	0.68
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	3	0.68
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	3	0.68
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	9	0.68
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	9	0.68
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	2	0.68
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	10	0.68
(1,485)	1:37:A:GLU:HB2	1:37:A:GLU:HA	5	0.68
(1,462)	1:61:A:THR:HG21	1:61:A:THR:H	10	0.68
(1,462)	1:61:A:THR:HG22	1:61:A:THR:H	10	0.68
(1,462)	1:61:A:THR:HG23	1:61:A:THR:H	10	0.68
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	5	0.68
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	10	0.68
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	10	0.68
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	10	0.68
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	8	0.68
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	3	0.68
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	3	0.68
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	4	0.68
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	4	0.68
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	4	0.68
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	4	0.68
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,193)	1:13:A:PRO:HA	1:13:A:PRO:HB3	1	0.68
(1,112)	1:67:A:ARG:HG3	1:67:A:ARG:HD3	2	0.68
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	4	0.68
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	9	0.68
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	9	0.68
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	9	0.68
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	6	0.68
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	6	0.68
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	10	0.68
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	10	0.68
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	6	0.68
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	2	0.68
(1,11)	1:76:A:GLN:HA	1:64:A:GLU:HG3	8	0.68
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HE2	7	0.67
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	6	0.67
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	6	0.67
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	8	0.67
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	8	0.67
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	8	0.67
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	3	0.67
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	7	0.67
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	4	0.67
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	2	0.67
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	2	0.67
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	5	0.67
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	5	0.67
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	5	0.67
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB2	9	0.67
(2,287)	1:53:A:GLY:H	1:52:A:GLN:HB3	9	0.67
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	10	0.67
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	2	0.67
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	4	0.67
(2,224)	1:19:A:ALA:H	1:18:A:LEU:HB2	10	0.67
(2,198)	1:74:A:SER:H	1:73:A:TYR:HB3	7	0.67
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	3	0.67
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	3	0.67
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	4	0.67
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	4	0.67
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	8	0.67
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	1	0.67
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	1	0.67
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	7	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	7	0.67
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	8	0.67
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	8	0.67
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	10	0.67
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	10	0.67
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	2	0.67
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	3	0.67
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	4	0.67
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	10	0.67
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	1	0.67
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	1	0.67
(1,485)	1:37:A:GLU:HB2	1:37:A:GLU:HA	10	0.67
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	3	0.67
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	4	0.67
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	10	0.67
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	3	0.67
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	3	0.67
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	6	0.67
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	6	0.67
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	6	0.67
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD11	9	0.67
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD12	9	0.67
(1,364)	1:27:A:ILE:HB	1:27:A:ILE:HD13	9	0.67
(1,324)	1:73:A:TYR:HA	1:67:A:ARG:HA	8	0.67
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	2	0.67
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	6	0.67
(1,112)	1:67:A:ARG:HG3	1:67:A:ARG:HD3	1	0.67
(1,112)	1:67:A:ARG:HG3	1:67:A:ARG:HD3	4	0.67
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	7	0.67
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	7	0.67
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	7	0.67
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	7	0.67
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	7	0.67
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	7	0.67
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	1	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	1	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	1	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	1	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	2	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	2	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	2	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	4	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	4	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	5	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	5	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	5	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	7	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	7	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	7	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	8	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	8	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	8	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	9	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	9	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	9	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	10	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	10	0.67
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	10	0.67
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	6	0.67
(1,11)	1:76:A:GLN:HA	1:64:A:GLU:HG3	10	0.67
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	5	0.66
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	5	0.66
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	7	0.66
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	7	0.66
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	7	0.66
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	6	0.66
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	1	0.66
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	5	0.66
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	9	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	1	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	2	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	3	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	5	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	6	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	7	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	8	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	9	0.66
(2,318)	1:6:A:ASP:H	1:6:A:ASP:HA	10	0.66
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	1	0.66
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	3	0.66
(2,103)	1:43:A:GLY:H	1:11:A:ALA:HA	1	0.66
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	9	0.66
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	9	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	1	0.66
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	5	0.66
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	9	0.66
(2,56)	1:58:A:LEU:H	1:58:A:LEU:HB2	10	0.66
(1,485)	1:37:A:GLU:HB2	1:37:A:GLU:HA	6	0.66
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	1	0.66
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	2	0.66
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	1	0.66
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	1	0.66
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	1	0.66
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	1	0.66
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	3	0.66
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	9	0.66
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	7	0.66
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	1	0.66
(1,112)	1:67:A:ARG:HG3	1:67:A:ARG:HD3	3	0.66
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	3	0.66
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	3	0.66
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	3	0.66
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB1	6	0.66
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB2	6	0.66
(1,40)	1:3:A:ALA:HA	1:3:A:ALA:HB3	6	0.66
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	7	0.66
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	10	0.65
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	10	0.65
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	6	0.65
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	6	0.65
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	2	0.65
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	2	0.65
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	7	0.65
(2,405)	1:62:A:GLY:H	1:62:A:GLY:HA2	8	0.65
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	6	0.65
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	9	0.65
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	9	0.65
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	1	0.65
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	1	0.65
(2,362)	1:69:A:ALA:H	1:68:A:GLY:HA3	2	0.65
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	7	0.65
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	6	0.65
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	7	0.65
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	7	0.65
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,284)	1:76:A:GLN:H	1:64:A:GLU:H	9	0.65
(2,176)	1:68:A:GLY:H	1:67:A:ARG:HG3	6	0.65
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD21	10	0.65
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD22	10	0.65
(2,165)	1:9:A:ILE:H	1:57:A:LEU:HD23	10	0.65
(2,160)	1:74:A:SER:H	1:74:A:SER:HB2	9	0.65
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	1	0.65
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	1	0.65
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	6	0.65
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	6	0.65
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	9	0.65
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	9	0.65
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	4	0.65
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	4	0.65
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB1	2	0.65
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB2	2	0.65
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB3	2	0.65
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	2	0.65
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	2	0.65
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB2	4	0.65
(2,76)	1:23:A:GLN:H	1:23:A:GLN:HB3	4	0.65
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	4	0.65
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	9	0.65
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	9	0.65
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	9	0.65
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	1	0.65
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	5	0.65
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	10	0.65
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	8	0.65
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	2	0.65
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	2	0.65
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	2	0.65
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	2	0.65
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	2	0.65
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	2	0.65
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	2	0.65
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	2	0.65
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	2	0.65
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	3	0.65
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	3	0.65
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	8	0.65
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	8	0.65
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	5	0.65
(1,53)	1:11:A:ALA:HA	1:43:A:GLY:HA3	10	0.65
(1,32)	1:67:A:ARG:HA	1:67:A:ARG:HB2	2	0.65
(1,16)	1:62:A:GLY:HA2	1:62:A:GLY:H	8	0.65
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	4	0.64
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	4	0.64
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	8	0.64
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	8	0.64
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	8	0.64
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	8	0.64
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	8	0.64
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	8	0.64
(3,21)	1:14:A:LEU:HD13	1:14:A:LEU:HA	8	0.64
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	2	0.64
(2,328)	1:37:A:GLU:H	1:33:A:THR:HB	7	0.64
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB1	4	0.64
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB2	4	0.64
(2,319)	1:34:A:ALA:H	1:34:A:ALA:HB3	4	0.64
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	10	0.64
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	10	0.64
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	10	0.64
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	3	0.64
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	1	0.64
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	1	0.64
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	1	0.64
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	8	0.64
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	6	0.64
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	10	0.64
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	10	0.64
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	10	0.64
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	3	0.64
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	1	0.64
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	3	0.64
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	10	0.64
(2,73)	1:21:A:PHE:H	1:21:A:PHE:HB3	7	0.64
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	10	0.64
(1,485)	1:37:A:GLU:HB2	1:37:A:GLU:HA	3	0.64
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	5	0.64
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	2	0.64
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	2	0.64
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	2	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	3	0.64
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	4	0.64
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	6	0.64
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	7	0.64
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	3	0.64
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	8	0.64
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	9	0.64
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	1	0.64
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	1	0.64
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	3	0.64
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	3	0.64
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	3	0.64
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD11	2	0.64
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD12	2	0.64
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD13	2	0.64
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	6	0.64
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	7	0.64
(1,53)	1:11:A:ALA:HA	1:43:A:GLY:HA3	3	0.64
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	9	0.64
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	9	0.64
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	9	0.64
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	2	0.64
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	2	0.64
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	4	0.64
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	4	0.64
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	8	0.64
(3,21)	1:14:A:LEU:HD12	1:14:A:LEU:HA	5	0.63
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	10	0.63
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	5	0.63
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	5	0.63
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	2	0.63
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	7	0.63
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	8	0.63
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	8	0.63
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	8	0.63
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	2	0.63
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	5	0.63
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	2	0.63
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	2	0.63
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	2	0.63
(2,176)	1:68:A:GLY:H	1:67:A:ARG:HG3	8	0.63
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	8	0.63
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	9	0.63
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	5	0.63
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD11	1	0.63
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD12	1	0.63
(2,30)	1:15:A:ALA:H	1:14:A:LEU:HD13	1	0.63
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	9	0.63
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	5	0.63
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	5	0.63
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	4	0.63
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	4	0.63
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	7	0.63
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	7	0.63
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	8	0.63
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	8	0.63
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	2	0.63
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	8	0.63
(1,261)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	9	0.63
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	2	0.63
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	2	0.63
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	2	0.63
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	7	0.63
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	1	0.63
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	1	0.63
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	1	0.63
(1,32)	1:67:A:ARG:HA	1:67:A:ARG:HB2	7	0.63
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	5	0.62
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	5	0.62
(3,34)	1:67:A:ARG:HG2	1:67:A:ARG:HA	3	0.62
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	5	0.62
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	5	0.62
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	6	0.62
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	6	0.62
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	3	0.62
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	8	0.62
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	10	0.62
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	1	0.62
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	1	0.62
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	4	0.62
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	4	0.62
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	10	0.62
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	10	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	5	0.62
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	4	0.62
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	1	0.62
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	1	0.62
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	1	0.62
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	1	0.62
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	6	0.62
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	6	0.62
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	6	0.62
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	2	0.62
(2,152)	1:12:A:GLY:H	1:40:A:SER:HB2	7	0.62
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB2	7	0.62
(2,137)	1:57:A:LEU:H	1:57:A:LEU:HB3	7	0.62
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	4	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	1	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	1	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	1	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	4	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	4	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	4	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	5	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	5	0.62
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	5	0.62
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	7	0.62
(2,34)	1:50:A:ILE:H	1:4:A:GLN:HA	2	0.62
(2,4)	1:73:A:TYR:H	1:28:A:LEU:HB2	10	0.62
(1,485)	1:37:A:GLU:HB2	1:37:A:GLU:HA	2	0.62
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	2	0.62
(1,428)	1:40:A:SER:HA	1:14:A:LEU:HD21	1	0.62
(1,428)	1:40:A:SER:HA	1:14:A:LEU:HD22	1	0.62
(1,428)	1:40:A:SER:HA	1:14:A:LEU:HD23	1	0.62
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	2	0.62
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	2	0.62
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	3	0.62
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	3	0.62
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	5	0.62
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	5	0.62
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	9	0.62
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	8	0.62
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	8	0.62
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	8	0.62
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	10	0.62
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	10	0.62
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	10	0.62
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	2	0.62
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	2	0.62
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	2	0.62
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	10	0.62
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	6	0.62
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	6	0.62
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	6	0.62
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	6	0.62
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	6	0.62
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	6	0.62
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	2	0.62
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	4	0.62
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	4	0.62
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	8	0.62
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	2	0.61
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	2	0.61
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	7	0.61
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	7	0.61
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	8	0.61
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	8	0.61
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	2	0.61
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	2	0.61
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	3	0.61
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	3	0.61
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	6	0.61
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	6	0.61
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	8	0.61
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	8	0.61
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	8	0.61
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD21	7	0.61
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD22	7	0.61
(2,270)	1:75:A:LEU:H	1:75:A:LEU:HD23	7	0.61
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	7	0.61
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	3	0.61
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	3	0.61
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	3	0.61
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	2	0.61
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	4	0.61
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	4	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	1	0.61
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	1	0.61
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	6	0.61
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	6	0.61
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	9	0.61
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	9	0.61
(1,330)	1:13:A:PRO:HA	1:40:A:SER:HB2	5	0.61
(1,280)	1:31:A:TYR:HB3	1:32:A:PRO:HD2	8	0.61
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	3	0.61
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	10	0.61
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	6	0.61
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	6	0.61
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	6	0.61
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	6	0.61
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	6	0.61
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	6	0.61
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	6	0.61
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	6	0.61
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	6	0.61
(1,170)	1:67:A:ARG:HG2	1:67:A:ARG:HD3	10	0.61
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	6	0.61
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	1	0.61
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	1	0.61
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	1	0.61
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	7	0.61
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	3	0.61
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	3	0.61
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	9	0.61
(1,32)	1:67:A:ARG:HA	1:67:A:ARG:HB2	5	0.61
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	7	0.61
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	7	0.6
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	7	0.6
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	7	0.6
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	7	0.6
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	7	0.6
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	7	0.6
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	6	0.6
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	10	0.6
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	4	0.6
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	4	0.6
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	4	0.6
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA2	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,384)	1:23:A:GLN:H	1:22:A:GLY:HA3	7	0.6
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	2	0.6
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	2	0.6
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	9	0.6
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	9	0.6
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	7	0.6
(2,313)	1:58:A:LEU:H	1:54:A:LEU:HA	5	0.6
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	3	0.6
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	9	0.6
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	5	0.6
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	9	0.6
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	1	0.6
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	2	0.6
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	5	0.6
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	7	0.6
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	10	0.6
(2,102)	1:43:A:GLY:H	1:41:A:THR:HA	1	0.6
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	10	0.6
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	2	0.6
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	6	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	2	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	2	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	2	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	6	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	6	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	6	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	7	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	7	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	7	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	9	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	9	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	9	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	10	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	10	0.6
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	10	0.6
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	1	0.6
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	1	0.6
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	1	0.6
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	3	0.6
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	3	0.6
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	6	0.6
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	6	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	8	0.6
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	8	0.6
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	3	0.6
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	10	0.6
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	10	0.6
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	6	0.6
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	8	0.6
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	3	0.6
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	3	0.6
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	3	0.6
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	4	0.6
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	8	0.6
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	1	0.6
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	1	0.6
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	1	0.6
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	1	0.6
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	1	0.6
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	1	0.6
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	1	0.6
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	1	0.6
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	1	0.6
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	5	0.6
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	5	0.6
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	5	0.6
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	5	0.6
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	5	0.6
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	5	0.6
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	5	0.6
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	5	0.6
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	5	0.6
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	7	0.6
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	10	0.6
(1,112)	1:67:A:ARG:HG3	1:67:A:ARG:HD3	6	0.6
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	8	0.6
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	1	0.6
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	5	0.59
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	5	0.59
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	2	0.59
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	2	0.59
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	3	0.59
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	3	0.59
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	3	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	3	0.59
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	6	0.59
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	8	0.59
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	7	0.59
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG2	3	0.59
(2,372)	1:64:A:GLU:H	1:64:A:GLU:HG3	3	0.59
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	4	0.59
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	4	0.59
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	4	0.59
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	4	0.59
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	3	0.59
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	1	0.59
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	8	0.59
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	8	0.59
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	8	0.59
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	8	0.59
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	4	0.59
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	3	0.59
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	3	0.59
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	3	0.59
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	3	0.59
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB1	8	0.59
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB2	8	0.59
(2,82)	1:25:A:ALA:H	1:25:A:ALA:HB3	8	0.59
(2,66)	1:17:A:ALA:H	1:16:A:PRO:HB2	9	0.59
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	3	0.59
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	3	0.59
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	8	0.59
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	8	0.59
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	1	0.59
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	3	0.59
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	5	0.59
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	5	0.59
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	5	0.59
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	2	0.59
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	2	0.59
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	4	0.59
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	4	0.59
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	1	0.59
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	2	0.59
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	3	0.59
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	4	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	5	0.59
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	7	0.59
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	10	0.59
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	9	0.59
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	9	0.59
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	8	0.59
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	10	0.58
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	10	0.58
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	10	0.58
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	10	0.58
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	4	0.58
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	4	0.58
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	8	0.58
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	8	0.58
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	10	0.58
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	10	0.58
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	7	0.58
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	8	0.58
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	7	0.58
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	6	0.58
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	6	0.58
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	10	0.58
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	10	0.58
(2,313)	1:58:A:LEU:H	1:54:A:LEU:HA	4	0.58
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	1	0.58
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	1	0.58
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	4	0.58
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	4	0.58
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	4	0.58
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	4	0.58
(2,227)	1:19:A:ALA:H	1:16:A:PRO:HB2	10	0.58
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	8	0.58
(2,128)	1:39:A:ARG:H	1:39:A:ARG:HA	6	0.58
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	7	0.58
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	3	0.58
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	3	0.58
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	6	0.58
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	6	0.58
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	6	0.58
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	8	0.58
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	7	0.58
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD1	8	0.58
(1,366)	1:31:A:TYR:HB3	1:31:A:TYR:HD2	8	0.58
(1,339)	1:53:A:GLY:HA3	1:53:A:GLY:H	9	0.58
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	1	0.58
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	1	0.58
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	1	0.58
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	1	0.58
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	1	0.58
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	5	0.58
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	7	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	3	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	3	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	3	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	3	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	3	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	3	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	3	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	3	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	3	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	6	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	6	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	6	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	6	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	6	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	6	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	6	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	6	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	6	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	8	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	8	0.58
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	8	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	8	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	8	0.58
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	8	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	8	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	8	0.58
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	8	0.58
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	9	0.58
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD21	10	0.58
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD22	10	0.58
(1,58)	1:57:A:LEU:HB2	1:58:A:LEU:HD23	10	0.58
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB1	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB2	5	0.58
(1,52)	1:16:A:PRO:HA	1:19:A:ALA:HB3	5	0.58
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	5	0.58
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	5	0.58
(1,32)	1:67:A:ARG:HA	1:67:A:ARG:HB2	6	0.58
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	6	0.58
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	5	0.57
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	5	0.57
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	1	0.57
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	1	0.57
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	1	0.57
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	1	0.57
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	2	0.57
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	10	0.57
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	3	0.57
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	10	0.57
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	7	0.57
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	7	0.57
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	2	0.57
(2,284)	1:76:A:GLN:H	1:64:A:GLU:H	5	0.57
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	8	0.57
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	3	0.57
(2,198)	1:74:A:SER:H	1:73:A:TYR:HB3	3	0.57
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	3	0.57
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	6	0.57
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	6	0.57
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	6	0.57
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	4	0.57
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	4	0.57
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	4	0.57
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB2	1	0.57
(2,93)	1:20:A:HIS:H	1:20:A:HIS:HB3	1	0.57
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	10	0.57
(2,34)	1:50:A:ILE:H	1:4:A:GLN:HA	7	0.57
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	9	0.57
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	9	0.57
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	9	0.57
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	4	0.57
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	6	0.57
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	6	0.57
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	6	0.57
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	2	0.57
(1,286)	1:47:A:ARG:HD2	1:47:A:ARG:HE	8	0.57
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	7	0.57
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	4	0.57
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	4	0.57
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	4	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	4	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	4	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	4	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	4	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	4	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	4	0.57
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	9	0.57
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	9	0.57
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	9	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	9	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	9	0.57
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	9	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	9	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	9	0.57
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	9	0.57
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	2	0.57
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	6	0.57
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	6	0.57
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	6	0.57
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	10	0.57
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	2	0.57
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	3	0.57
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	4	0.57
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	10	0.57
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	8	0.57
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	8	0.57
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	10	0.57
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	4	0.57
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	4	0.57
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	4	0.57
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	3	0.56
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	3	0.56
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	4	0.56
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	4	0.56
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	1	0.56
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	5	0.56
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	9	0.56
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	5	0.56
(2,466)	1:39:A:ARG:HE	1:39:A:ARG:HD2	6	0.56
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	10	0.56
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	2	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	2	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	2	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	2	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	8	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	8	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	8	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	9	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	9	0.56
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	9	0.56
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	5	0.56
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	6	0.56
(2,198)	1:74:A:SER:H	1:73:A:TYR:HB3	8	0.56
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	4	0.56
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	4	0.56
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	4	0.56
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	7	0.56
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	7	0.56
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	7	0.56
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	3	0.56
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	3	0.56
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	3	0.56
(2,176)	1:68:A:GLY:H	1:67:A:ARG:HG3	10	0.56
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	6	0.56
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	5	0.56
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	8	0.56
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	10	0.56
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	2	0.56
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	1	0.56
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	8	0.56
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	8	0.56
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	4	0.56
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	7	0.56
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	8	0.56
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB2	8	0.56
(2,12)	1:35:A:LEU:H	1:32:A:PRO:HB3	8	0.56
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	2	0.56
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	4	0.56
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	5	0.56
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	7	0.56
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	8	0.56
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	9	0.56
(1,494)	1:24:A:SER:HA	1:24:A:SER:HB3	10	0.56
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD11	7	0.56
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD12	7	0.56
(1,492)	1:54:A:LEU:HB3	1:58:A:LEU:HD13	7	0.56
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	10	0.56
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	10	0.56
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	10	0.56
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	10	0.56
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	10	0.56
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	10	0.56
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	10	0.56
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	10	0.56
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	10	0.56
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	6	0.56
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	8	0.56
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	6	0.56
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	6	0.56
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	6	0.56
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	3	0.56
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	7	0.56
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	4	0.56
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	4	0.56
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	2	0.56
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	2	0.56
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	2	0.56
(1,310)	1:47:A:ARG:HA	1:47:A:ARG:HG2	4	0.56
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	7	0.56
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	7	0.56
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	7	0.56
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD11	6	0.56
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD12	6	0.56
(1,208)	1:54:A:LEU:HA	1:54:A:LEU:HD13	6	0.56
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	2	0.56
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	2	0.56
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	2	0.56
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	2	0.56
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	2	0.56
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	2	0.56
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	2	0.56
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	2	0.56
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	2	0.56
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	2	0.56
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	2	0.56
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	7	0.56
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	7	0.56
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	7	0.56
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	4	0.56
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD11	6	0.56
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD12	6	0.56
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD13	6	0.56
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	1	0.56
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	5	0.56
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	9	0.56
(1,32)	1:67:A:ARG:HA	1:67:A:ARG:HB2	8	0.56
(1,13)	1:73:A:TYR:HA	1:73:A:TYR:HB2	1	0.56
(1,13)	1:73:A:TYR:HA	1:73:A:TYR:HB2	4	0.56
(1,13)	1:73:A:TYR:HA	1:73:A:TYR:HB2	5	0.56
(1,11)	1:76:A:GLN:HA	1:64:A:GLU:HG3	1	0.56
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	1	0.56
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	8	0.56
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	8	0.56
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	8	0.56
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	9	0.55
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	9	0.55
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	2	0.55
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	2	0.55
(2,490)	1:63:A:LEU:H	1:63:A:LEU:HA	4	0.55
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	2	0.55
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	9	0.55
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	9	0.55
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	5	0.55
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	1	0.55
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB1	5	0.55
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB2	5	0.55
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB3	5	0.55
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	2	0.55
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	3	0.55
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	3	0.55
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	3	0.55
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	10	0.55
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	10	0.55
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	10	0.55
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	1	0.55
(2,189)	1:68:A:GLY:H	1:73:A:TYR:HA	5	0.55
(2,169)	1:9:A:ILE:H	1:45:A:ALA:HA	1	0.55
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	4	0.55
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	2	0.55
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	3	0.55
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	7	0.55
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	7	0.55
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	9	0.55
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	9	0.55
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	2	0.55
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	5	0.55
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	2	0.55
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB2	10	0.55
(1,400)	1:57:A:LEU:HA	1:44:A:LEU:HB3	10	0.55
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	3	0.55
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	3	0.55
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	3	0.55
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	10	0.55
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	2	0.55
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	4	0.55
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	10	0.55
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	10	0.55
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	10	0.55
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	2	0.55
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	2	0.55
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	6	0.55
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	6	0.55
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	7	0.55
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	7	0.55
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	2	0.55
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	2	0.55
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	3	0.55
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	5	0.55
(1,254)	1:9:A:ILE:HA	1:10:A:PRO:HD3	10	0.55
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	3	0.55
(1,199)	1:11:A:ALA:HB1	1:43:A:GLY:HA3	1	0.55
(1,199)	1:11:A:ALA:HB2	1:43:A:GLY:HA3	1	0.55
(1,199)	1:11:A:ALA:HB3	1:43:A:GLY:HA3	1	0.55
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	2	0.55
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	6	0.55
(1,170)	1:67:A:ARG:HG2	1:67:A:ARG:HD3	1	0.55
(1,170)	1:67:A:ARG:HG2	1:67:A:ARG:HD3	3	0.55
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	3	0.55
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	5	0.55
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD11	7	0.55
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD12	7	0.55
(1,85)	1:39:A:ARG:HB3	1:14:A:LEU:HD13	7	0.55
(1,69)	1:40:A:SER:HB3	1:40:A:SER:HA	5	0.55
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	7	0.55
(1,32)	1:67:A:ARG:HA	1:67:A:ARG:HB2	10	0.55
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	5	0.55
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	5	0.55
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	5	0.55
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	1	0.54
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	1	0.54
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	6	0.54
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	6	0.54
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	4	0.54
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	4	0.54
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	1	0.54
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	1	0.54
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	1	0.54
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	1	0.54
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	1	0.54
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	1	0.54
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	3	0.54
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	3	0.54
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	4	0.54
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	4	0.54
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	9	0.54
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	9	0.54
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	10	0.54
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	10	0.54
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	8	0.54
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	8	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	6	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	6	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	6	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	6	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	6	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	9	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	9	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	9	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	9	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	9	0.54
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	9	0.54
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	2	0.54
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	2	0.54
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	4	0.54
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	4	0.54
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	6	0.54
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	6	0.54
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD11	7	0.54
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD12	7	0.54
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD13	7	0.54
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	2	0.54
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	9	0.54
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	9	0.54
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	10	0.54
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	5	0.54
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	5	0.54
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	5	0.54
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	7	0.54
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	10	0.54
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	9	0.54
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	8	0.54
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	1	0.54
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	7	0.54
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	8	0.54
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	10	0.54
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	7	0.54
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	9	0.54
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	8	0.54
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	9	0.54
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	10	0.54
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	8	0.54
(2,113)	1:41:A:THR:H	1:40:A:SER:HB3	9	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	1	0.54
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	4	0.54
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	5	0.54
(2,89)	1:52:A:GLN:H	1:51:A:ASP:HB2	7	0.54
(2,66)	1:17:A:ALA:H	1:16:A:PRO:HB2	2	0.54
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	2	0.54
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	3	0.54
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	6	0.54
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	9	0.54
(2,34)	1:50:A:ILE:H	1:4:A:GLN:HA	1	0.54
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	2	0.54
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	2	0.54
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	3	0.54
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	3	0.54
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	8	0.54
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	8	0.54
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	5	0.54
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	5	0.54
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	5	0.54
(1,283)	1:39:A:ARG:HD3	1:39:A:ARG:HB3	2	0.54
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	1	0.54
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	4	0.54
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	6	0.54
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	7	0.54
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	8	0.54
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	9	0.54
(1,264)	1:37:A:GLU:HG3	1:37:A:GLU:HG2	10	0.54
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	4	0.54
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	4	0.54
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	9	0.54
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	1	0.54
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	3	0.54
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	7	0.54
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	8	0.54
(1,170)	1:67:A:ARG:HG2	1:67:A:ARG:HD3	4	0.54
(1,170)	1:67:A:ARG:HG2	1:67:A:ARG:HD3	7	0.54
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	7	0.54
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	7	0.54
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	7	0.54
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	7	0.54
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	7	0.54
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	7	0.54
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	7	0.54
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	7	0.54
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD11	10	0.54
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD12	10	0.54
(1,136)	1:63:A:LEU:HD21	1:63:A:LEU:HD13	10	0.54
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD11	10	0.54
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD12	10	0.54
(1,136)	1:63:A:LEU:HD22	1:63:A:LEU:HD13	10	0.54
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD11	10	0.54
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD12	10	0.54
(1,136)	1:63:A:LEU:HD23	1:63:A:LEU:HD13	10	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	1	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	2	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	4	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	5	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	6	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	7	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	8	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	9	0.54
(1,134)	1:48:A:PHE:HB3	1:48:A:PHE:HB2	10	0.54
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	3	0.54
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	3	0.54
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	3	0.54
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	4	0.54
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	4	0.54
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	4	0.54
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	4	0.54
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	4	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	1	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	1	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	1	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	7	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	7	0.54
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	7	0.54
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	2	0.53
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	2	0.53
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	6	0.53
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	6	0.53
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	8	0.53
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	8	0.53
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	9	0.53
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	1	0.53
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	1	0.53
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	2	0.53
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	2	0.53
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	7	0.53
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	7	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	2	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	2	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	2	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	2	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	2	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	2	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	3	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	3	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	3	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	3	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	3	0.53
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	3	0.53
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	5	0.53
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	5	0.53
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	7	0.53
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	7	0.53
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	8	0.53
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	8	0.53
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	4	0.53
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	4	0.53
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	4	0.53
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	4	0.53
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	4	0.53
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	2	0.53
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	2	0.53
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	5	0.53
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	4	0.53
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	10	0.53
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	10	0.53
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	10	0.53
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	1	0.53
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	6	0.53
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	8	0.53
(2,317)	1:76:A:GLN:H	1:75:A:LEU:HB3	5	0.53
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	2	0.53
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	2	0.53
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	8	0.53
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	5	0.53
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	5	0.53
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	5	0.53
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	2	0.53
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	10	0.53
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	2	0.53
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	7	0.53
(2,189)	1:68:A:GLY:H	1:73:A:TYR:HA	8	0.53
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	1	0.53
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	4	0.53
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	5	0.53
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	5	0.53
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	9	0.53
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	2	0.53
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	3	0.53
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	9	0.53
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	10	0.53
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	5	0.53
(2,59)	1:66:A:SER:H	1:66:A:SER:HB3	3	0.53
(2,59)	1:66:A:SER:H	1:66:A:SER:HB3	7	0.53
(2,59)	1:66:A:SER:H	1:66:A:SER:HB3	10	0.53
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	6	0.53
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	6	0.53
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	6	0.53
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	2	0.53
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD11	10	0.53
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD12	10	0.53
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD13	10	0.53
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	10	0.53
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	5	0.53
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	5	0.53
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	10	0.53
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	10	0.53
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	6	0.53
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	6	0.53
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	6	0.53
(1,283)	1:39:A:ARG:HD3	1:39:A:ARG:HB3	7	0.53
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	1	0.53
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	8	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	8	0.53
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	9	0.53
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	9	0.53
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	4	0.53
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	4	0.53
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	4	0.53
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	4	0.53
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	10	0.53
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	1	0.53
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	1	0.53
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	1	0.53
(1,170)	1:67:A:ARG:HG2	1:67:A:ARG:HD3	2	0.53
(1,170)	1:67:A:ARG:HG2	1:67:A:ARG:HD3	8	0.53
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	7	0.53
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	8	0.53
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	1	0.53
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	9	0.53
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	3	0.53
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	8	0.53
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	2	0.53
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	2	0.53
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	5	0.53
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	10	0.53
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	2	0.53
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	2	0.53
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	2	0.53
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	9	0.52
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	9	0.52
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB2	7	0.52
(5,20)	1:21:A:PHE:H	1:21:A:PHE:HB3	7	0.52
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	5	0.52
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	5	0.52
(3,14)	1:14:A:LEU:HB3	1:14:A:LEU:HA	10	0.52
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	5	0.52
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	5	0.52
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	6	0.52
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	6	0.52
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	10	0.52
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	10	0.52
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	10	0.52
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	10	0.52
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	10	0.52
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	9	0.52
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	9	0.52
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	10	0.52
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	10	0.52
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	8	0.52
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	10	0.52
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	2	0.52
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	5	0.52
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	6	0.52
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	7	0.52
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	8	0.52
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	10	0.52
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	4	0.52
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	4	0.52
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	4	0.52
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	9	0.52
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	5	0.52
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	5	0.52
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	6	0.52
(2,347)	1:22:A:GLY:H	1:21:A:PHE:H	4	0.52
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	4	0.52
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	4	0.52
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	4	0.52
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	9	0.52
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	9	0.52
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	9	0.52
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	1	0.52
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	2	0.52
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	7	0.52
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	8	0.52
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	3	0.52
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	6	0.52
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	8	0.52
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	10	0.52
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	6	0.52
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	1	0.52
(2,185)	1:74:A:SER:H	1:67:A:ARG:HA	5	0.52
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	8	0.52
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	8	0.52
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	8	0.52
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	10	0.52
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	10	0.52
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	9	0.52
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	9	0.52
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	9	0.52
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	6	0.52
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	7	0.52
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	2	0.52
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	3	0.52
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	4	0.52
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	10	0.52
(2,66)	1:17:A:ALA:H	1:16:A:PRO:HB2	5	0.52
(2,66)	1:17:A:ALA:H	1:16:A:PRO:HB2	6	0.52
(2,59)	1:66:A:SER:H	1:66:A:SER:HB3	4	0.52
(2,59)	1:66:A:SER:H	1:66:A:SER:HB3	8	0.52
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	5	0.52
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	8	0.52
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	8	0.52
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	8	0.52
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	8	0.52
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	8	0.52
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	8	0.52
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	8	0.52
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	8	0.52
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	8	0.52
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	8	0.52
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	8	0.52
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	9	0.52
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	9	0.52
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	9	0.52
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	9	0.52
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	9	0.52
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	9	0.52
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	9	0.52
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	9	0.52
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	9	0.52
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	1	0.52
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	2	0.52
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	4	0.52
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	4	0.52
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	4	0.52
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	3	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	3	0.52
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	4	0.52
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	4	0.52
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	4	0.52
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	4	0.52
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	5	0.52
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	5	0.52
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	5	0.52
(1,177)	1:56:A:ILE:HB	1:56:A:ILE:H	9	0.52
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	7	0.52
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	7	0.52
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	7	0.52
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	5	0.52
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	8	0.52
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	9	0.52
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	9	0.52
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	1	0.52
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	3	0.52
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	9	0.52
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	1	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	3	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	3	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	3	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	6	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	6	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	6	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	10	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	10	0.52
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	10	0.52
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	2	0.51
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	2	0.51
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	7	0.51
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	7	0.51
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	10	0.51
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	10	0.51
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	4	0.51
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	4	0.51
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	10	0.51
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	10	0.51
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	6	0.51
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	6	0.51
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	7	0.51
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	4	0.51
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	5	0.51
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	6	0.51
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	7	0.51
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	10	0.51
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	1	0.51
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	1	0.51
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA2	3	0.51
(2,481)	1:47:A:ARG:H	1:46:A:GLY:HA3	3	0.51
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	1	0.51
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	4	0.51
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	1	0.51
(2,441)	1:71:A:ALA:H	1:71:A:ALA:HA	3	0.51
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	1	0.51
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	4	0.51
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	3	0.51
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	6	0.51
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	8	0.51
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	6	0.51
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	6	0.51
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	6	0.51
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	2	0.51
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	5	0.51
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	8	0.51
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	9	0.51
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	1	0.51
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	5	0.51
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	7	0.51
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	2	0.51
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	4	0.51
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB1	7	0.51
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB2	7	0.51
(2,260)	1:15:A:ALA:H	1:15:A:ALA:HB3	7	0.51
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	3	0.51
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	6	0.51
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	1	0.51
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	5	0.51
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	9	0.51
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	5	0.51
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	6	0.51
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	7	0.51
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB1	3	0.51
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB2	3	0.51
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB3	3	0.51
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB1	10	0.51
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB2	10	0.51
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB3	10	0.51
(2,39)	1:50:A:ILE:H	1:50:A:ILE:HA	1	0.51
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	8	0.51
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	8	0.51
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	8	0.51
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	4	0.51
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	3	0.51
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	1	0.51
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	1	0.51
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	2	0.51
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	2	0.51
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	6	0.51
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	6	0.51
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	7	0.51
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	7	0.51
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	7	0.51
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	7	0.51
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	5	0.51
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	5	0.51
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	5	0.51
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	1	0.51
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	6	0.51
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	8	0.51
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	6	0.5
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	6	0.5
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	3	0.5
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	3	0.5
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB2	8	0.5
(5,23)	1:47:A:ARG:H	1:47:A:ARG:HB3	8	0.5
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD2	6	0.5
(5,10)	1:17:A:ALA:H	1:16:A:PRO:HD3	6	0.5
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	3	0.5
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	3	0.5
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	9	0.5
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	9	0.5
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	2	0.5
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	4	0.5
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	7	0.5
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	2	0.5
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	8	0.5
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	9	0.5
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	3	0.5
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	1	0.5
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	1	0.5
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	2	0.5
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	10	0.5
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	7	0.5
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	1	0.5
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	1	0.5
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	10	0.5
(2,281)	1:41:A:THR:H	1:13:A:PRO:HA	6	0.5
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	5	0.5
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	2	0.5
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	7	0.5
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	10	0.5
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	2	0.5
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	4	0.5
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	10	0.5
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	1	0.5
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	5	0.5
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	10	0.5
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	2	0.5
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	3	0.5
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	4	0.5
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	6	0.5
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	9	0.5
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	10	0.5
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	8	0.5
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	8	0.5
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	3	0.5
(2,66)	1:17:A:ALA:H	1:16:A:PRO:HB2	3	0.5
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD11	1	0.5
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD12	1	0.5
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD13	1	0.5
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD11	9	0.5
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD12	9	0.5
(1,487)	1:73:A:TYR:HB2	1:29:A:LEU:HD13	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	3	0.5
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	4	0.5
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	4	0.5
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	4	0.5
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	4	0.5
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	4	0.5
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	4	0.5
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	4	0.5
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	4	0.5
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	4	0.5
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	4	0.5
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	10	0.5
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	8	0.5
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	9	0.5
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	4	0.5
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	8	0.5
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	4	0.5
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	4	0.5
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	4	0.5
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	1	0.5
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	1	0.5
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	2	0.5
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	2	0.5
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	2	0.5
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	3	0.5
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	2	0.5
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	2	0.5
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	5	0.5
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	5	0.5
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	8	0.5
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	8	0.5
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	5	0.5
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	5	0.5
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	5	0.5
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	7	0.5
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	7	0.5
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	7	0.5
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	7	0.5
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	7	0.5
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	7	0.5
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	7	0.5
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	7	0.5
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	1	0.5
(1,96)	1:37:A:GLU:HB3	1:37:A:GLU:H	5	0.5
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	10	0.5
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	10	0.5
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	10	0.5
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	4	0.5
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	5	0.5
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	7	0.5
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	7	0.5
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	7	0.5
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	2	0.5
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	4	0.5
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	7	0.5
(1,43)	1:23:A:GLN:HB3	1:23:A:GLN:H	4	0.5
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	6	0.5
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	6	0.5
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	6	0.5
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	3	0.5
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	1	0.49
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	1	0.49
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	3	0.49
(3,18)	1:12:A:GLY:HA3	1:13:A:PRO:HD3	3	0.49
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	1	0.49
(2,484)	1:47:A:ARG:H	1:47:A:ARG:HA	3	0.49
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	5	0.49
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	9	0.49
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	1	0.49
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	2	0.49
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	4	0.49
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	7	0.49
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	5	0.49
(2,440)	1:27:A:ILE:H	1:22:A:GLY:HA3	9	0.49
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	7	0.49
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	10	0.49
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	8	0.49
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	10	0.49
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	6	0.49
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	6	0.49
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	1	0.49
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	2	0.49
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	9	0.49
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	10	0.49
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	7	0.49
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	8	0.49
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	1	0.49
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	3	0.49
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	4	0.49
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	7	0.49
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	7	0.49
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	7	0.49
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	9	0.49
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	1	0.49
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	1	0.49
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	1	0.49
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	2	0.49
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	2	0.49
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	2	0.49
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	3	0.49
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	6	0.49
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	1	0.49
(2,221)	1:23:A:GLN:H	1:22:A:GLY:HA2	9	0.49
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	2	0.49
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	4	0.49
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	7	0.49
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	8	0.49
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	3	0.49
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	1	0.49
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	5	0.49
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	7	0.49
(2,143)	1:56:A:ILE:H	1:56:A:ILE:HA	8	0.49
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	6	0.49
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	10	0.49
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	4	0.49
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	8	0.49
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	7	0.49
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	4	0.49
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	5	0.49
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	6	0.49
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB1	1	0.49
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB2	1	0.49
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB3	1	0.49
(2,28)	1:14:A:LEU:H	1:40:A:SER:HA	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	5	0.49
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	5	0.49
(2,7)	1:30:A:SER:H	1:29:A:LEU:HB3	9	0.49
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	10	0.49
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	7	0.49
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	7	0.49
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	7	0.49
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	7	0.49
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	7	0.49
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	7	0.49
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	7	0.49
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	7	0.49
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	7	0.49
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	10	0.49
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	6	0.49
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	7	0.49
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	9	0.49
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	10	0.49
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	10	0.49
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	10	0.49
(1,280)	1:31:A:TYR:HB3	1:32:A:PRO:HD2	9	0.49
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	3	0.49
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	3	0.49
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	3	0.49
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	9	0.49
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	4	0.49
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD1	10	0.49
(1,225)	1:48:A:PHE:HB3	1:48:A:PHE:HD2	10	0.49
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	7	0.49
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	10	0.49
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	2	0.49
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	2	0.49
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	2	0.49
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	3	0.49
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	3	0.49
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	3	0.49
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	4	0.49
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	4	0.49
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	4	0.49
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	6	0.49
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	6	0.49
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	9	0.49
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	9	0.49
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	9	0.49
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	10	0.49
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	10	0.49
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	10	0.49
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	1	0.49
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	6	0.49
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	1	0.49
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	1	0.49
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	1	0.49
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	1	0.49
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	1	0.49
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	1	0.49
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	1	0.49
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	1	0.49
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	1	0.49
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	8	0.49
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	8	0.49
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	8	0.49
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	8	0.49
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	8	0.49
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	8	0.49
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD11	9	0.49
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD12	9	0.49
(1,98)	1:75:A:LEU:HA	1:75:A:LEU:HD13	9	0.49
(1,96)	1:37:A:GLU:HB3	1:37:A:GLU:H	10	0.49
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	6	0.49
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	9	0.49
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	10	0.49
(1,34)	1:8:A:ASP:HA	1:8:A:ASP:HB2	6	0.49
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD11	9	0.49
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD12	9	0.49
(1,2)	1:58:A:LEU:HB3	1:58:A:LEU:HD13	9	0.49
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	5	0.48
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	5	0.48
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	5	0.48
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	5	0.48
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	5	0.48
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	5	0.48
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	5	0.48
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	7	0.48
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	7	0.48
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	1	0.48
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	2	0.48
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	4	0.48
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	10	0.48
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	10	0.48
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	5	0.48
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	8	0.48
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	10	0.48
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	9	0.48
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	10	0.48
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD11	9	0.48
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD12	9	0.48
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD13	9	0.48
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	3	0.48
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	5	0.48
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	6	0.48
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	8	0.48
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	9	0.48
(2,446)	1:25:A:ALA:H	1:25:A:ALA:HA	10	0.48
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB2	4	0.48
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB3	4	0.48
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	2	0.48
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	3	0.48
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	5	0.48
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	5	0.48
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	6	0.48
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	1	0.48
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	10	0.48
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	10	0.48
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	9	0.48
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	3	0.48
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	4	0.48
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	8	0.48
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	9	0.48
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	7	0.48
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	7	0.48
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	7	0.48
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	4	0.48
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	10	0.48
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	3	0.48
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	9	0.48
(2,211)	1:58:A:LEU:H	1:59:A:ALA:H	10	0.48
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	5	0.48
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	3	0.48
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	5	0.48
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	7	0.48
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	9	0.48
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	2	0.48
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	7	0.48
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	1	0.48
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	1	0.48
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	2	0.48
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	7	0.48
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	8	0.48
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	9	0.48
(2,91)	1:4:A:GLN:H	1:4:A:GLN:HA	10	0.48
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	6	0.48
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	8	0.48
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	8	0.48
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	5	0.48
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	7	0.48
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	7	0.48
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	7	0.48
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	9	0.48
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	9	0.48
(1,286)	1:47:A:ARG:HD2	1:47:A:ARG:HE	7	0.48
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	8	0.48
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	8	0.48
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	1	0.48
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	5	0.48
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	2	0.48
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	3	0.48
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	6	0.48
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	6	0.48
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB2	10	0.48
(1,216)	1:67:A:ARG:HG2	1:67:A:ARG:HB3	10	0.48
(1,174)	1:75:A:LEU:HD11	1:75:A:LEU:HG	8	0.48
(1,174)	1:75:A:LEU:HD12	1:75:A:LEU:HG	8	0.48
(1,174)	1:75:A:LEU:HD13	1:75:A:LEU:HG	8	0.48
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	7	0.48
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	6	0.48
(1,96)	1:37:A:GLU:HB3	1:37:A:GLU:H	6	0.48
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	3	0.48
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	2	0.48
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	5	0.48
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	8	0.48
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	10	0.48
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	4	0.48
(1,11)	1:76:A:GLN:HA	1:64:A:GLU:HG3	6	0.48
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	6	0.47
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	8	0.47
(3,5)	1:66:A:SER:HB2	1:66:A:SER:H	1	0.47
(3,5)	1:66:A:SER:HB3	1:66:A:SER:H	1	0.47
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	9	0.47
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	4	0.47
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	10	0.47
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	6	0.47
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	2	0.47
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	5	0.47
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	7	0.47
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	6	0.47
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	6	0.47
(2,411)	1:51:A:ASP:H	1:51:A:ASP:HA	7	0.47
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	1	0.47
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	5	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	1	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	2	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	3	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	4	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	5	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	6	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	7	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	8	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	9	0.47
(2,392)	1:70:A:ASN:HD22	1:70:A:ASN:HD21	10	0.47
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	7	0.47
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	2	0.47
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	3	0.47
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	6	0.47
(2,313)	1:58:A:LEU:H	1:54:A:LEU:HA	9	0.47
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	1	0.47
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	5	0.47
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	6	0.47
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	7	0.47
(2,290)	1:48:A:PHE:H	1:48:A:PHE:HA	10	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	1	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	2	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	3	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	4	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	5	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	6	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	7	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	8	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	9	0.47
(2,279)	1:4:A:GLN:HE21	1:4:A:GLN:HE22	10	0.47
(2,278)	1:70:A:ASN:H	1:70:A:ASN:HA	1	0.47
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	2	0.47
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	2	0.47
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	2	0.47
(2,246)	1:25:A:ALA:H	1:26:A:HIS:H	1	0.47
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	8	0.47
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	5	0.47
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	6	0.47
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	3	0.47
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	1	0.47
(2,216)	1:40:A:SER:H	1:40:A:SER:HA	5	0.47
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	9	0.47
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	4	0.47
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	6	0.47
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	7	0.47
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	8	0.47
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	10	0.47
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	4	0.47
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD11	3	0.47
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD12	3	0.47
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD13	3	0.47
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	3	0.47
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	9	0.47
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	8	0.47
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	3	0.47
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	3	0.47
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	3	0.47
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	10	0.47
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	6	0.47
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	9	0.47
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	10	0.47
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	2	0.47
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	7	0.47
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	3	0.47
(2,59)	1:66:A:SER:H	1:66:A:SER:HB3	5	0.47
(2,34)	1:50:A:ILE:H	1:4:A:GLN:HA	10	0.47
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	9	0.47
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	10	0.47
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	3	0.47
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	3	0.47
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	3	0.47
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	3	0.47
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	3	0.47
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	3	0.47
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	3	0.47
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	3	0.47
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	3	0.47
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	5	0.47
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	5	0.47
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	5	0.47
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	5	0.47
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	6	0.47
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	4	0.47
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	4	0.47
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	4	0.47
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	10	0.47
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	10	0.47
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	10	0.47
(1,296)	1:27:A:ILE:HG13	1:27:A:ILE:H	5	0.47
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	5	0.47
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	6	0.47
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	9	0.47
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	4	0.47
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	6	0.47
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	1	0.47
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	1	0.47
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	1	0.47
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	2	0.47
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	9	0.47
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	9	0.47
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	9	0.47
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	4	0.47
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	9	0.47
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	5	0.47
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	3	0.46
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	3	0.46
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	3	0.46
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	10	0.46
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	10	0.46
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	5	0.46
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	2	0.46
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	2	0.46
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	9	0.46
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	5	0.46
(2,466)	1:39:A:ARG:HE	1:39:A:ARG:HD2	5	0.46
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB2	3	0.46
(2,457)	1:70:A:ASN:H	1:70:A:ASN:HB3	3	0.46
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	10	0.46
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	3	0.46
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	6	0.46
(2,450)	1:15:A:ALA:H	1:15:A:ALA:HA	9	0.46
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	4	0.46
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	5	0.46
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	8	0.46
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	1	0.46
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	4	0.46
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	9	0.46
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	1	0.46
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	1	0.46
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	4	0.46
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	8	0.46
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	9	0.46
(2,398)	1:49:A:ASP:H	1:49:A:ASP:HA	10	0.46
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	9	0.46
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	4	0.46
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	5	0.46
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	2	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	3	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	3	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	4	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	4	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	4	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	6	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	6	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	6	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	8	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	8	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	8	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	9	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	9	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	9	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	10	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	10	0.46
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	10	0.46
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	5	0.46
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	1	0.46
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	9	0.46
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	4	0.46
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	10	0.46
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	3	0.46
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	2	0.46
(2,200)	1:74:A:SER:H	1:74:A:SER:HA	9	0.46
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	3	0.46
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	6	0.46
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	7	0.46
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	3	0.46
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	4	0.46
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	5	0.46
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	7	0.46
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	8	0.46
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	10	0.46
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	2	0.46
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	9	0.46
(2,119)	1:31:A:TYR:H	1:31:A:TYR:HA	1	0.46
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	8	0.46
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	2	0.46
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB1	4	0.46
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB2	4	0.46
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB3	4	0.46
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	3	0.46
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:17:A:ALA:H	1:16:A:PRO:HB2	7	0.46
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	4	0.46
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	4	0.46
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	9	0.46
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	5	0.46
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	6	0.46
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	6	0.46
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	6	0.46
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	6	0.46
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	6	0.46
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	6	0.46
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	6	0.46
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	6	0.46
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	6	0.46
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	6	0.46
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	9	0.46
(1,383)	1:12:A:GLY:HA3	1:12:A:GLY:H	1	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	1	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	2	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	4	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	5	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	6	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	7	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	8	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	9	0.46
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	10	0.46
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	2	0.46
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	3	0.46
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	4	0.46
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	6	0.46
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	7	0.46
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	8	0.46
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	10	0.46
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	6	0.46
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	10	0.46
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	6	0.46
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	6	0.46
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	6	0.46
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	9	0.46
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	9	0.46
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	9	0.46
(1,286)	1:47:A:ARG:HD2	1:47:A:ARG:HE	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	1	0.46
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	5	0.46
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	3	0.46
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	5	0.46
(1,235)	1:74:A:SER:HB3	1:74:A:SER:HA	9	0.46
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	4	0.46
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	5	0.46
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	8	0.46
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	4	0.46
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	4	0.46
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	9	0.46
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	3	0.46
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	4	0.46
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	6	0.46
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	9	0.46
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	3	0.46
(1,96)	1:37:A:GLU:HB3	1:37:A:GLU:H	3	0.46
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	9	0.46
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	5	0.46
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	5	0.46
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	9	0.46
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	10	0.46
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	7	0.45
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	7	0.45
(4,39)	1:12:A:GLY:H	1:41:A:THR:O	10	0.45
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	9	0.45
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	10	0.45
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	4	0.45
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	4	0.45
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	5	0.45
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	5	0.45
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	7	0.45
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	7	0.45
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	8	0.45
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	8	0.45
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	1	0.45
(2,492)	1:47:A:ARG:H	1:46:A:GLY:HA2	3	0.45
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	7	0.45
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	6	0.45
(2,429)	1:31:A:TYR:H	1:30:A:SER:HA	1	0.45
(2,410)	1:4:A:GLN:H	1:4:A:GLN:HG2	8	0.45
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	8	0.45
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	3	0.45
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	1	0.45
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	3	0.45
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	3	0.45
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	6	0.45
(2,346)	1:73:A:TYR:H	1:72:A:SER:HA	8	0.45
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	10	0.45
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	5	0.45
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	1	0.45
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	1	0.45
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	1	0.45
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB1	5	0.45
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB2	5	0.45
(2,272)	1:55:A:ALA:H	1:55:A:ALA:HB3	5	0.45
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	4	0.45
(2,245)	1:30:A:SER:H	1:30:A:SER:HA	5	0.45
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	3	0.45
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	8	0.45
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	3	0.45
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	1	0.45
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	7	0.45
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD21	8	0.45
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD22	8	0.45
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD23	8	0.45
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	1	0.45
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	2	0.45
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	4	0.45
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	5	0.45
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	8	0.45
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	9	0.45
(2,175)	1:69:A:ALA:H	1:69:A:ALA:HA	10	0.45
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	2	0.45
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	3	0.45
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	3	0.45
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	1	0.45
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	5	0.45
(2,115)	1:26:A:HIS:H	1:26:A:HIS:HB2	7	0.45
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	3	0.45
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	1	0.45
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	6	0.45
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	9	0.45
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	5	0.45
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	8	0.45
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	5	0.45
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	4	0.45
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	3	0.45
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	4	0.45
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	9	0.45
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	2	0.45
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	3	0.45
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	5	0.45
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	6	0.45
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	7	0.45
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	8	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	1	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	2	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	3	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	4	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	5	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	6	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	7	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	8	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	9	0.45
(1,450)	1:46:A:GLY:HA3	1:46:A:GLY:HA2	10	0.45
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	8	0.45
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	7	0.45
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	7	0.45
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	4	0.45
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	8	0.45
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	6	0.45
(1,346)	1:22:A:GLY:HA3	1:22:A:GLY:HA2	3	0.45
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	1	0.45
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	5	0.45
(1,336)	1:43:A:GLY:HA2	1:43:A:GLY:HA3	9	0.45
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	2	0.45
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	5	0.45
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	7	0.45
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	8	0.45
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	8	0.45
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	7	0.45
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	7	0.45
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	3	0.45
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	3	0.45
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	3	0.45
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	10	0.45
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	10	0.45
(1,269)	1:16:A:PRO:HD2	1:17:A:ALA:H	6	0.45
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	2	0.45
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	3	0.45
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	6	0.45
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	7	0.45
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	8	0.45
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	9	0.45
(1,251)	1:73:A:TYR:HB2	1:73:A:TYR:HB3	10	0.45
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	6	0.45
(1,228)	1:39:A:ARG:HD3	1:38:A:GLY:HA3	1	0.45
(1,223)	1:30:A:SER:HA	1:31:A:TYR:H	1	0.45
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	3	0.45
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	8	0.45
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	2	0.45
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	2	0.45
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	2	0.45
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	8	0.45
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	5	0.45
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	2	0.45
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	2	0.45
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	2	0.45
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	2	0.45
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	2	0.45
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	2	0.45
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	2	0.45
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	2	0.45
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	2	0.45
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	9	0.45
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	9	0.45
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	9	0.45
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	9	0.45
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	9	0.45
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	9	0.45
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	9	0.45
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	9	0.45
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	9	0.45
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	10	0.45
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	1	0.45
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	2	0.45
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	5	0.45
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	7	0.45
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	10	0.45
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	1	0.45
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	2	0.45
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	9	0.45
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	4	0.45
(1,46)	1:73:A:TYR:HA	1:68:A:GLY:H	5	0.45
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	1	0.45
(1,45)	1:46:A:GLY:HA2	1:47:A:ARG:H	3	0.45
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	1	0.45
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	7	0.45
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	7	0.45
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	7	0.45
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	5	0.44
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	5	0.44
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	9	0.44
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	9	0.44
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	2	0.44
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	8	0.44
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	8	0.44
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	5	0.44
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	9	0.44
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	9	0.44
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	4	0.44
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	4	0.44
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	9	0.44
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	9	0.44
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	1	0.44
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	1	0.44
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	1	0.44
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	2	0.44
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	5	0.44
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	4	0.44
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	2	0.44
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	5	0.44
(2,344)	1:36:A:THR:H	1:32:A:PRO:HG2	4	0.44
(2,344)	1:36:A:THR:H	1:32:A:PRO:HG3	4	0.44
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,324)	1:61:A:THR:H	1:61:A:THR:HB	10	0.44
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	7	0.44
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	2	0.44
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	6	0.44
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	6	0.44
(2,185)	1:74:A:SER:H	1:67:A:ARG:HA	8	0.44
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD11	9	0.44
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD12	9	0.44
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD13	9	0.44
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	3	0.44
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	3	0.44
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	3	0.44
(2,173)	1:45:A:ALA:H	1:45:A:ALA:HA	6	0.44
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	2	0.44
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	9	0.44
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	9	0.44
(2,120)	1:25:A:ALA:H	1:24:A:SER:HB2	1	0.44
(2,115)	1:26:A:HIS:H	1:26:A:HIS:HB2	4	0.44
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	5	0.44
(2,71)	1:60:A:GLY:H	1:60:A:GLY:HA3	7	0.44
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	6	0.44
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	6	0.44
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	1	0.44
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	8	0.44
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	2	0.44
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	3	0.44
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	5	0.44
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	7	0.44
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	1	0.44
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	2	0.44
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	6	0.44
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	7	0.44
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	8	0.44
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	10	0.44
(1,466)	1:12:A:GLY:HA3	1:12:A:GLY:HA2	1	0.44
(1,424)	1:40:A:SER:HB3	1:41:A:THR:H	9	0.44
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	1	0.44
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	2	0.44
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	3	0.44
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	5	0.44
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	6	0.44
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:32:A:PRO:HD3	1:32:A:PRO:HD2	10	0.44
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	10	0.44
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	10	0.44
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	10	0.44
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	10	0.44
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	8	0.44
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	9	0.44
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	3	0.44
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	3	0.44
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	3	0.44
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	1	0.44
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	3	0.44
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	4	0.44
(1,334)	1:39:A:ARG:HD2	1:39:A:ARG:HD3	9	0.44
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	4	0.44
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	4	0.44
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	4	0.44
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	2	0.44
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	1	0.44
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	3	0.44
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	10	0.44
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	10	0.44
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	10	0.44
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	10	0.44
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	7	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	3	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	3	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	3	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	3	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	3	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	3	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	3	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	3	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	3	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	4	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	4	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	4	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	4	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	4	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	4	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	4	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	4	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	6	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	6	0.44
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	6	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	6	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	6	0.44
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	6	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	6	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	6	0.44
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	6	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	1	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	3	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	4	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	5	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	6	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	7	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	8	0.44
(1,130)	1:31:A:TYR:HB3	1:31:A:TYR:HB2	9	0.44
(1,127)	1:29:A:LEU:HB2	1:29:A:LEU:HB3	8	0.44
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	8	0.44
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	8	0.44
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	8	0.44
(1,76)	1:21:A:PHE:HB3	1:21:A:PHE:H	7	0.44
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	3	0.44
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	2	0.44
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	8	0.43
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	8	0.43
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	2	0.43
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	2	0.43
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	5	0.43
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	6	0.43
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	10	0.43
(4,28)	1:9:A:ILE:N	1:44:A:LEU:O	7	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	4	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	4	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	4	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	4	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	4	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	4	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	5	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	5	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	5	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	5	0.43
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	5	0.43
(2,485)	1:55:A:ALA:H	1:54:A:LEU:HB3	10	0.43
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	9	0.43
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	9	0.43
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	9	0.43
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD11	2	0.43
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD12	2	0.43
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD13	2	0.43
(2,419)	1:72:A:SER:H	1:70:A:ASN:HA	3	0.43
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	1	0.43
(2,351)	1:68:A:GLY:H	1:68:A:GLY:HA3	4	0.43
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	4	0.43
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	4	0.43
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	3	0.43
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	6	0.43
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	7	0.43
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	9	0.43
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	8	0.43
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	10	0.43
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	2	0.43
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	4	0.43
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	4	0.43
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	5	0.43
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	7	0.43
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	9	0.43
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	3	0.43
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	6	0.43
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	8	0.43
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	6	0.43
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	6	0.43
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	6	0.43
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	6	0.43
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	8	0.43
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	8	0.43
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	8	0.43
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	9	0.43
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	9	0.43
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	9	0.43
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	1	0.43
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:57:A:LEU:H	1:56:A:ILE:HB	4	0.43
(2,139)	1:56:A:ILE:H	1:57:A:LEU:H	1	0.43
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	10	0.43
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	10	0.43
(2,115)	1:26:A:HIS:H	1:26:A:HIS:HB2	2	0.43
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	1	0.43
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	10	0.43
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	1	0.43
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	3	0.43
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	7	0.43
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	8	0.43
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	1	0.43
(1,477)	1:67:A:ARG:HG2	1:67:A:ARG:HG3	5	0.43
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	2	0.43
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	2	0.43
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	2	0.43
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	2	0.43
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	2	0.43
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	2	0.43
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	2	0.43
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	2	0.43
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	2	0.43
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD11	10	0.43
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD12	10	0.43
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD13	10	0.43
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	5	0.43
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	4	0.43
(1,410)	1:55:A:ALA:HB1	1:52:A:GLN:HA	10	0.43
(1,410)	1:55:A:ALA:HB2	1:52:A:GLN:HA	10	0.43
(1,410)	1:55:A:ALA:HB3	1:52:A:GLN:HA	10	0.43
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	5	0.43
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	5	0.43
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	9	0.43
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	9	0.43
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD11	4	0.43
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD12	4	0.43
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD13	4	0.43
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	2	0.43
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	8	0.43
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	8	0.43
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	8	0.43
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	9	0.43
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	9	0.43
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	9	0.43
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	9	0.43
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	9	0.43
(1,283)	1:39:A:ARG:HD3	1:39:A:ARG:HB3	10	0.43
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	2	0.43
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	4	0.43
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	4	0.43
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	4	0.43
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	4	0.43
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	4	0.43
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	4	0.43
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	6	0.43
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	6	0.43
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	6	0.43
(1,46)	1:73:A:TYR:HA	1:68:A:GLY:H	8	0.43
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	8	0.43
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	2	0.43
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	1	0.42
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	1	0.42
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	3	0.42
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	3	0.42
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	4	0.42
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	4	0.42
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA2	9	0.42
(5,25)	1:38:A:GLY:H	1:38:A:GLY:HA3	9	0.42
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	4	0.42
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	4	0.42
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	4	0.42
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	4	0.42
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	4	0.42
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	4	0.42
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	4	0.42
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	1	0.42
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	1	0.42
(3,18)	1:12:A:GLY:HA3	1:13:A:PRO:HD3	4	0.42
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	5	0.42
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	5	0.42
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	1	0.42
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	1	0.42
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	5	0.42
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	5	0.42
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	5	0.42
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD11	3	0.42
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD12	3	0.42
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD13	3	0.42
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	4	0.42
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	5	0.42
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	6	0.42
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	9	0.42
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	9	0.42
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	9	0.42
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	3	0.42
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	2	0.42
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	6	0.42
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	10	0.42
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	7	0.42
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	10	0.42
(2,331)	1:50:A:ILE:H	1:51:A:ASP:H	10	0.42
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	9	0.42
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	2	0.42
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	4	0.42
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	5	0.42
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	8	0.42
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	10	0.42
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	2	0.42
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	1	0.42
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	1	0.42
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	3	0.42
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	5	0.42
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	7	0.42
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	1	0.42
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	10	0.42
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	1	0.42
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	4	0.42
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	10	0.42
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	3	0.42
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	6	0.42
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	2	0.42
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	3	0.42
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	4	0.42
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	7	0.42
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	2	0.42
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	4	0.42
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	6	0.42
(2,26)	1:14:A:LEU:H	1:13:A:PRO:HB3	10	0.42
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	9	0.42
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD11	1	0.42
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD12	1	0.42
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD13	1	0.42
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	5	0.42
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	6	0.42
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	8	0.42
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	8	0.42
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	5	0.42
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	9	0.42
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	1	0.42
(1,436)	1:67:A:ARG:HA	1:67:A:ARG:HG2	3	0.42
(1,436)	1:67:A:ARG:HA	1:67:A:ARG:HG2	9	0.42
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	5	0.42
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	10	0.42
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	10	0.42
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	10	0.42
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	5	0.42
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	4	0.42
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	4	0.42
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	3	0.42
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	2	0.42
(1,371)	1:49:A:ASP:HA	1:49:A:ASP:HB3	10	0.42
(1,327)	1:13:A:PRO:HA	1:40:A:SER:HA	5	0.42
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	2	0.42
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	2	0.42
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	2	0.42
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	1	0.42
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	1	0.42
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	1	0.42
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	8	0.42
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	8	0.42
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	8	0.42
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	4	0.42
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	5	0.42
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	6	0.42
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	5	0.42
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	10	0.42
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	1	0.42
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	8	0.42
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	8	0.42
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	1	0.42
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	1	0.42
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	1	0.42
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	6	0.42
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	6	0.42
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	6	0.42
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB2	9	0.41
(5,4)	1:73:A:TYR:H	1:73:A:TYR:HB3	9	0.41
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	10	0.41
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	6	0.41
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	6	0.41
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	8	0.41
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	5	0.41
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	5	0.41
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	6	0.41
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	6	0.41
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	10	0.41
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	10	0.41
(3,18)	1:12:A:GLY:HA3	1:13:A:PRO:HD3	7	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	2	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	2	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	2	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	3	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	3	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	3	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	4	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	4	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	4	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	8	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	8	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	8	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	10	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	10	0.41
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	10	0.41
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	4	0.41
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	8	0.41
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	8	0.41
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	10	0.41
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	8	0.41
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	4	0.41
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	8	0.41
(2,300)	1:46:A:GLY:H	1:46:A:GLY:HA3	1	0.41
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	9	0.41
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD11	10	0.41
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD12	10	0.41
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD13	10	0.41
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	8	0.41
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	2	0.41
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	7	0.41
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	9	0.41
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	4	0.41
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	4	0.41
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	1	0.41
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	1	0.41
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	1	0.41
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	2	0.41
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	6	0.41
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	7	0.41
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	8	0.41
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	9	0.41
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	2	0.41
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	2	0.41
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	1	0.41
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	7	0.41
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	8	0.41
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	6	0.41
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	10	0.41
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	1	0.41
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	1	0.41
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	3	0.41
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	3	0.41
(2,43)	1:54:A:LEU:H	1:54:A:LEU:HG	9	0.41
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	3	0.41
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	4	0.41
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	1	0.41
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	5	0.41
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	5	0.41
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	5	0.41
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	5	0.41
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	5	0.41
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	5	0.41
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	5	0.41
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	5	0.41
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD21	10	0.41
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD22	10	0.41
(1,431)	1:14:A:LEU:HA	1:14:A:LEU:HD23	10	0.41
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	7	0.41
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	8	0.41
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	9	0.41
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	1	0.41
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	6	0.41
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	10	0.41
(1,333)	1:13:A:PRO:HB2	1:16:A:PRO:HD2	10	0.41
(1,324)	1:73:A:TYR:HA	1:67:A:ARG:HA	10	0.41
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	3	0.41
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	3	0.41
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	3	0.41
(1,283)	1:39:A:ARG:HD3	1:39:A:ARG:HB3	8	0.41
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	9	0.41
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	7	0.41
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	8	0.41
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	10	0.41
(1,259)	1:6:A:ASP:HB3	1:6:A:ASP:H	7	0.41
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	2	0.41
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	5	0.41
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	5	0.41
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	5	0.41
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	5	0.41
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	5	0.41
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	5	0.41
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	5	0.41
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	5	0.41
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	5	0.41
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	8	0.41
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	8	0.41
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	8	0.41
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	8	0.41
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	8	0.41
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	8	0.41
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	8	0.41
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	8	0.41
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	8	0.41
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	8	0.41
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	8	0.41
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	2	0.41
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	8	0.41
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	8	0.41
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	8	0.41
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	10	0.41
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	10	0.41
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	5	0.41
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD11	5	0.41
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD12	5	0.41
(1,37)	1:65:A:ALA:HA	1:75:A:LEU:HD13	5	0.41
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	8	0.4
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	8	0.4
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	6	0.4
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	5	0.4
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD11	1	0.4
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD12	1	0.4
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD13	1	0.4
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD21	1	0.4
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD22	1	0.4
(3,2)	1:29:A:LEU:HB3	1:29:A:LEU:HD23	1	0.4
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	7	0.4
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	7	0.4
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	7	0.4
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	1	0.4
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	8	0.4
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	10	0.4
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	1	0.4
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	1	0.4
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	1	0.4
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	5	0.4
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	5	0.4
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	5	0.4
(2,409)	1:21:A:PHE:H	1:18:A:LEU:HA	8	0.4
(2,404)	1:4:A:GLN:H	1:3:A:ALA:HA	3	0.4
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	2	0.4
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	2	0.4
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	3	0.4
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	8	0.4
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	4	0.4
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	5	0.4
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	3	0.4
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	5	0.4
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	8	0.4
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	10	0.4
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	2	0.4
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	7	0.4
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	8	0.4
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	10	0.4
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	1	0.4
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	2	0.4
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	3	0.4
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	6	0.4
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	7	0.4
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	8	0.4
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	10	0.4
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	5	0.4
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	3	0.4
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	6	0.4
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	5	0.4
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	10	0.4
(2,224)	1:19:A:ALA:H	1:18:A:LEU:HB2	5	0.4
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	8	0.4
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	7	0.4
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD21	4	0.4
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD22	4	0.4
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD23	4	0.4
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	2	0.4
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	8	0.4
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	5	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	2	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	2	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	2	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	5	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	5	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	5	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	7	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	7	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	9	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	9	0.4
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	9	0.4
(2,176)	1:68:A:GLY:H	1:67:A:ARG:HG3	5	0.4
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	3	0.4
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	4	0.4
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	4	0.4
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	6	0.4
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	6	0.4
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	7	0.4
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	7	0.4
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	8	0.4
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB1	5	0.4
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB2	5	0.4
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB3	5	0.4
(2,78)	1:27:A:ILE:H	1:26:A:HIS:H	9	0.4
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	5	0.4
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	8	0.4
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	3	0.4
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	7	0.4
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	3	0.4
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	4	0.4
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	4	0.4
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	5	0.4
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	5	0.4
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	7	0.4
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	7	0.4
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB2	10	0.4
(2,27)	1:14:A:LEU:H	1:14:A:LEU:HB3	10	0.4
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	1	0.4
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	10	0.4
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	1	0.4
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	6	0.4
(1,480)	1:50:A:ILE:HG13	1:50:A:ILE:HB	10	0.4
(1,436)	1:67:A:ARG:HA	1:67:A:ARG:HG2	1	0.4
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	7	0.4
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	9	0.4
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	8	0.4
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	8	0.4
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	8	0.4
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	9	0.4
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	9	0.4
(1,409)	1:78:A:SER:HB2	1:78:A:SER:HA	10	0.4
(1,409)	1:78:A:SER:HB3	1:78:A:SER:HA	10	0.4
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	4	0.4
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	3	0.4
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	4	0.4
(1,373)	1:32:A:PRO:HD3	1:32:A:PRO:HG3	5	0.4
(1,371)	1:49:A:ASP:HA	1:49:A:ASP:HB3	4	0.4
(1,330)	1:13:A:PRO:HA	1:40:A:SER:HB2	8	0.4
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	7	0.4
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	7	0.4
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	7	0.4
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	3	0.4
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	3	0.4
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	3	0.4
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	5	0.4
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	5	0.4
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	5	0.4
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	10	0.4
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	10	0.4
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	10	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	3	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	3	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	5	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	5	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	7	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	7	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	10	0.4
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	10	0.4
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	2	0.4
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	7	0.4
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	8	0.4
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	10	0.4
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	8	0.4
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	3	0.4
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	3	0.4
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	3	0.4
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD21	10	0.4
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD22	10	0.4
(1,144)	1:14:A:LEU:HD11	1:14:A:LEU:HD23	10	0.4
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD21	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD22	10	0.4
(1,144)	1:14:A:LEU:HD12	1:14:A:LEU:HD23	10	0.4
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD21	10	0.4
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD22	10	0.4
(1,144)	1:14:A:LEU:HD13	1:14:A:LEU:HD23	10	0.4
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	3	0.4
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	3	0.4
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	3	0.4
(1,97)	1:35:A:LEU:HB2	1:35:A:LEU:H	3	0.4
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	5	0.4
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	10	0.4
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	3	0.4
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	6	0.4
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	8	0.39
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	4	0.39
(3,35)	1:66:A:SER:HB2	1:66:A:SER:HA	2	0.39
(3,35)	1:66:A:SER:HB3	1:66:A:SER:HA	2	0.39
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	4	0.39
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	4	0.39
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB1	6	0.39
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB2	6	0.39
(2,475)	1:69:A:ALA:H	1:69:A:ALA:HB3	6	0.39
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	9	0.39
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	1	0.39
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	3	0.39
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	4	0.39
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	7	0.39
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	9	0.39
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	6	0.39
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	8	0.39
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	1	0.39
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	9	0.39
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	3	0.39
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	2	0.39
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	2	0.39
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	5	0.39
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	5	0.39
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	10	0.39
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	10	0.39
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	6	0.39
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	1	0.39
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	4	0.39
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	9	0.39
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	10	0.39
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	10	0.39
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	10	0.39
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	10	0.39
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB1	6	0.39
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB2	6	0.39
(2,288)	1:3:A:ALA:H	1:3:A:ALA:HB3	6	0.39
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	1	0.39
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	6	0.39
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	3	0.39
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	4	0.39
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	6	0.39
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	4	0.39
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	5	0.39
(2,256)	1:20:A:HIS:H	1:20:A:HIS:HA	9	0.39
(2,195)	1:63:A:LEU:H	1:62:A:GLY:HA3	7	0.39
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD11	7	0.39
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD12	7	0.39
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD13	7	0.39
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	3	0.39
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	4	0.39
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	4	0.39
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	4	0.39
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB1	6	0.39
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB2	6	0.39
(2,177)	1:11:A:ALA:H	1:11:A:ALA:HB3	6	0.39
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	9	0.39
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	1	0.39
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD1	1	0.39
(2,131)	1:22:A:GLY:H	1:21:A:PHE:HD2	1	0.39
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	5	0.39
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	4	0.39
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	2	0.39
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	4	0.39
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	10	0.39
(2,53)	1:38:A:GLY:H	1:37:A:GLU:HG3	10	0.39
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	2	0.39
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	2	0.39
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	7	0.39
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	2	0.39
(1,377)	1:40:A:SER:HA	1:14:A:LEU:H	1	0.39
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	6	0.39
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	6	0.39
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	6	0.39
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	1	0.39
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	1	0.39
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	1	0.39
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	2	0.39
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	2	0.39
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	2	0.39
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	6	0.39
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	6	0.39
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	6	0.39
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	1	0.39
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	1	0.39
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	4	0.39
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	4	0.39
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	3	0.39
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	4	0.39
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	6	0.39
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	1	0.39
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	9	0.39
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG21	6	0.39
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG22	6	0.39
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG23	6	0.39
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	10	0.39
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	4	0.39
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	5	0.39
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	5	0.39
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	5	0.39
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	9	0.39
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	4	0.39
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	9	0.39
(1,38)	1:26:A:HIS:HB2	1:26:A:HIS:HA	2	0.39
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	4	0.39
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	4	0.39
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	4	0.39
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	2	0.38
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	2	0.38
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	2	0.38
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	2	0.38
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	2	0.38
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	5	0.38
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	1	0.38
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	10	0.38
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	10	0.38
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	7	0.38
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	7	0.38
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	3	0.38
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	6	0.38
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	2	0.38
(2,447)	1:79:A:ALA:H	1:78:A:SER:HA	5	0.38
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	3	0.38
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	7	0.38
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	10	0.38
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	9	0.38
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	9	0.38
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	10	0.38
(2,335)	1:19:A:ALA:H	1:20:A:HIS:H	10	0.38
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	1	0.38
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	6	0.38
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	1	0.38
(2,262)	1:22:A:GLY:H	1:22:A:GLY:HA3	5	0.38
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	9	0.38
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	9	0.38
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	9	0.38
(2,243)	1:29:A:LEU:H	1:29:A:LEU:HB2	9	0.38
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	10	0.38
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	2	0.38
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	10	0.38
(2,206)	1:21:A:PHE:H	1:20:A:HIS:HA	4	0.38
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	5	0.38
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	9	0.38
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	1	0.38
(2,171)	1:48:A:PHE:H	1:47:A:ARG:HA	5	0.38
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	2	0.38
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	2	0.38
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	2	0.38
(2,152)	1:12:A:GLY:H	1:40:A:SER:HB2	2	0.38
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	2	0.38
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	9	0.38
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	4	0.38
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	7	0.38
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	1	0.38
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	9	0.38
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	9	0.38
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA2	10	0.38
(2,44)	1:54:A:LEU:H	1:53:A:GLY:HA3	10	0.38
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	6	0.38
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	1	0.38
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	1	0.38
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	10	0.38
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	10	0.38
(1,420)	1:37:A:GLU:HB2	1:37:A:GLU:HG3	9	0.38
(1,410)	1:55:A:ALA:HB1	1:52:A:GLN:HA	5	0.38
(1,410)	1:55:A:ALA:HB2	1:52:A:GLN:HA	5	0.38
(1,410)	1:55:A:ALA:HB3	1:52:A:GLN:HA	5	0.38
(1,410)	1:55:A:ALA:HB1	1:52:A:GLN:HA	9	0.38
(1,410)	1:55:A:ALA:HB2	1:52:A:GLN:HA	9	0.38
(1,410)	1:55:A:ALA:HB3	1:52:A:GLN:HA	9	0.38
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	1	0.38
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	5	0.38
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	7	0.38
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	10	0.38
(1,316)	1:50:A:ILE:HD11	1:50:A:ILE:HA	9	0.38
(1,316)	1:50:A:ILE:HD12	1:50:A:ILE:HA	9	0.38
(1,316)	1:50:A:ILE:HD13	1:50:A:ILE:HA	9	0.38
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	5	0.38
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	5	0.38
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	5	0.38
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	1	0.38
(1,273)	1:22:A:GLY:HA3	1:22:A:GLY:H	5	0.38
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	9	0.38
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	10	0.38
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	4	0.38
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	4	0.38
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	4	0.38
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	10	0.38
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	10	0.38
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	10	0.38
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	4	0.38
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	4	0.38
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	3	0.38
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	6	0.38
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	2	0.38
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	7	0.38
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	8	0.38
(1,38)	1:26:A:HIS:HB2	1:26:A:HIS:HA	4	0.38
(1,26)	1:29:A:LEU:HB2	1:29:A:LEU:H	9	0.38
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	1	0.37
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	10	0.37
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	9	0.37
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	8	0.37
(3,18)	1:12:A:GLY:HA3	1:13:A:PRO:HD3	8	0.37
(3,18)	1:12:A:GLY:HA3	1:13:A:PRO:HD3	9	0.37
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	10	0.37
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	10	0.37
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	8	0.37
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	2	0.37
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	5	0.37
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	9	0.37
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	5	0.37
(2,355)	1:20:A:HIS:H	1:20:A:HIS:HB3	3	0.37
(2,355)	1:20:A:HIS:H	1:20:A:HIS:HB3	6	0.37
(2,350)	1:41:A:THR:H	1:40:A:SER:HB2	6	0.37
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	5	0.37
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	8	0.37
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	5	0.37
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	7	0.37
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	6	0.37
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	7	0.37
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	7	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	1	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	2	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	3	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	4	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	5	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	6	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	7	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	8	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	9	0.37
(2,254)	1:52:A:GLN:HE22	1:52:A:GLN:HE21	10	0.37
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	7	0.37
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	2	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	1	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	2	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	3	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	4	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	5	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	6	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	7	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	8	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	9	0.37
(2,141)	1:76:A:GLN:HE22	1:76:A:GLN:HE21	10	0.37
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	3	0.37
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	9	0.37
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	3	0.37
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	5	0.37
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	6	0.37
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	9	0.37
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	5	0.37
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	9	0.37
(2,68)	1:19:A:ALA:H	1:17:A:ALA:H	8	0.37
(2,51)	1:80:A:SER:H	1:80:A:SER:HB3	9	0.37
(2,43)	1:54:A:LEU:H	1:54:A:LEU:HG	10	0.37
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	9	0.37
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	8	0.37
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	8	0.37
(1,473)	1:7:A:PHE:HB2	1:44:A:LEU:HG	1	0.37
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	6	0.37
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	6	0.37
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	6	0.37
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	7	0.37
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	7	0.37
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	7	0.37
(1,420)	1:37:A:GLU:HB2	1:37:A:GLU:HG3	1	0.37
(1,410)	1:55:A:ALA:HB1	1:52:A:GLN:HA	1	0.37
(1,410)	1:55:A:ALA:HB2	1:52:A:GLN:HA	1	0.37
(1,410)	1:55:A:ALA:HB3	1:52:A:GLN:HA	1	0.37
(1,404)	1:11:A:ALA:HB1	1:42:A:SER:HA	1	0.37
(1,404)	1:11:A:ALA:HB2	1:42:A:SER:HA	1	0.37
(1,404)	1:11:A:ALA:HB3	1:42:A:SER:HA	1	0.37
(1,384)	1:48:A:PHE:HB3	1:48:A:PHE:HA	6	0.37
(1,354)	1:75:A:LEU:HD11	1:75:A:LEU:HB3	1	0.37
(1,354)	1:75:A:LEU:HD12	1:75:A:LEU:HB3	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:75:A:LEU:HD13	1:75:A:LEU:HB3	1	0.37
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	3	0.37
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	1	0.37
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	5	0.37
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	5	0.37
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	5	0.37
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB1	8	0.37
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB2	8	0.37
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB3	8	0.37
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	2	0.37
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	2	0.37
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	8	0.37
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	8	0.37
(1,283)	1:39:A:ARG:HD3	1:39:A:ARG:HB3	6	0.37
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	2	0.37
(1,228)	1:39:A:ARG:HD3	1:38:A:GLY:HA3	8	0.37
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	2	0.37
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	9	0.37
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	8	0.37
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	10	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	1	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	1	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	1	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	2	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	2	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	2	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	3	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	3	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	3	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	4	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	4	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	4	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	5	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	5	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	5	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	6	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	6	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	6	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	7	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	7	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	7	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	8	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	8	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	9	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	9	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	9	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB1	10	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB2	10	0.37
(1,124)	1:69:A:ALA:HA	1:69:A:ALA:HB3	10	0.37
(1,122)	1:26:A:HIS:HB3	1:26:A:HIS:HA	6	0.37
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	2	0.37
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	3	0.37
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	1	0.37
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	4	0.37
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	10	0.37
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	3	0.37
(1,38)	1:26:A:HIS:HB2	1:26:A:HIS:HA	7	0.37
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	7	0.37
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	6	0.36
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	5	0.36
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	5	0.36
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	4	0.36
(2,469)	1:55:A:ALA:H	1:55:A:ALA:HA	2	0.36
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD11	6	0.36
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD12	6	0.36
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD13	6	0.36
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB2	6	0.36
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB3	6	0.36
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	1	0.36
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	5	0.36
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	5	0.36
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	5	0.36
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	8	0.36
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	8	0.36
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	8	0.36
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	4	0.36
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	4	0.36
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	8	0.36
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	5	0.36
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	5	0.36
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	1	0.36
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	6	0.36
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	8	0.36
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	7	0.36
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	7	0.36
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	1	0.36
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	8	0.36
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	8	0.36
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	8	0.36
(2,238)	1:63:A:LEU:H	1:62:A:GLY:HA2	9	0.36
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	4	0.36
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	2	0.36
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	10	0.36
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	1	0.36
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	2	0.36
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	8	0.36
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	9	0.36
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	5	0.36
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	5	0.36
(2,88)	1:51:A:ASP:H	1:51:A:ASP:HB2	4	0.36
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB1	9	0.36
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB2	9	0.36
(2,86)	1:60:A:GLY:H	1:59:A:ALA:HB3	9	0.36
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	1	0.36
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	1	0.36
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	1	0.36
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	2	0.36
(2,51)	1:80:A:SER:H	1:80:A:SER:HB3	3	0.36
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	3	0.36
(1,420)	1:37:A:GLU:HB2	1:37:A:GLU:HG3	8	0.36
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	1	0.36
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	2	0.36
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	3	0.36
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	4	0.36
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	5	0.36
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	9	0.36
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	10	0.36
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	6	0.36
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD11	5	0.36
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD12	5	0.36
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD13	5	0.36
(1,393)	1:72:A:SER:HA	1:28:A:LEU:HB2	2	0.36
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	1	0.36
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	1	0.36
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	1	0.36
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	1	0.36
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	1	0.36
(1,329)	1:72:A:SER:HB3	1:72:A:SER:HA	3	0.36
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	7	0.36
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD1	5	0.36
(1,288)	1:21:A:PHE:HB3	1:21:A:PHE:HD2	5	0.36
(1,276)	1:4:A:GLN:HA	1:49:A:ASP:HA	7	0.36
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	10	0.36
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	10	0.36
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	10	0.36
(1,228)	1:39:A:ARG:HD3	1:38:A:GLY:HA3	6	0.36
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	1	0.36
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	3	0.36
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	2	0.36
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	3	0.36
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	1	0.36
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	2	0.36
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	4	0.36
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	7	0.36
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	8	0.36
(1,122)	1:26:A:HIS:HB3	1:26:A:HIS:HA	10	0.36
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	9	0.36
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	9	0.36
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	9	0.36
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	6	0.36
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	6	0.36
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	2	0.36
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	2	0.36
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	2	0.36
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	8	0.36
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	8	0.36
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	8	0.36
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	9	0.36
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	9	0.36
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	9	0.36
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	3	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	3	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	3	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	3	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	3	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	10	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	10	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	10	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	10	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	10	0.35
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	10	0.35
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	2	0.35
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	2	0.35
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	10	0.35
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	6	0.35
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	4	0.35
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	7	0.35
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	7	0.35
(2,430)	1:5:A:ALA:H	1:5:A:ALA:HA	4	0.35
(2,428)	1:7:A:PHE:H	1:6:A:ASP:HA	3	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	7	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	7	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	7	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	8	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	8	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	8	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	10	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	10	0.35
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	10	0.35
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	7	0.35
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	7	0.35
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	7	0.35
(2,406)	1:7:A:PHE:H	1:47:A:ARG:HA	8	0.35
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	9	0.35
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	9	0.35
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	2	0.35
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	9	0.35
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	2	0.35
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	3	0.35
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	9	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	2	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	2	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	4	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	4	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	6	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	7	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	7	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	10	0.35
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	10	0.35
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	3	0.35
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	4	0.35
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	6	0.35
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	2	0.35
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	3	0.35
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	3	0.35
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	3	0.35
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	3	0.35
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB2	3	0.35
(2,255)	1:70:A:ASN:HD21	1:70:A:ASN:HB3	3	0.35
(2,250)	1:55:A:ALA:H	1:54:A:LEU:HG	8	0.35
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	4	0.35
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	8	0.35
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	5	0.35
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD21	6	0.35
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD22	6	0.35
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD23	6	0.35
(2,183)	1:41:A:THR:H	1:41:A:THR:HG1	10	0.35
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	1	0.35
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	2	0.35
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	6	0.35
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	4	0.35
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	10	0.35
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	2	0.35
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	9	0.35
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	3	0.35
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	3	0.35
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD11	10	0.35
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD12	10	0.35
(1,446)	1:14:A:LEU:HD11	1:18:A:LEU:HD13	10	0.35
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD11	10	0.35
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD12	10	0.35
(1,446)	1:14:A:LEU:HD12	1:18:A:LEU:HD13	10	0.35
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD11	10	0.35
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD12	10	0.35
(1,446)	1:14:A:LEU:HD13	1:18:A:LEU:HD13	10	0.35
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	5	0.35
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	5	0.35
(1,420)	1:37:A:GLU:HB2	1:37:A:GLU:HG3	7	0.35
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	5	0.35
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	8	0.35
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	6	0.35
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	8	0.35
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	10	0.35
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	3	0.35
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	6	0.35
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	7	0.35
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	7	0.35
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	7	0.35
(1,286)	1:47:A:ARG:HD2	1:47:A:ARG:HE	1	0.35
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	7	0.35
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	7	0.35
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	7	0.35
(1,272)	1:6:A:ASP:HA	1:7:A:PHE:H	3	0.35
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	7	0.35
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	2	0.35
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	4	0.35
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	6	0.35
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	5	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	1	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	3	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	4	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	5	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	6	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	7	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	8	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	9	0.35
(1,160)	1:62:A:GLY:HA3	1:62:A:GLY:HA2	10	0.35
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	6	0.35
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	6	0.35
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	6	0.35
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	7	0.35
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	6	0.35
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	8	0.35
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	3	0.35
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	3	0.35
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	3	0.35
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	5	0.35
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	5	0.35
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	2	0.35
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	10	0.35
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	3	0.35
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	3	0.35
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	3	0.35
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	10	0.35
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	10	0.35
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	10	0.35
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	7	0.34
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	7	0.34
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	7	0.34
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	2	0.34
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	9	0.34
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	8	0.34
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	2	0.34
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	7	0.34
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	1	0.34
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	1	0.34
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	2	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	2	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	2	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	2	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	3	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	3	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	3	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	4	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	4	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	4	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	6	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	6	0.34
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	6	0.34
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	10	0.34
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	9	0.34
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	1	0.34
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	1	0.34
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	1	0.34
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	6	0.34
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	7	0.34
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	6	0.34
(2,326)	1:17:A:ALA:H	1:16:A:PRO:HA	7	0.34
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	3	0.34
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	8	0.34
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	8	0.34
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	10	0.34
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	10	0.34
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	5	0.34
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	2	0.34
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	4	0.34
(2,251)	1:12:A:GLY:H	1:43:A:GLY:HA2	10	0.34
(2,227)	1:19:A:ALA:H	1:16:A:PRO:HB2	5	0.34
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	2	0.34
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	4	0.34
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	9	0.34
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	3	0.34
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	6	0.34
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	9	0.34
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	3	0.34
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	2	0.34
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD21	2	0.34
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD22	2	0.34
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD23	2	0.34
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	2	0.34
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	4	0.34
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	6	0.34
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	1	0.34
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	1	0.34
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	3	0.34
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	7	0.34
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	8	0.34
(2,113)	1:41:A:THR:H	1:40:A:SER:HB3	3	0.34
(2,112)	1:42:A:SER:H	1:41:A:THR:HA	7	0.34
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	1	0.34
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	3	0.34
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	10	0.34
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	9	0.34
(2,47)	1:61:A:THR:H	1:60:A:GLY:HA2	5	0.34
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	7	0.34
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	2	0.34
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	5	0.34
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	10	0.34
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	8	0.34
(2,11)	1:35:A:LEU:H	1:34:A:ALA:H	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	2	0.34
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	2	0.34
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	4	0.34
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	4	0.34
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	5	0.34
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	5	0.34
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	6	0.34
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	6	0.34
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	7	0.34
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	7	0.34
(1,488)	1:10:A:PRO:HG2	1:10:A:PRO:HD3	9	0.34
(1,488)	1:10:A:PRO:HG3	1:10:A:PRO:HD3	9	0.34
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	1	0.34
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	8	0.34
(1,436)	1:67:A:ARG:HA	1:67:A:ARG:HG2	4	0.34
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	4	0.34
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	8	0.34
(1,413)	1:63:A:LEU:HA	1:77:A:ALA:HA	7	0.34
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD11	8	0.34
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD12	8	0.34
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD13	8	0.34
(1,393)	1:72:A:SER:HA	1:28:A:LEU:HB2	3	0.34
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	1	0.34
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	5	0.34
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	10	0.34
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	4	0.34
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	5	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	1	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	2	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	4	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	5	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	6	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	7	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	8	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	9	0.34
(1,326)	1:68:A:GLY:HA3	1:68:A:GLY:HA2	10	0.34
(1,292)	1:34:A:ALA:HB1	1:34:A:ALA:H	4	0.34
(1,292)	1:34:A:ALA:HB2	1:34:A:ALA:H	4	0.34
(1,292)	1:34:A:ALA:HB3	1:34:A:ALA:H	4	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	1	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	2	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	4	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	5	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	6	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	7	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	8	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	9	0.34
(1,291)	1:26:A:HIS:HB2	1:26:A:HIS:HB3	10	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	1	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	2	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	3	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	4	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	5	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	6	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	7	0.34
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	9	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	1	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	2	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	3	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	4	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	5	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	6	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	7	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	8	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	9	0.34
(1,255)	1:8:A:ASP:HB3	1:8:A:ASP:HB2	10	0.34
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	8	0.34
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	10	0.34
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	9	0.34
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	9	0.34
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	10	0.34
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	2	0.34
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	3	0.34
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	6	0.34
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	9	0.34
(1,122)	1:26:A:HIS:HB3	1:26:A:HIS:HA	5	0.34
(1,122)	1:26:A:HIS:HB3	1:26:A:HIS:HA	8	0.34
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	1	0.34
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	2	0.34
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	4	0.34
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	5	0.34
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	6	0.34
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	6	0.34
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	10	0.34
(1,62)	1:60:A:GLY:HA3	1:60:A:GLY:H	7	0.34
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	2	0.34
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	2	0.34
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	2	0.34
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	7	0.34
(1,27)	1:67:A:ARG:HA	1:67:A:ARG:HG3	1	0.34
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	3	0.33
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	3	0.33
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	3	0.33
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	10	0.33
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HD2	5	0.33
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	9	0.33
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB1	9	0.33
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB2	9	0.33
(2,424)	1:19:A:ALA:H	1:19:A:ALA:HB3	9	0.33
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	8	0.33
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	9	0.33
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	9	0.33
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	9	0.33
(2,355)	1:20:A:HIS:H	1:20:A:HIS:HB3	1	0.33
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	2	0.33
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB2	9	0.33
(2,322)	1:44:A:LEU:H	1:44:A:LEU:HB3	9	0.33
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	4	0.33
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	9	0.33
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	1	0.33
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	1	0.33
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	1	0.33
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	4	0.33
(2,274)	1:67:A:ARG:H	1:67:A:ARG:HG3	5	0.33
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	4	0.33
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	9	0.33
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	6	0.33
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	6	0.33
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	6	0.33
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	9	0.33
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	6	0.33
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	3	0.33
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	5	0.33
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	7	0.33
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	1	0.33
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	10	0.33
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	10	0.33
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	9	0.33
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	1	0.33
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	3	0.33
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	4	0.33
(2,162)	1:4:A:GLN:H	1:4:A:GLN:HB2	10	0.33
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	4	0.33
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	10	0.33
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	2	0.33
(2,47)	1:61:A:THR:H	1:60:A:GLY:HA2	1	0.33
(2,34)	1:50:A:ILE:H	1:4:A:GLN:HA	6	0.33
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	6	0.33
(2,7)	1:30:A:SER:H	1:29:A:LEU:HB3	4	0.33
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	9	0.33
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	1	0.33
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	1	0.33
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	9	0.33
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	9	0.33
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	9	0.33
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	4	0.33
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	9	0.33
(1,425)	1:71:A:ALA:HB1	1:71:A:ALA:H	3	0.33
(1,425)	1:71:A:ALA:HB2	1:71:A:ALA:H	3	0.33
(1,425)	1:71:A:ALA:HB3	1:71:A:ALA:H	3	0.33
(1,420)	1:37:A:GLU:HB2	1:37:A:GLU:HG3	4	0.33
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	6	0.33
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	7	0.33
(1,415)	1:60:A:GLY:HA2	1:60:A:GLY:HA3	8	0.33
(1,410)	1:55:A:ALA:HB1	1:52:A:GLN:HA	2	0.33
(1,410)	1:55:A:ALA:HB2	1:52:A:GLN:HA	2	0.33
(1,410)	1:55:A:ALA:HB3	1:52:A:GLN:HA	2	0.33
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	9	0.33
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	2	0.33
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	2	0.33
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	2	0.33
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	6	0.33
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	1	0.33
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	2	0.33
(1,303)	1:78:A:SER:HA	1:78:A:SER:HB2	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD1	6	0.33
(1,284)	1:7:A:PHE:HB2	1:7:A:PHE:HD2	6	0.33
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	8	0.33
(1,270)	1:16:A:PRO:HB2	1:16:A:PRO:HB3	10	0.33
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG21	5	0.33
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG22	5	0.33
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG23	5	0.33
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	2	0.33
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	9	0.33
(1,241)	1:39:A:ARG:HD3	1:35:A:LEU:HG	1	0.33
(1,241)	1:39:A:ARG:HD3	1:35:A:LEU:HG	9	0.33
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	6	0.33
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	4	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	4	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	4	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	4	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	6	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	6	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	6	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	7	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	7	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	7	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	9	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	9	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	9	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	10	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	10	0.33
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	10	0.33
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	2	0.33
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	6	0.33
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	6	0.33
(1,122)	1:26:A:HIS:HB3	1:26:A:HIS:HA	3	0.33
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	3	0.33
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	8	0.33
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	9	0.33
(1,118)	1:10:A:PRO:HB3	1:10:A:PRO:HB2	10	0.33
(1,96)	1:37:A:GLU:HB3	1:37:A:GLU:H	2	0.33
(1,83)	1:37:A:GLU:HB3	1:37:A:GLU:HA	5	0.33
(1,33)	1:18:A:LEU:HB2	1:18:A:LEU:HD11	8	0.33
(1,33)	1:18:A:LEU:HB2	1:18:A:LEU:HD12	8	0.33
(1,33)	1:18:A:LEU:HB2	1:18:A:LEU:HD13	8	0.33
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	5	0.33
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	5	0.33
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	9	0.32
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	9	0.32
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	6	0.32
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	1	0.32
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	3	0.32
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	8	0.32
(2,473)	1:78:A:SER:H	1:63:A:LEU:HA	3	0.32
(2,438)	1:5:A:ALA:H	1:4:A:GLN:HB2	9	0.32
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB2	5	0.32
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB3	5	0.32
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	8	0.32
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	8	0.32
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	9	0.32
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	6	0.32
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	3	0.32
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	3	0.32
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	8	0.32
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	9	0.32
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	10	0.32
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	3	0.32
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	3	0.32
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	3	0.32
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD11	6	0.32
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD12	6	0.32
(2,258)	1:21:A:PHE:H	1:9:A:ILE:HD13	6	0.32
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	6	0.32
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	7	0.32
(2,244)	1:61:A:THR:H	1:63:A:LEU:H	8	0.32
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	7	0.32
(2,220)	1:22:A:GLY:H	1:23:A:GLN:H	1	0.32
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	2	0.32
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	4	0.32
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	8	0.32
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	5	0.32
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	9	0.32
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	8	0.32
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	9	0.32
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	5	0.32
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	5	0.32
(2,144)	1:56:A:ILE:H	1:56:A:ILE:HB	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	10	0.32
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	1	0.32
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	1	0.32
(2,53)	1:38:A:GLY:H	1:37:A:GLU:HG3	6	0.32
(2,51)	1:80:A:SER:H	1:80:A:SER:HB3	1	0.32
(2,51)	1:80:A:SER:H	1:80:A:SER:HB3	4	0.32
(2,47)	1:61:A:THR:H	1:60:A:GLY:HA2	4	0.32
(2,47)	1:61:A:THR:H	1:60:A:GLY:HA2	9	0.32
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD11	10	0.32
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD12	10	0.32
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD13	10	0.32
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	10	0.32
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	9	0.32
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	9	0.32
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	6	0.32
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	4	0.32
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	4	0.32
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	4	0.32
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	9	0.32
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	9	0.32
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	9	0.32
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	7	0.32
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	2	0.32
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	4	0.32
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	7	0.32
(1,325)	1:41:A:THR:HA	1:41:A:THR:HG1	10	0.32
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	8	0.32
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	10	0.32
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	2	0.32
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB1	5	0.32
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB2	5	0.32
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB3	5	0.32
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	10	0.32
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	4	0.32
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	10	0.32
(1,228)	1:39:A:ARG:HD3	1:38:A:GLY:HA3	10	0.32
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	8	0.32
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	7	0.32
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	2	0.32
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	5	0.32
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	6	0.32
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	8	0.32
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	10	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	2	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	2	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	2	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	3	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	3	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	3	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	5	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	5	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	5	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	8	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	8	0.32
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	8	0.32
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	1	0.32
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	6	0.32
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	3	0.32
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	3	0.32
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	3	0.32
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	5	0.32
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	5	0.32
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	5	0.32
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	6	0.32
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	6	0.32
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	6	0.32
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	7	0.32
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	7	0.32
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	8	0.32
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	8	0.32
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	10	0.32
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	10	0.32
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	5	0.32
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	1	0.32
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	1	0.32
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	1	0.32
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	4	0.32
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	4	0.32
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	4	0.32
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	5	0.32
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	5	0.32
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	5	0.32
(1,95)	1:63:A:LEU:HA	1:78:A:SER:H	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	1	0.32
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	10	0.32
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	10	0.32
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	10	0.32
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	5	0.32
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	5	0.32
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	5	0.32
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	6	0.32
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	9	0.32
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	6	0.31
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	6	0.31
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	6	0.31
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	6	0.31
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	6	0.31
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	6	0.31
(4,48)	1:76:A:GLN:N	1:64:A:GLU:O	9	0.31
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	3	0.31
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	6	0.31
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	5	0.31
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	6	0.31
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	7	0.31
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	5	0.31
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	10	0.31
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	2	0.31
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	7	0.31
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	7	0.31
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	9	0.31
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	10	0.31
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	10	0.31
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	2	0.31
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	6	0.31
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	2	0.31
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG2	3	0.31
(2,399)	1:35:A:LEU:H	1:32:A:PRO:HG3	3	0.31
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	1	0.31
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	1	0.31
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	1	0.31
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	4	0.31
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	9	0.31
(2,365)	1:34:A:ALA:H	1:33:A:THR:HB	4	0.31
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	4	0.31
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	4	0.31
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	6	0.31
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	8	0.31
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	5	0.31
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	4	0.31
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	6	0.31
(2,215)	1:47:A:ARG:H	1:46:A:GLY:HA3	7	0.31
(2,189)	1:68:A:GLY:H	1:73:A:TYR:HA	6	0.31
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	7	0.31
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	7	0.31
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	7	0.31
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	10	0.31
(2,94)	1:6:A:ASP:H	1:6:A:ASP:HB3	7	0.31
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	5	0.31
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	5	0.31
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	5	0.31
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	10	0.31
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	10	0.31
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	10	0.31
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	10	0.31
(2,51)	1:80:A:SER:H	1:80:A:SER:HB3	10	0.31
(2,17)	1:78:A:SER:H	1:77:A:ALA:HA	2	0.31
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	1	0.31
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	1	0.31
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	10	0.31
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	2	0.31
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	3	0.31
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	3	0.31
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	3	0.31
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	5	0.31
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	5	0.31
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	5	0.31
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	10	0.31
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	10	0.31
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	10	0.31
(1,348)	1:39:A:ARG:HB3	1:39:A:ARG:HA	5	0.31
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	6	0.31
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	10	0.31
(1,337)	1:27:A:ILE:HD11	1:18:A:LEU:HD11	8	0.31
(1,337)	1:27:A:ILE:HD11	1:18:A:LEU:HD12	8	0.31
(1,337)	1:27:A:ILE:HD11	1:18:A:LEU:HD13	8	0.31
(1,337)	1:27:A:ILE:HD12	1:18:A:LEU:HD11	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:27:A:ILE:HD12	1:18:A:LEU:HD12	8	0.31
(1,337)	1:27:A:ILE:HD12	1:18:A:LEU:HD13	8	0.31
(1,337)	1:27:A:ILE:HD13	1:18:A:LEU:HD11	8	0.31
(1,337)	1:27:A:ILE:HD13	1:18:A:LEU:HD12	8	0.31
(1,337)	1:27:A:ILE:HD13	1:18:A:LEU:HD13	8	0.31
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	9	0.31
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	9	0.31
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	9	0.31
(1,328)	1:2:A:SER:HA	1:2:A:SER:HB3	9	0.31
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	1	0.31
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	4	0.31
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	10	0.31
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	8	0.31
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	1	0.31
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	4	0.31
(1,254)	1:9:A:ILE:HA	1:10:A:PRO:HD3	1	0.31
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	4	0.31
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	10	0.31
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	2	0.31
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	6	0.31
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	7	0.31
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	8	0.31
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	9	0.31
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	5	0.31
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	1	0.31
(1,204)	1:71:A:ALA:HA	1:71:A:ALA:H	3	0.31
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	5	0.31
(1,200)	1:14:A:LEU:HD11	1:36:A:THR:HB	10	0.31
(1,200)	1:14:A:LEU:HD12	1:36:A:THR:HB	10	0.31
(1,200)	1:14:A:LEU:HD13	1:36:A:THR:HB	10	0.31
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD21	1	0.31
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD22	1	0.31
(1,195)	1:44:A:LEU:HG	1:44:A:LEU:HD23	1	0.31
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	2	0.31
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	4	0.31
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	7	0.31
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	10	0.31
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	3	0.31
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	4	0.31
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	9	0.31
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	9	0.31
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:54:A:LEU:HB3	1:51:A:ASP:HA	9	0.31
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	6	0.31
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	1	0.31
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	1	0.31
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	8	0.31
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	8	0.31
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	8	0.31
(1,149)	1:50:A:ILE:HA	1:50:A:ILE:H	1	0.31
(1,122)	1:26:A:HIS:HB3	1:26:A:HIS:HA	1	0.31
(1,122)	1:26:A:HIS:HB3	1:26:A:HIS:HA	9	0.31
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	9	0.31
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	1	0.31
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	1	0.31
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	1	0.31
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	4	0.31
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	4	0.31
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	4	0.31
(1,42)	1:63:A:LEU:HA	1:63:A:LEU:HB3	6	0.31
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	2	0.31
(1,19)	1:15:A:ALA:HB1	1:15:A:ALA:H	7	0.31
(1,19)	1:15:A:ALA:HB2	1:15:A:ALA:H	7	0.31
(1,19)	1:15:A:ALA:HB3	1:15:A:ALA:H	7	0.31
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	9	0.31
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	9	0.31
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	9	0.31
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB2	6	0.3
(5,16)	1:21:A:PHE:H	1:20:A:HIS:HB3	6	0.3
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	3	0.3
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	6	0.3
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	5	0.3
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	9	0.3
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	1	0.3
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	9	0.3
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	4	0.3
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	10	0.3
(3,36)	1:73:A:TYR:HB2	1:29:A:LEU:HA	5	0.3
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	2	0.3
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	2	0.3
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	6	0.3
(2,422)	1:76:A:GLN:H	1:75:A:LEU:HA	7	0.3
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	6	0.3
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	4	0.3
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	8	0.3
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	5	0.3
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	8	0.3
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	2	0.3
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	6	0.3
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	3	0.3
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	3	0.3
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	3	0.3
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	6	0.3
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	6	0.3
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	6	0.3
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB1	1	0.3
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB2	1	0.3
(2,330)	1:74:A:SER:H	1:65:A:ALA:HB3	1	0.3
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	4	0.3
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	4	0.3
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	4	0.3
(2,323)	1:68:A:GLY:H	1:67:A:ARG:HB2	4	0.3
(2,321)	1:60:A:GLY:H	1:59:A:ALA:HA	2	0.3
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	1	0.3
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	9	0.3
(2,235)	1:26:A:HIS:H	1:22:A:GLY:HA2	9	0.3
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	8	0.3
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	7	0.3
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	9	0.3
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	2	0.3
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	8	0.3
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	10	0.3
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	8	0.3
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	2	0.3
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	6	0.3
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	8	0.3
(2,106)	1:42:A:SER:H	1:43:A:GLY:H	1	0.3
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	2	0.3
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	2	0.3
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	2	0.3
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	7	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	2	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	2	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	2	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	8	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	8	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	9	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	9	0.3
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	9	0.3
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	2	0.3
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	2	0.3
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	4	0.3
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	4	0.3
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	6	0.3
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	6	0.3
(2,14)	1:35:A:LEU:H	1:35:A:LEU:HB2	3	0.3
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	9	0.3
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	3	0.3
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	4	0.3
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	5	0.3
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	6	0.3
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	3	0.3
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	3	0.3
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	3	0.3
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	5	0.3
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	5	0.3
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	5	0.3
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	6	0.3
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	6	0.3
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	6	0.3
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	8	0.3
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD11	5	0.3
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD12	5	0.3
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD13	5	0.3
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD11	8	0.3
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD12	8	0.3
(1,449)	1:14:A:LEU:HA	1:14:A:LEU:HD13	8	0.3
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	6	0.3
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	7	0.3
(1,435)	1:60:A:GLY:HA2	1:60:A:GLY:H	8	0.3
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	2	0.3
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	2	0.3
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	2	0.3
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	8	0.3
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	8	0.3
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	9	0.3
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	9	0.3
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	9	0.3
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	7	0.3
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	7	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	3	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	3	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	3	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	4	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	4	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	4	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	5	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	5	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	5	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	6	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	6	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	6	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	10	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	10	0.3
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	10	0.3
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	8	0.3
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	10	0.3
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	4	0.3
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	6	0.3
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	6	0.3
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	1	0.3
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	3	0.3
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	6	0.3
(1,237)	1:75:A:LEU:HB3	1:75:A:LEU:H	7	0.3
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	3	0.3
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	8	0.3
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	7	0.3
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	1	0.3
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	7	0.3
(1,181)	1:75:A:LEU:HA	1:76:A:GLN:H	7	0.3
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	9	0.3
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	5	0.3
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	6	0.3
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	8	0.3
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	9	0.3
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	7	0.3
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	7	0.3
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	7	0.3
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	8	0.3
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	6	0.3
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	10	0.3
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	10	0.3
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	10	0.3
(1,142)	1:57:A:LEU:HD21	1:43:A:GLY:HA3	1	0.3
(1,142)	1:57:A:LEU:HD22	1:43:A:GLY:HA3	1	0.3
(1,142)	1:57:A:LEU:HD23	1:43:A:GLY:HA3	1	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	1	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	1	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	1	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	5	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	5	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	5	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	7	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	7	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	7	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	9	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	9	0.3
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	9	0.3
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	2	0.3
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	2	0.3
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	2	0.3
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	6	0.3
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	6	0.3
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	6	0.3
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	7	0.3
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	7	0.3
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	7	0.3
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	9	0.3
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	9	0.3
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	9	0.3
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	10	0.3
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	10	0.3
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	10	0.3
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	4	0.3
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	9	0.3
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	4	0.3
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	3	0.3
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	8	0.3
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	9	0.3
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	10	0.3
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	1	0.3
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	1	0.3
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	1	0.3
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	2	0.3
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	6	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	2	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	2	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	2	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	3	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	3	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	3	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	6	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	6	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	6	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	7	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	7	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	7	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	8	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	8	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	8	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	9	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	9	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	9	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD11	10	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD12	10	0.3
(1,60)	1:27:A:ILE:HG13	1:27:A:ILE:HD13	10	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	1	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	1	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	1	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	2	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	2	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	2	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	3	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	3	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	3	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	4	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	4	0.3
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	4	0.3
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	1	0.29
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	4	0.29
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	5	0.29
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	3	0.29
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	5	0.29
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	5	0.29
(2,487)	1:8:A:ASP:H	1:8:A:ASP:HB3	6	0.29
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	9	0.29
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	1	0.29
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	4	0.29
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	5	0.29
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	10	0.29
(2,468)	1:77:A:ALA:H	1:64:A:GLU:HG3	1	0.29
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	1	0.29
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB2	2	0.29
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB3	2	0.29
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	2	0.29
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	6	0.29
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	7	0.29
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	8	0.29
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	7	0.29
(2,380)	1:52:A:GLN:H	1:52:A:GLN:HB3	9	0.29
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	1	0.29
(2,358)	1:64:A:GLU:H	1:75:A:LEU:HD21	1	0.29
(2,358)	1:64:A:GLU:H	1:75:A:LEU:HD22	1	0.29
(2,358)	1:64:A:GLU:H	1:75:A:LEU:HD23	1	0.29
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	5	0.29
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	5	0.29
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	5	0.29
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	2	0.29
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	4	0.29
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	2	0.29
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	3	0.29
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	4	0.29
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	5	0.29
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	6	0.29
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	10	0.29
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	10	0.29
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	10	0.29
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	10	0.29
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	10	0.29
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	6	0.29
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	4	0.29
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	6	0.29
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	10	0.29
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	9	0.29
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	9	0.29
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	9	0.29
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	1	0.29
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	5	0.29
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	5	0.29
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	2	0.29
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	7	0.29
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	10	0.29
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	5	0.29
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	7	0.29
(2,166)	1:9:A:ILE:H	1:8:A:ASP:HA	10	0.29
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	6	0.29
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	4	0.29
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	4	0.29
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	4	0.29
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	10	0.29
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	1	0.29
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	2	0.29
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	3	0.29
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	4	0.29
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	5	0.29
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	7	0.29
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	10	0.29
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	3	0.29
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	3	0.29
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	3	0.29
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	6	0.29
(2,47)	1:61:A:THR:H	1:60:A:GLY:HA2	3	0.29
(2,6)	1:33:A:THR:H	1:33:A:THR:HG1	7	0.29
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	2	0.29
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	7	0.29
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	8	0.29
(2,2)	1:28:A:LEU:H	1:28:A:LEU:HA	10	0.29
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	4	0.29
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	5	0.29
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	5	0.29
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	1	0.29
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	1	0.29
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	2	0.29
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	2	0.29
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	2	0.29
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	8	0.29
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	8	0.29
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	8	0.29
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	10	0.29
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	10	0.29
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	10	0.29
(1,429)	1:9:A:ILE:HB	1:9:A:ILE:H	3	0.29
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	1	0.29
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	1	0.29
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	1	0.29
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	4	0.29
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	4	0.29
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	4	0.29
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	1	0.29
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	4	0.29
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	5	0.29
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	10	0.29
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	3	0.29
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	3	0.29
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	3	0.29
(1,388)	1:48:A:PHE:HB2	1:49:A:ASP:H	5	0.29
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	7	0.29
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	7	0.29
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	7	0.29
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	1	0.29
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	3	0.29
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	8	0.29
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	9	0.29
(1,365)	1:37:A:GLU:HA	1:37:A:GLU:HG2	5	0.29
(1,365)	1:37:A:GLU:HA	1:37:A:GLU:HG2	10	0.29
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	1	0.29
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	1	0.29
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	1	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	1	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	1	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	1	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	2	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	2	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	7	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	7	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	7	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB1	8	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB2	8	0.29
(1,332)	1:77:A:ALA:HA	1:77:A:ALA:HB3	8	0.29
(1,331)	1:74:A:SER:HB2	1:74:A:SER:HA	9	0.29
(1,331)	1:74:A:SER:HB3	1:74:A:SER:HA	9	0.29
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	1	0.29
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	3	0.29
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	4	0.29
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	7	0.29
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	9	0.29
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	1	0.29
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	3	0.29
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	6	0.29
(1,304)	1:14:A:LEU:HD11	1:36:A:THR:HA	10	0.29
(1,304)	1:14:A:LEU:HD12	1:36:A:THR:HA	10	0.29
(1,304)	1:14:A:LEU:HD13	1:36:A:THR:HA	10	0.29
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	1	0.29
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	1	0.29
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	2	0.29
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	2	0.29
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	5	0.29
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	5	0.29
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG21	7	0.29
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG22	7	0.29
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG23	7	0.29
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	2	0.29
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	6	0.29
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	7	0.29
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	8	0.29
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	3	0.29
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	10	0.29
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	7	0.29
(1,176)	1:56:A:ILE:HB	1:56:A:ILE:HG13	10	0.29
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	9	0.29
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	4	0.29
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	4	0.29
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	2	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	2	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	2	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	3	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	3	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	3	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	4	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	4	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	4	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	6	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	6	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	6	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	8	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	8	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	8	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB1	10	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB2	10	0.29
(1,132)	1:45:A:ALA:HA	1:45:A:ALA:HB3	10	0.29
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	3	0.29
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	3	0.29
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	3	0.29
(1,128)	1:25:A:ALA:HB1	1:25:A:ALA:H	8	0.29
(1,128)	1:25:A:ALA:HB2	1:25:A:ALA:H	8	0.29
(1,128)	1:25:A:ALA:HB3	1:25:A:ALA:H	8	0.29
(1,103)	1:37:A:GLU:HB2	1:37:A:GLU:H	4	0.29
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	2	0.29
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	4	0.29
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	5	0.29
(1,92)	1:45:A:ALA:HA	1:46:A:GLY:H	6	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	2	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	2	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	2	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	3	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	3	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	3	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	4	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	4	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	4	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	5	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	5	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	5	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	6	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	6	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	7	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	7	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	7	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	8	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	8	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	8	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	9	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	9	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	9	0.29
(1,89)	1:25:A:ALA:HB1	1:25:A:ALA:HA	10	0.29
(1,89)	1:25:A:ALA:HB2	1:25:A:ALA:HA	10	0.29
(1,89)	1:25:A:ALA:HB3	1:25:A:ALA:HA	10	0.29
(1,50)	1:27:A:ILE:HG13	1:27:A:ILE:HB	8	0.29
(1,36)	1:52:A:GLN:HB3	1:52:A:GLN:H	9	0.29
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	4	0.29
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	5	0.29
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	5	0.29
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	5	0.29
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	5	0.29
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	10	0.29
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	10	0.29
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	10	0.29
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	1	0.29
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	2	0.29
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	4	0.29
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	5	0.29
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	6	0.29
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	9	0.29
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD11	9	0.28
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD12	9	0.28
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD13	9	0.28
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD21	9	0.28
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD22	9	0.28
(5,14)	1:30:A:SER:H	1:29:A:LEU:HD23	9	0.28
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	8	0.28
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	8	0.28
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	2	0.28
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	9	0.28
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	2	0.28
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	2	0.28
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	3	0.28
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	10	0.28
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	8	0.28
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	3	0.28
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	3	0.28
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	4	0.28
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	4	0.28
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	8	0.28
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	8	0.28
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	3	0.28
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	8	0.28
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	4	0.28
(2,425)	1:5:A:ALA:H	1:4:A:GLN:HB3	9	0.28
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	1	0.28
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	3	0.28
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	9	0.28
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	1	0.28
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	3	0.28
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	4	0.28
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	1	0.28
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	1	0.28
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	1	0.28
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD21	3	0.28
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD22	3	0.28
(2,401)	1:8:A:ASP:H	1:57:A:LEU:HD23	3	0.28
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	2	0.28
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	3	0.28
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	6	0.28
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	10	0.28
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	8	0.28
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	8	0.28
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	8	0.28
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	8	0.28
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	1	0.28
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	1	0.28
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	1	0.28
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	10	0.28
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	10	0.28
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	10	0.28
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	2	0.28
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	7	0.28
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	7	0.28
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	8	0.28
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	9	0.28
(2,280)	1:9:A:ILE:H	1:9:A:ILE:HA	10	0.28
(2,231)	1:53:A:GLY:H	1:48:A:PHE:HB2	7	0.28
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	4	0.28
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	5	0.28
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	9	0.28
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	1	0.28
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	8	0.28
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD21	3	0.28
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD22	3	0.28
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD23	3	0.28
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	1	0.28
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	1	0.28
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	1	0.28
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	10	0.28
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	10	0.28
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	10	0.28
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	2	0.28
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	4	0.28
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	7	0.28
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	8	0.28
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	10	0.28
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	2	0.28
(2,110)	1:53:A:GLY:H	1:53:A:GLY:HA3	9	0.28
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	6	0.28
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	8	0.28
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	4	0.28
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	4	0.28
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	4	0.28
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	6	0.28
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	4	0.28
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	4	0.28
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	4	0.28
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	6	0.28
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	6	0.28
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	6	0.28
(2,63)	1:17:A:ALA:H	1:14:A:LEU:HA	4	0.28
(2,38)	1:50:A:ILE:H	1:49:A:ASP:HB2	4	0.28
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	3	0.28
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	6	0.28
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	4	0.28
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	4	0.28
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	4	0.28
(1,474)	1:65:A:ALA:HB1	1:65:A:ALA:HA	7	0.28
(1,474)	1:65:A:ALA:HB2	1:65:A:ALA:HA	7	0.28
(1,474)	1:65:A:ALA:HB3	1:65:A:ALA:HA	7	0.28
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	3	0.28
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	3	0.28
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	8	0.28
(1,393)	1:72:A:SER:HA	1:28:A:LEU:HB2	8	0.28
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	4	0.28
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	4	0.28
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	4	0.28
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	6	0.28
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	6	0.28
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	6	0.28
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	2	0.28
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	2	0.28
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	2	0.28
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	5	0.28
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	5	0.28
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	5	0.28
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	6	0.28
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	6	0.28
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	6	0.28
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	7	0.28
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	7	0.28
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	7	0.28
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	9	0.28
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	9	0.28
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	9	0.28
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	5	0.28
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	2	0.28
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	5	0.28
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	6	0.28
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	7	0.28
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	2	0.28
(1,312)	1:78:A:SER:HA	1:79:A:ALA:H	5	0.28
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	8	0.28
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	5	0.28
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	5	0.28
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	5	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	3	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	3	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	3	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	4	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	4	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	4	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	6	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	6	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	6	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	7	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	7	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	7	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	8	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	8	0.28
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	8	0.28
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	7	0.28
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	7	0.28
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG21	9	0.28
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG22	9	0.28
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG23	9	0.28
(1,253)	1:40:A:SER:HA	1:41:A:THR:H	6	0.28
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	1	0.28
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	3	0.28
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	9	0.28
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	5	0.28
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	1	0.28
(1,229)	1:47:A:ARG:HA	1:48:A:PHE:H	5	0.28
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	1	0.28
(1,178)	1:43:A:GLY:HA2	1:44:A:LEU:H	5	0.28
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	10	0.28
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	10	0.28
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	10	0.28
(1,166)	1:45:A:ALA:HA	1:8:A:ASP:HA	7	0.28
(1,161)	1:16:A:PRO:HD2	1:13:A:PRO:HG3	2	0.28
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	8	0.28
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	3	0.28
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	3	0.28
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	3	0.28
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	1	0.28
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	8	0.28
(1,86)	1:35:A:LEU:HD11	1:35:A:LEU:HA	9	0.28
(1,86)	1:35:A:LEU:HD12	1:35:A:LEU:HA	9	0.28
(1,86)	1:35:A:LEU:HD13	1:35:A:LEU:HA	9	0.28
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	7	0.28
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	7	0.28
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB1	7	0.28
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB2	7	0.28
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB3	7	0.28
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	7	0.28
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	3	0.27
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	4	0.27
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	2	0.27
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	1	0.27
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	6	0.27
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	1	0.27
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	2	0.27
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	5	0.27
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	9	0.27
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	9	0.27
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	1	0.27
(2,478)	1:27:A:ILE:H	1:27:A:ILE:HG13	5	0.27
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	2	0.27
(2,468)	1:77:A:ALA:H	1:64:A:GLU:HG3	10	0.27
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	5	0.27
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	10	0.27
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	7	0.27
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	4	0.27
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	5	0.27
(2,417)	1:27:A:ILE:H	1:27:A:ILE:HA	10	0.27
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	8	0.27
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	10	0.27
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	2	0.27
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	10	0.27
(2,382)	1:43:A:GLY:H	1:57:A:LEU:HA	5	0.27
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	4	0.27
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	5	0.27
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	5	0.27
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	5	0.27
(2,323)	1:68:A:GLY:H	1:67:A:ARG:HB2	3	0.27
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	3	0.27
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	5	0.27
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	5	0.27
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	2	0.27
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	2	0.27
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	2	0.27
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	2	0.27
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	10	0.27
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	1	0.27
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	8	0.27
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD21	7	0.27
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD22	7	0.27
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD23	7	0.27
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	1	0.27
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	1	0.27
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	1	0.27
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	5	0.27
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	5	0.27
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	5	0.27
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	8	0.27
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	8	0.27
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	8	0.27
(2,186)	1:70:A:ASN:H	1:69:A:ALA:HA	6	0.27
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD11	2	0.27
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD12	2	0.27
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD13	2	0.27
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD11	4	0.27
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD12	4	0.27
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD13	4	0.27
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	1	0.27
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD11	5	0.27
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD12	5	0.27
(2,154)	1:64:A:GLU:H	1:63:A:LEU:HD13	5	0.27
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	6	0.27
(2,108)	1:59:A:ALA:H	1:59:A:ALA:HA	7	0.27
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	1	0.27
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	2	0.27
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	3	0.27
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	8	0.27
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB1	7	0.27
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB2	7	0.27
(2,67)	1:17:A:ALA:H	1:17:A:ALA:HB3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:66:A:SER:H	1:65:A:ALA:HA	9	0.27
(2,47)	1:61:A:THR:H	1:60:A:GLY:HA2	2	0.27
(2,47)	1:61:A:THR:H	1:60:A:GLY:HA2	10	0.27
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD11	6	0.27
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD12	6	0.27
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD13	6	0.27
(2,5)	1:30:A:SER:H	1:29:A:LEU:HB2	9	0.27
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	3	0.27
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	3	0.27
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	4	0.27
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD21	2	0.27
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD22	2	0.27
(1,427)	1:58:A:LEU:HA	1:58:A:LEU:HD23	2	0.27
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	2	0.27
(1,390)	1:17:A:ALA:HB1	1:17:A:ALA:H	7	0.27
(1,390)	1:17:A:ALA:HB2	1:17:A:ALA:H	7	0.27
(1,390)	1:17:A:ALA:HB3	1:17:A:ALA:H	7	0.27
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	10	0.27
(1,365)	1:37:A:GLU:HA	1:37:A:GLU:HG2	6	0.27
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	3	0.27
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	3	0.27
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	3	0.27
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	8	0.27
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	8	0.27
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	8	0.27
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	10	0.27
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	10	0.27
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	10	0.27
(1,354)	1:75:A:LEU:HD11	1:75:A:LEU:HB3	9	0.27
(1,354)	1:75:A:LEU:HD12	1:75:A:LEU:HB3	9	0.27
(1,354)	1:75:A:LEU:HD13	1:75:A:LEU:HB3	9	0.27
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	1	0.27
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	7	0.27
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	2	0.27
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	5	0.27
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	7	0.27
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	1	0.27
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	3	0.27
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	10	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	1	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	1	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	2	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	2	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	2	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	5	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	5	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	5	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	9	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	9	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	9	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB1	10	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB2	10	0.27
(1,295)	1:5:A:ALA:HA	1:5:A:ALA:HB3	10	0.27
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	6	0.27
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	10	0.27
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	4	0.27
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	4	0.27
(1,254)	1:9:A:ILE:HA	1:10:A:PRO:HD3	8	0.27
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	4	0.27
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	5	0.27
(1,242)	1:27:A:ILE:HA	1:27:A:ILE:H	10	0.27
(1,241)	1:39:A:ARG:HD3	1:35:A:LEU:HG	4	0.27
(1,241)	1:39:A:ARG:HD3	1:35:A:LEU:HG	7	0.27
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	6	0.27
(1,218)	1:40:A:SER:HB2	1:41:A:THR:H	6	0.27
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	7	0.27
(1,200)	1:14:A:LEU:HD11	1:36:A:THR:HB	2	0.27
(1,200)	1:14:A:LEU:HD12	1:36:A:THR:HB	2	0.27
(1,200)	1:14:A:LEU:HD13	1:36:A:THR:HB	2	0.27
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	2	0.27
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	2	0.27
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	2	0.27
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	2	0.27
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	5	0.27
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	3	0.27
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	6	0.27
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	9	0.27
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	4	0.27
(1,87)	1:63:A:LEU:HD21	1:64:A:GLU:H	6	0.27
(1,87)	1:63:A:LEU:HD22	1:64:A:GLU:H	6	0.27
(1,87)	1:63:A:LEU:HD23	1:64:A:GLU:H	6	0.27
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	10	0.27
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	4	0.27
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	4	0.27
(1,27)	1:67:A:ARG:HA	1:67:A:ARG:HG3	9	0.27
(1,17)	1:20:A:HIS:HB3	1:20:A:HIS:H	3	0.27
(1,17)	1:20:A:HIS:HB3	1:20:A:HIS:H	6	0.27
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	1	0.27
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	9	0.26
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	9	0.26
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	8	0.26
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	5	0.26
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	8	0.26
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	4	0.26
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	3	0.26
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	5	0.26
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	3	0.26
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	3	0.26
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	10	0.26
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	10	0.26
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	8	0.26
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	8	0.26
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HD2	2	0.26
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	9	0.26
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	9	0.26
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	4	0.26
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	5	0.26
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	7	0.26
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	8	0.26
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	10	0.26
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	7	0.26
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB2	10	0.26
(2,435)	1:31:A:TYR:H	1:30:A:SER:HB3	10	0.26
(2,422)	1:76:A:GLN:H	1:75:A:LEU:HA	5	0.26
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	6	0.26
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	6	0.26
(2,382)	1:43:A:GLY:H	1:57:A:LEU:HA	4	0.26
(2,374)	1:52:A:GLN:H	1:51:A:ASP:HA	7	0.26
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	2	0.26
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	2	0.26
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	2	0.26
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	10	0.26
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	10	0.26
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	5	0.26
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	6	0.26
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	6	0.26
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	6	0.26
(2,325)	1:70:A:ASN:HD22	1:70:A:ASN:HB3	1	0.26
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	8	0.26
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	7	0.26
(2,294)	1:48:A:PHE:H	1:48:A:PHE:HB2	3	0.26
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	8	0.26
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	8	0.26
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	8	0.26
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	9	0.26
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	9	0.26
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	9	0.26
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	3	0.26
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	3	0.26
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	3	0.26
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	5	0.26
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	8	0.26
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	3	0.26
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	7	0.26
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	3	0.26
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	2	0.26
(2,213)	1:40:A:SER:H	1:39:A:ARG:HA	6	0.26
(2,211)	1:58:A:LEU:H	1:59:A:ALA:H	1	0.26
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	4	0.26
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD21	9	0.26
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD22	9	0.26
(2,196)	1:44:A:LEU:H	1:57:A:LEU:HD23	9	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	2	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	2	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	2	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	4	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	4	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	4	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	7	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	7	0.26
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	7	0.26
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	2	0.26
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	3	0.26
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	4	0.26
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	3	0.26
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	5	0.26
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	8	0.26
(2,113)	1:41:A:THR:H	1:40:A:SER:HB3	2	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	7	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	7	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	7	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	8	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	8	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	8	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	10	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	10	0.26
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	10	0.26
(2,97)	1:55:A:ALA:H	1:52:A:GLN:HA	2	0.26
(2,69)	1:39:A:ARG:HE	1:39:A:ARG:HB2	6	0.26
(2,53)	1:38:A:GLY:H	1:37:A:GLU:HG3	5	0.26
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	1	0.26
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	10	0.26
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	8	0.26
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	8	0.26
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	8	0.26
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	10	0.26
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	2	0.26
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	5	0.26
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	6	0.26
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	7	0.26
(1,464)	1:10:A:PRO:HD3	1:10:A:PRO:HG3	9	0.26
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	3	0.26
(1,440)	1:18:A:LEU:HA	1:21:A:PHE:HB2	10	0.26
(1,412)	1:42:A:SER:HA	1:42:A:SER:H	1	0.26
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	7	0.26
(1,393)	1:72:A:SER:HA	1:28:A:LEU:HB2	7	0.26
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	2	0.26
(1,360)	1:17:A:ALA:HB1	1:17:A:ALA:HA	4	0.26
(1,360)	1:17:A:ALA:HB2	1:17:A:ALA:HA	4	0.26
(1,360)	1:17:A:ALA:HB3	1:17:A:ALA:HA	4	0.26
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	2	0.26
(1,330)	1:13:A:PRO:HA	1:40:A:SER:HB2	6	0.26
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	3	0.26
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	6	0.26
(1,321)	1:15:A:ALA:HA	1:15:A:ALA:H	9	0.26
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	1:14:A:LEU:HD11	1:36:A:THR:HA	1	0.26
(1,304)	1:14:A:LEU:HD12	1:36:A:THR:HA	1	0.26
(1,304)	1:14:A:LEU:HD13	1:36:A:THR:HA	1	0.26
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	8	0.26
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	8	0.26
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	8	0.26
(1,298)	1:14:A:LEU:HD11	1:14:A:LEU:HB3	10	0.26
(1,298)	1:14:A:LEU:HD12	1:14:A:LEU:HB3	10	0.26
(1,298)	1:14:A:LEU:HD13	1:14:A:LEU:HB3	10	0.26
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	2	0.26
(1,226)	1:58:A:LEU:HG	1:58:A:LEU:H	4	0.26
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	9	0.26
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	1	0.26
(1,181)	1:75:A:LEU:HA	1:76:A:GLN:H	5	0.26
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	4	0.26
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	4	0.26
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	4	0.26
(1,172)	1:9:A:ILE:HG21	1:9:A:ILE:HA	8	0.26
(1,172)	1:9:A:ILE:HG22	1:9:A:ILE:HA	8	0.26
(1,172)	1:9:A:ILE:HG23	1:9:A:ILE:HA	8	0.26
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	3	0.26
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	4	0.26
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	2	0.26
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	2	0.26
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	2	0.26
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	10	0.26
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	10	0.26
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	10	0.26
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	2	0.26
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	4	0.26
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	7	0.26
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	8	0.26
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	7	0.26
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	4	0.26
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB1	9	0.26
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB2	9	0.26
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB3	9	0.26
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	5	0.26
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	4	0.26
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	9	0.26
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	6	0.26
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	6	0.26
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	7	0.26
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	7	0.26
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	7	0.26
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	3	0.26
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	5	0.26
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	8	0.25
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	7	0.25
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	1	0.25
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	4	0.25
(4,14)	1:56:A:ILE:N	1:52:A:GLN:O	1	0.25
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	4	0.25
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	1	0.25
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	3	0.25
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	4	0.25
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	4	0.25
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	5	0.25
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	5	0.25
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	7	0.25
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	7	0.25
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	8	0.25
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	8	0.25
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	7	0.25
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	7	0.25
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	2	0.25
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	2	0.25
(3,10)	1:30:A:SER:HB2	1:30:A:SER:H	3	0.25
(2,489)	1:69:A:ALA:H	1:68:A:GLY:HA2	1	0.25
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	2	0.25
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	3	0.25
(2,486)	1:65:A:ALA:H	1:65:A:ALA:HA	6	0.25
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	10	0.25
(2,419)	1:72:A:SER:H	1:70:A:ASN:HA	6	0.25
(2,414)	1:66:A:SER:H	1:66:A:SER:HA	5	0.25
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	3	0.25
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	8	0.25
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	8	0.25
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	8	0.25
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	8	0.25
(2,349)	1:21:A:PHE:H	1:21:A:PHE:HB2	8	0.25
(2,333)	1:37:A:GLU:H	1:37:A:GLU:HG2	7	0.25
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,284)	1:76:A:GLN:H	1:64:A:GLU:H	3	0.25
(2,284)	1:76:A:GLN:H	1:64:A:GLU:H	10	0.25
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	10	0.25
(2,266)	1:30:A:SER:H	1:29:A:LEU:HA	9	0.25
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	10	0.25
(2,225)	1:18:A:LEU:H	1:19:A:ALA:H	10	0.25
(2,204)	1:21:A:PHE:H	1:23:A:GLN:H	4	0.25
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	8	0.25
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB1	6	0.25
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB2	6	0.25
(2,187)	1:70:A:ASN:H	1:69:A:ALA:HB3	6	0.25
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	2	0.25
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	7	0.25
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	6	0.25
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	10	0.25
(2,142)	1:59:A:ALA:H	1:56:A:ILE:HA	8	0.25
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	4	0.25
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	10	0.25
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	8	0.25
(2,65)	1:17:A:ALA:H	1:18:A:LEU:H	10	0.25
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	8	0.25
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	10	0.25
(2,34)	1:50:A:ILE:H	1:4:A:GLN:HA	8	0.25
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	1	0.25
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	1	0.25
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	4	0.25
(2,21)	1:34:A:ALA:H	1:34:A:ALA:HA	7	0.25
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	7	0.25
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	2	0.25
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	3	0.25
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	5	0.25
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	9	0.25
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	4	0.25
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	4	0.25
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	10	0.25
(1,438)	1:74:A:SER:HA	1:75:A:LEU:H	1	0.25
(1,438)	1:74:A:SER:HA	1:75:A:LEU:H	7	0.25
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	8	0.25
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	10	0.25
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	1	0.25
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	1	0.25
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	2	0.25
(1,365)	1:37:A:GLU:HA	1:37:A:GLU:HG2	3	0.25
(1,329)	1:72:A:SER:HB3	1:72:A:SER:HA	1	0.25
(1,314)	1:72:A:SER:HA	1:72:A:SER:H	9	0.25
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	4	0.25
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	9	0.25
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	8	0.25
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	3	0.25
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	4	0.25
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	9	0.25
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	9	0.25
(1,253)	1:40:A:SER:HA	1:41:A:THR:H	1	0.25
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	8	0.25
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	3	0.25
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	6	0.25
(1,211)	1:72:A:SER:HA	1:73:A:TYR:H	8	0.25
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	2	0.25
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	5	0.25
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	9	0.25
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	3	0.25
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	2	0.25
(1,103)	1:37:A:GLU:HB2	1:37:A:GLU:H	1	0.25
(1,103)	1:37:A:GLU:HB2	1:37:A:GLU:H	9	0.25
(1,78)	1:57:A:LEU:HD21	1:57:A:LEU:HB3	4	0.25
(1,78)	1:57:A:LEU:HD22	1:57:A:LEU:HB3	4	0.25
(1,78)	1:57:A:LEU:HD23	1:57:A:LEU:HB3	4	0.25
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE1	9	0.25
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE2	9	0.25
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	9	0.25
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	9	0.25
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	9	0.25
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	5	0.25
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	2	0.25
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	7	0.25
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	7	0.25
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG21	8	0.25
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG22	8	0.25
(1,10)	1:61:A:THR:HB	1:61:A:THR:HG23	8	0.25
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	8	0.25
(1,8)	1:10:A:PRO:HA	1:10:A:PRO:HB3	10	0.25
(4,41)	1:43:A:GLY:H	1:41:A:THR:OG1	7	0.24
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	5	0.24
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	1	0.24
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	2	0.24
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	3	0.24
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	9	0.24
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	8	0.24
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	9	0.24
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	9	0.24
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	2	0.24
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	2	0.24
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	3	0.24
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	3	0.24
(3,10)	1:30:A:SER:HB2	1:30:A:SER:H	7	0.24
(2,470)	1:45:A:ALA:H	1:44:A:LEU:HA	6	0.24
(2,468)	1:77:A:ALA:H	1:64:A:GLU:HG3	8	0.24
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	2	0.24
(2,453)	1:19:A:ALA:H	1:16:A:PRO:HA	5	0.24
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	3	0.24
(2,409)	1:21:A:PHE:H	1:18:A:LEU:HA	10	0.24
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	5	0.24
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	10	0.24
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	4	0.24
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	7	0.24
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	3	0.24
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	8	0.24
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	10	0.24
(2,333)	1:37:A:GLU:H	1:37:A:GLU:HG2	8	0.24
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	1	0.24
(2,304)	1:58:A:LEU:H	1:58:A:LEU:HA	10	0.24
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	9	0.24
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	7	0.24
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	7	0.24
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	7	0.24
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	9	0.24
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	9	0.24
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	9	0.24
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	1	0.24
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	9	0.24
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	2	0.24
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	6	0.24
(2,189)	1:68:A:GLY:H	1:73:A:TYR:HA	2	0.24
(2,189)	1:68:A:GLY:H	1:73:A:TYR:HA	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,157)	1:53:A:GLY:H	1:48:A:PHE:HB3	5	0.24
(2,149)	1:12:A:GLY:H	1:42:A:SER:HA	10	0.24
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	3	0.24
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	3	0.24
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	3	0.24
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	6	0.24
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	6	0.24
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	6	0.24
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	5	0.24
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	4	0.24
(2,51)	1:80:A:SER:H	1:80:A:SER:HB3	5	0.24
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	3	0.24
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	1	0.24
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	6	0.24
(2,1)	1:29:A:LEU:H	1:28:A:LEU:HA	7	0.24
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	5	0.24
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	8	0.24
(1,481)	1:58:A:LEU:HG	1:57:A:LEU:HB3	4	0.24
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	9	0.24
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	10	0.24
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	1	0.24
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	1	0.24
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	2	0.24
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	2	0.24
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	4	0.24
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	4	0.24
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	6	0.24
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	6	0.24
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	2	0.24
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	5	0.24
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	10	0.24
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	9	0.24
(1,424)	1:40:A:SER:HB3	1:41:A:THR:H	3	0.24
(1,396)	1:44:A:LEU:HA	1:45:A:ALA:H	6	0.24
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	3	0.24
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	6	0.24
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	9	0.24
(1,369)	1:23:A:GLN:HB2	1:23:A:GLN:HA	4	0.24
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	3	0.24
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	4	0.24
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	8	0.24
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	4	0.24
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	6	0.24
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD11	8	0.24
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD12	8	0.24
(1,299)	1:21:A:PHE:HB3	1:18:A:LEU:HD13	8	0.24
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	3	0.24
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	5	0.24
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	7	0.24
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	1	0.24
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	1	0.24
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	5	0.24
(1,238)	1:73:A:TYR:HB3	1:73:A:TYR:HD2	5	0.24
(1,220)	1:23:A:GLN:HB2	1:23:A:GLN:H	5	0.24
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	3	0.24
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	8	0.24
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	1	0.24
(1,164)	1:57:A:LEU:HA	1:57:A:LEU:H	10	0.24
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	3	0.24
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	3	0.24
(1,145)	1:11:A:ALA:HA	1:12:A:GLY:H	1	0.24
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	10	0.24
(1,119)	1:50:A:ILE:HD11	1:55:A:ALA:H	8	0.24
(1,119)	1:50:A:ILE:HD12	1:55:A:ALA:H	8	0.24
(1,119)	1:50:A:ILE:HD13	1:55:A:ALA:H	8	0.24
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	1	0.24
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	7	0.24
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	5	0.24
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	7	0.24
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	8	0.24
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	8	0.24
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	8	0.24
(1,54)	1:11:A:ALA:HB1	1:11:A:ALA:H	10	0.24
(1,54)	1:11:A:ALA:HB2	1:11:A:ALA:H	10	0.24
(1,54)	1:11:A:ALA:HB3	1:11:A:ALA:H	10	0.24
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	7	0.24
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	3	0.24
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	8	0.24
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	10	0.24
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	5	0.24
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB2	1	0.23
(5,5)	1:75:A:LEU:H	1:74:A:SER:HB3	1	0.23
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	7	0.23
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	4	0.23
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	7	0.23
(4,40)	1:12:A:GLY:N	1:41:A:THR:O	6	0.23
(4,37)	1:14:A:LEU:H	1:39:A:ARG:O	10	0.23
(4,34)	1:21:A:PHE:N	1:17:A:ALA:O	4	0.23
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	2	0.23
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	3	0.23
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	8	0.23
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	5	0.23
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	7	0.23
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	8	0.23
(3,27)	1:68:A:GLY:HA3	1:68:A:GLY:H	4	0.23
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	1	0.23
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	1	0.23
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	7	0.23
(2,419)	1:72:A:SER:H	1:70:A:ASN:HA	2	0.23
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	7	0.23
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	4	0.23
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	5	0.23
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB1	7	0.23
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB2	7	0.23
(2,361)	1:27:A:ILE:H	1:25:A:ALA:HB3	7	0.23
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	3	0.23
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	6	0.23
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	7	0.23
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	9	0.23
(2,350)	1:41:A:THR:H	1:40:A:SER:HB2	4	0.23
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	5	0.23
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	7	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	2	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	2	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	2	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	7	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	7	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	7	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	8	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	8	0.23
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	8	0.23
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	5	0.23
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	1	0.23
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	3	0.23
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	4	0.23
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	5	0.23
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	6	0.23
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	8	0.23
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	10	0.23
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	7	0.23
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	7	0.23
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	7	0.23
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	7	0.23
(2,227)	1:19:A:ALA:H	1:16:A:PRO:HB2	1	0.23
(2,227)	1:19:A:ALA:H	1:16:A:PRO:HB2	8	0.23
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	10	0.23
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	10	0.23
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	9	0.23
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	9	0.23
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	7	0.23
(2,97)	1:55:A:ALA:H	1:52:A:GLN:HA	1	0.23
(2,96)	1:52:A:GLN:H	1:52:A:GLN:HA	9	0.23
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	1	0.23
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	5	0.23
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	6	0.23
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	7	0.23
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	9	0.23
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	10	0.23
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	1	0.23
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	2	0.23
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	4	0.23
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	5	0.23
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	5	0.23
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	5	0.23
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	10	0.23
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	10	0.23
(2,16)	1:36:A:THR:H	1:35:A:LEU:H	6	0.23
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	4	0.23
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	6	0.23
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	3	0.23
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	3	0.23
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	5	0.23
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	5	0.23
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	7	0.23
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	8	0.23
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	8	0.23
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	9	0.23
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	9	0.23
(1,443)	1:10:A:PRO:HG2	1:10:A:PRO:HB3	10	0.23
(1,443)	1:10:A:PRO:HG3	1:10:A:PRO:HB3	10	0.23
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	6	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	1	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	2	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	3	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	4	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	5	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	6	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	8	0.23
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	10	0.23
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	1	0.23
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	2	0.23
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	3	0.23
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	4	0.23
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	6	0.23
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	7	0.23
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	8	0.23
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	10	0.23
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	9	0.23
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	1	0.23
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	3	0.23
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	5	0.23
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	5	0.23
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	5	0.23
(1,296)	1:27:A:ILE:HG13	1:27:A:ILE:H	8	0.23
(1,241)	1:39:A:ARG:HD3	1:35:A:LEU:HG	2	0.23
(1,155)	1:44:A:LEU:HB3	1:44:A:LEU:HD21	1	0.23
(1,155)	1:44:A:LEU:HB3	1:44:A:LEU:HD22	1	0.23
(1,155)	1:44:A:LEU:HB3	1:44:A:LEU:HD23	1	0.23
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	4	0.23
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	4	0.23
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	6	0.23
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	6	0.23
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	6	0.23
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	3	0.23
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	3	0.23
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	6	0.23
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	8	0.23
(1,121)	1:20:A:HIS:HB2	1:20:A:HIS:HA	7	0.23
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	6	0.23
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	6	0.23
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	6	0.23
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	3	0.23
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	3	0.23
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	6	0.23
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	7	0.23
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	9	0.23
(1,93)	1:70:A:ASN:HB3	1:70:A:ASN:HD21	3	0.23
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	4	0.23
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	9	0.23
(1,79)	1:39:A:ARG:HD3	1:39:A:ARG:HE	8	0.23
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	1	0.23
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	2	0.23
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	3	0.23
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	5	0.23
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	6	0.23
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	8	0.23
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	9	0.23
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	9	0.23
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	9	0.23
(1,30)	1:73:A:TYR:HB3	1:73:A:TYR:HA	1	0.23
(1,17)	1:20:A:HIS:HB3	1:20:A:HIS:H	1	0.23
(5,11)	1:34:A:ALA:H	1:32:A:PRO:HG2	7	0.22
(5,11)	1:34:A:ALA:H	1:32:A:PRO:HG3	7	0.22
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	4	0.22
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	5	0.22
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	9	0.22
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	10	0.22
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	7	0.22
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	1	0.22
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	5	0.22
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	1	0.22
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	6	0.22
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	8	0.22
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	10	0.22
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	2	0.22
(3,36)	1:73:A:TYR:HB2	1:29:A:LEU:HA	1	0.22
(3,36)	1:73:A:TYR:HB2	1:29:A:LEU:HA	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	1	0.22
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	1	0.22
(3,22)	1:30:A:SER:HB2	1:30:A:SER:HA	4	0.22
(3,22)	1:30:A:SER:HB3	1:30:A:SER:HA	4	0.22
(2,489)	1:69:A:ALA:H	1:68:A:GLY:HA2	2	0.22
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	6	0.22
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	6	0.22
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	2	0.22
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	4	0.22
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	6	0.22
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	8	0.22
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	9	0.22
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	2	0.22
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	5	0.22
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	6	0.22
(2,382)	1:43:A:GLY:H	1:57:A:LEU:HA	6	0.22
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	4	0.22
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	4	0.22
(2,360)	1:5:A:ALA:H	1:48:A:PHE:H	7	0.22
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	1	0.22
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	2	0.22
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	5	0.22
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	8	0.22
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	10	0.22
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	2	0.22
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	4	0.22
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	6	0.22
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	9	0.22
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	4	0.22
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	7	0.22
(2,325)	1:70:A:ASN:HD22	1:70:A:ASN:HB3	10	0.22
(2,313)	1:58:A:LEU:H	1:54:A:LEU:HA	2	0.22
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	1	0.22
(2,291)	1:26:A:HIS:H	1:26:A:HIS:HA	7	0.22
(2,284)	1:76:A:GLN:H	1:64:A:GLU:H	1	0.22
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	4	0.22
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	5	0.22
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	1	0.22
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	1	0.22
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	10	0.22
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	10	0.22
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	2	0.22
(2,217)	1:28:A:LEU:H	1:27:A:ILE:HA	5	0.22
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	6	0.22
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	6	0.22
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	4	0.22
(2,189)	1:68:A:GLY:H	1:73:A:TYR:HA	10	0.22
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	6	0.22
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	10	0.22
(2,178)	1:64:A:GLU:H	1:64:A:GLU:HA	5	0.22
(2,164)	1:65:A:ALA:H	1:64:A:GLU:HA	3	0.22
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	8	0.22
(2,142)	1:59:A:ALA:H	1:56:A:ILE:HA	6	0.22
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	5	0.22
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	9	0.22
(2,103)	1:43:A:GLY:H	1:11:A:ALA:HA	5	0.22
(2,103)	1:43:A:GLY:H	1:11:A:ALA:HA	7	0.22
(2,103)	1:43:A:GLY:H	1:11:A:ALA:HA	9	0.22
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	2	0.22
(2,95)	1:53:A:GLY:H	1:52:A:GLN:HA	3	0.22
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	3	0.22
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	6	0.22
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	7	0.22
(2,62)	1:17:A:ALA:H	1:17:A:ALA:HA	9	0.22
(2,51)	1:80:A:SER:H	1:80:A:SER:HB3	2	0.22
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	8	0.22
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	2	0.22
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	2	0.22
(2,16)	1:36:A:THR:H	1:35:A:LEU:H	2	0.22
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	3	0.22
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	5	0.22
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	6	0.22
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	8	0.22
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	7	0.22
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	7	0.22
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	8	0.22
(1,433)	1:26:A:HIS:HA	1:26:A:HIS:H	7	0.22
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	5	0.22
(1,430)	1:64:A:GLU:HG2	1:64:A:GLU:HG3	9	0.22
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	8	0.22
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	9	0.22
(1,308)	1:50:A:ILE:HB	1:50:A:ILE:HA	5	0.22
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB1	1	0.22
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB2	1	0.22
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB3	1	0.22
(1,286)	1:47:A:ARG:HD2	1:47:A:ARG:HE	10	0.22
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	8	0.22
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	8	0.22
(1,214)	1:66:A:SER:HA	1:67:A:ARG:H	1	0.22
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	6	0.22
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	8	0.22
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	8	0.22
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	8	0.22
(1,145)	1:11:A:ALA:HA	1:12:A:GLY:H	8	0.22
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	2	0.22
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	9	0.22
(1,114)	1:20:A:HIS:HB2	1:20:A:HIS:H	6	0.22
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	6	0.22
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	1	0.22
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	2	0.22
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	5	0.22
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	8	0.22
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	10	0.22
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	8	0.22
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	3	0.22
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	3	0.22
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	3	0.22
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD21	2	0.22
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD22	2	0.22
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD23	2	0.22
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD21	2	0.22
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD22	2	0.22
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD23	2	0.22
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD21	2	0.22
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD22	2	0.22
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD23	2	0.22
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD21	4	0.22
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD22	4	0.22
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD23	4	0.22
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD21	4	0.22
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD22	4	0.22
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD23	4	0.22
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD21	4	0.22
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD22	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD23	4	0.22
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	9	0.22
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	1	0.22
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	1	0.22
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	1	0.22
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	5	0.22
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	5	0.22
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	5	0.22
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	2	0.22
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	4	0.22
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	6	0.22
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	9	0.22
(1,13)	1:73:A:TYR:HA	1:73:A:TYR:HB2	9	0.22
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	2	0.22
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	6	0.22
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	10	0.22
(5,1)	1:78:A:SER:H	1:78:A:SER:HB2	3	0.21
(5,1)	1:78:A:SER:H	1:78:A:SER:HB3	3	0.21
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	5	0.21
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	1	0.21
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	9	0.21
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	10	0.21
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	6	0.21
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	6	0.21
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	10	0.21
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	10	0.21
(2,489)	1:69:A:ALA:H	1:68:A:GLY:HA2	4	0.21
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	3	0.21
(2,466)	1:39:A:ARG:HE	1:39:A:ARG:HD2	8	0.21
(2,455)	1:15:A:ALA:H	1:16:A:PRO:HD2	3	0.21
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	10	0.21
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	2	0.21
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	2	0.21
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	2	0.21
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	6	0.21
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	6	0.21
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	6	0.21
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	5	0.21
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	9	0.21
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	9	0.21
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	2	0.21
(2,380)	1:52:A:GLN:H	1:52:A:GLN:HB3	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	3	0.21
(2,354)	1:22:A:GLY:H	1:22:A:GLY:HA2	4	0.21
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	7	0.21
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	10	0.21
(2,325)	1:70:A:ASN:HD22	1:70:A:ASN:HB3	5	0.21
(2,325)	1:70:A:ASN:HD22	1:70:A:ASN:HB3	8	0.21
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	8	0.21
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	8	0.21
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	8	0.21
(2,305)	1:72:A:SER:H	1:71:A:ALA:H	7	0.21
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	3	0.21
(2,284)	1:76:A:GLN:H	1:64:A:GLU:H	4	0.21
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	6	0.21
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	8	0.21
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	9	0.21
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	1	0.21
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	1	0.21
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	1	0.21
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	9	0.21
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	10	0.21
(2,211)	1:58:A:LEU:H	1:59:A:ALA:H	7	0.21
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	8	0.21
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	8	0.21
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	8	0.21
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	2	0.21
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	10	0.21
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD21	9	0.21
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD22	9	0.21
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD23	9	0.21
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	3	0.21
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	5	0.21
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	7	0.21
(2,147)	1:12:A:GLY:H	1:12:A:GLY:HA2	10	0.21
(2,147)	1:12:A:GLY:H	1:12:A:GLY:HA3	10	0.21
(2,146)	1:49:A:ASP:H	1:48:A:PHE:HA	4	0.21
(2,142)	1:59:A:ALA:H	1:56:A:ILE:HA	7	0.21
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	3	0.21
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	4	0.21
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	5	0.21
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	6	0.21
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	9	0.21
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	9	0.21
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD11	8	0.21
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD12	8	0.21
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD13	8	0.21
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	5	0.21
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	6	0.21
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD11	8	0.21
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD12	8	0.21
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD13	8	0.21
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	7	0.21
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	7	0.21
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	3	0.21
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	4	0.21
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG21	1	0.21
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG22	1	0.21
(1,459)	1:17:A:ALA:HB1	1:9:A:ILE:HG23	1	0.21
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG21	1	0.21
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG22	1	0.21
(1,459)	1:17:A:ALA:HB2	1:9:A:ILE:HG23	1	0.21
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG21	1	0.21
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG22	1	0.21
(1,459)	1:17:A:ALA:HB3	1:9:A:ILE:HG23	1	0.21
(1,438)	1:74:A:SER:HA	1:75:A:LEU:H	9	0.21
(1,410)	1:55:A:ALA:HB1	1:52:A:GLN:HA	3	0.21
(1,410)	1:55:A:ALA:HB2	1:52:A:GLN:HA	3	0.21
(1,410)	1:55:A:ALA:HB3	1:52:A:GLN:HA	3	0.21
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	1	0.21
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	4	0.21
(1,329)	1:72:A:SER:HB3	1:72:A:SER:HA	7	0.21
(1,329)	1:72:A:SER:HB3	1:72:A:SER:HA	10	0.21
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	6	0.21
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	6	0.21
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	9	0.21
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	6	0.21
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD21	6	0.21
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD22	6	0.21
(1,278)	1:75:A:LEU:HB3	1:58:A:LEU:HD23	6	0.21
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	9	0.21
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	7	0.21
(1,214)	1:66:A:SER:HA	1:67:A:ARG:H	4	0.21
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	2	0.21
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.21
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.21
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	9	0.21
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	9	0.21
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	9	0.21
(1,167)	1:54:A:LEU:HB3	1:51:A:ASP:HA	5	0.21
(1,106)	1:22:A:GLY:HA2	1:22:A:GLY:H	4	0.21
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	9	0.21
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	3	0.21
(1,78)	1:57:A:LEU:HD21	1:57:A:LEU:HB3	2	0.21
(1,78)	1:57:A:LEU:HD22	1:57:A:LEU:HB3	2	0.21
(1,78)	1:57:A:LEU:HD23	1:57:A:LEU:HB3	2	0.21
(1,78)	1:57:A:LEU:HD21	1:57:A:LEU:HB3	8	0.21
(1,78)	1:57:A:LEU:HD22	1:57:A:LEU:HB3	8	0.21
(1,78)	1:57:A:LEU:HD23	1:57:A:LEU:HB3	8	0.21
(1,73)	1:76:A:GLN:HA	1:77:A:ALA:H	7	0.21
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE1	3	0.21
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE2	3	0.21
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	2	0.21
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	2	0.21
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	2	0.21
(1,46)	1:73:A:TYR:HA	1:68:A:GLY:H	6	0.21
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	2	0.21
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	2	0.21
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	2	0.21
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	3	0.21
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	3	0.21
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	3	0.21
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	4	0.21
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	4	0.21
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	4	0.21
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	8	0.21
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	8	0.21
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	8	0.21
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	10	0.21
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	10	0.21
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	10	0.21
(1,36)	1:52:A:GLN:HB3	1:52:A:GLN:H	5	0.21
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB1	2	0.21
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB2	2	0.21
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB3	2	0.21
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	8	0.21
(1,1)	1:15:A:ALA:HB1	1:16:A:PRO:HB2	5	0.21
(1,1)	1:15:A:ALA:HB2	1:16:A:PRO:HB2	5	0.21
(1,1)	1:15:A:ALA:HB3	1:16:A:PRO:HB2	5	0.21
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	1	0.2
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	9	0.2
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	3	0.2
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	6	0.2
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	5	0.2
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	4	0.2
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	5	0.2
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	7	0.2
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	10	0.2
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	6	0.2
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	10	0.2
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	5	0.2
(3,1)	1:66:A:SER:HB2	1:66:A:SER:H	9	0.2
(3,1)	1:66:A:SER:HB3	1:66:A:SER:H	9	0.2
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB2	9	0.2
(2,488)	1:28:A:LEU:H	1:28:A:LEU:HB3	9	0.2
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	1	0.2
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	9	0.2
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	10	0.2
(2,459)	1:66:A:SER:H	1:73:A:TYR:HB2	6	0.2
(2,449)	1:55:A:ALA:H	1:56:A:ILE:H	5	0.2
(2,422)	1:76:A:GLN:H	1:75:A:LEU:HA	1	0.2
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	1	0.2
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	1	0.2
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	1	0.2
(2,419)	1:72:A:SER:H	1:70:A:ASN:HA	7	0.2
(2,419)	1:72:A:SER:H	1:70:A:ASN:HA	8	0.2
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	5	0.2
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	9	0.2
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	7	0.2
(2,394)	1:14:A:LEU:H	1:13:A:PRO:HA	8	0.2
(2,382)	1:43:A:GLY:H	1:57:A:LEU:HA	2	0.2
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	9	0.2
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	2	0.2
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	9	0.2
(2,325)	1:70:A:ASN:HD22	1:70:A:ASN:HB3	2	0.2
(2,325)	1:70:A:ASN:HD22	1:70:A:ASN:HB3	4	0.2
(2,325)	1:70:A:ASN:HD22	1:70:A:ASN:HB3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	1	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	1	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	1	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	5	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	5	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	5	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	10	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	10	0.2
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	10	0.2
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	10	0.2
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	3	0.2
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	7	0.2
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	8	0.2
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	9	0.2
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	10	0.2
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	1	0.2
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	1	0.2
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	1	0.2
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	4	0.2
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	4	0.2
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	4	0.2
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	1	0.2
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	2	0.2
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	3	0.2
(2,282)	1:61:A:THR:H	1:61:A:THR:HA	10	0.2
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	9	0.2
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	9	0.2
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	5	0.2
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	5	0.2
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	5	0.2
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	3	0.2
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	5	0.2
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	7	0.2
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD21	5	0.2
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD22	5	0.2
(2,261)	1:21:A:PHE:H	1:57:A:LEU:HD23	5	0.2
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	8	0.2
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	7	0.2
(2,211)	1:58:A:LEU:H	1:59:A:ALA:H	3	0.2
(2,211)	1:58:A:LEU:H	1:59:A:ALA:H	8	0.2
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	3	0.2
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	5	0.2
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	7	0.2
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	3	0.2
(2,199)	1:75:A:LEU:H	1:74:A:SER:HA	10	0.2
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	6	0.2
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	8	0.2
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD11	7	0.2
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD12	7	0.2
(2,155)	1:76:A:GLN:H	1:63:A:LEU:HD13	7	0.2
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	7	0.2
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	9	0.2
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	9	0.2
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	2	0.2
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	2	0.2
(2,46)	1:55:A:ALA:H	1:54:A:LEU:H	2	0.2
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	4	0.2
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	10	0.2
(2,16)	1:36:A:THR:H	1:35:A:LEU:H	5	0.2
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	1	0.2
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	2	0.2
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	7	0.2
(1,489)	1:6:A:ASP:HA	1:6:A:ASP:HB2	10	0.2
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	1	0.2
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	10	0.2
(1,483)	1:64:A:GLU:HB3	1:64:A:GLU:HA	9	0.2
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	8	0.2
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	7	0.2
(1,354)	1:75:A:LEU:HD11	1:75:A:LEU:HB3	3	0.2
(1,354)	1:75:A:LEU:HD12	1:75:A:LEU:HB3	3	0.2
(1,354)	1:75:A:LEU:HD13	1:75:A:LEU:HB3	3	0.2
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	1	0.2
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	1	0.2
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	1	0.2
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	4	0.2
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	4	0.2
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	4	0.2
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	10	0.2
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	6	0.2
(1,244)	1:27:A:ILE:HA	1:27:A:ILE:HB	5	0.2
(1,241)	1:39:A:ARG:HD3	1:35:A:LEU:HG	3	0.2
(1,231)	1:14:A:LEU:HB3	1:14:A:LEU:H	1	0.2
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	10	0.2
(1,214)	1:66:A:SER:HA	1:67:A:ARG:H	5	0.2
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	1	0.2
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	1	0.2
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	1	0.2
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	6	0.2
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	6	0.2
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	6	0.2
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD11	7	0.2
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD12	7	0.2
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD13	7	0.2
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD11	7	0.2
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD12	7	0.2
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD13	7	0.2
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD11	7	0.2
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD12	7	0.2
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD13	7	0.2
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	3	0.2
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	3	0.2
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	3	0.2
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	10	0.2
(1,181)	1:75:A:LEU:HA	1:76:A:GLN:H	1	0.2
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	4	0.2
(1,159)	1:4:A:GLN:HA	1:4:A:GLN:HB2	9	0.2
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	3	0.2
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	3	0.2
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	3	0.2
(1,145)	1:11:A:ALA:HA	1:12:A:GLY:H	3	0.2
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	9	0.2
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	1	0.2
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	9	0.2
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE1	7	0.2
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE2	7	0.2
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	5	0.2
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	5	0.2
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	5	0.2
(1,48)	1:16:A:PRO:HB3	1:16:A:PRO:HA	10	0.2
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	7	0.2
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	7	0.2
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	7	0.2
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD11	8	0.2
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD12	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:39:A:ARG:HD2	1:63:A:LEU:HD13	8	0.2
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	6	0.2
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	8	0.2
(1,12)	1:3:A:ALA:HA	1:4:A:GLN:H	3	0.2
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	3	0.19
(4,46)	1:19:A:ALA:N	1:15:A:ALA:O	8	0.19
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	3	0.19
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	3	0.19
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	7	0.19
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	9	0.19
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	9	0.19
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	4	0.19
(4,22)	1:59:A:ALA:N	1:56:A:ILE:O	9	0.19
(4,20)	1:58:A:LEU:N	1:54:A:LEU:O	6	0.19
(4,18)	1:54:A:LEU:N	1:50:A:ILE:O	7	0.19
(4,12)	1:64:A:GLU:N	1:76:A:GLN:O	7	0.19
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	2	0.19
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	3	0.19
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	4	0.19
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	8	0.19
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	9	0.19
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	3	0.19
(3,23)	1:66:A:SER:HB2	1:66:A:SER:HA	2	0.19
(3,23)	1:66:A:SER:HB3	1:66:A:SER:HA	2	0.19
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	1	0.19
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	1	0.19
(2,468)	1:77:A:ALA:H	1:64:A:GLU:HG3	6	0.19
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	1	0.19
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	8	0.19
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	2	0.19
(2,380)	1:52:A:GLN:H	1:52:A:GLN:HB3	10	0.19
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	5	0.19
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	10	0.19
(2,345)	1:14:A:LEU:H	1:14:A:LEU:HA	1	0.19
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB1	3	0.19
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB2	3	0.19
(2,329)	1:65:A:ALA:H	1:65:A:ALA:HB3	3	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	2	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	2	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	2	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	4	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	4	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	6	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	6	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	6	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB1	7	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB2	7	0.19
(2,314)	1:72:A:SER:H	1:71:A:ALA:HB3	7	0.19
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	2	0.19
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	4	0.19
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	5	0.19
(2,295)	1:46:A:GLY:H	1:45:A:ALA:HA	6	0.19
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	9	0.19
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	9	0.19
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	9	0.19
(2,284)	1:76:A:GLN:H	1:64:A:GLU:H	8	0.19
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	8	0.19
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	8	0.19
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	1	0.19
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	6	0.19
(2,228)	1:60:A:GLY:H	1:60:A:GLY:HA2	9	0.19
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	8	0.19
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	1	0.19
(2,202)	1:77:A:ALA:H	1:76:A:GLN:HA	5	0.19
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	10	0.19
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	6	0.19
(2,37)	1:50:A:ILE:H	1:49:A:ASP:HA	9	0.19
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	7	0.19
(1,483)	1:64:A:GLU:HB3	1:64:A:GLU:HA	5	0.19
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	2	0.19
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	2	0.19
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	1	0.19
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	3	0.19
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	6	0.19
(1,387)	1:3:A:ALA:HB1	1:3:A:ALA:H	6	0.19
(1,387)	1:3:A:ALA:HB2	1:3:A:ALA:H	6	0.19
(1,387)	1:3:A:ALA:HB3	1:3:A:ALA:H	6	0.19
(1,365)	1:37:A:GLU:HA	1:37:A:GLU:HG2	2	0.19
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	4	0.19
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	5	0.19
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	7	0.19
(1,319)	1:8:A:ASP:HA	1:9:A:ILE:H	10	0.19
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	7	0.19
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	9	0.19
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	9	0.19
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	5	0.19
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	5	0.19
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	5	0.19
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	2	0.19
(1,271)	1:31:A:TYR:HB3	1:31:A:TYR:HA	1	0.19
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	1	0.19
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD1	3	0.19
(1,266)	1:48:A:PHE:HA	1:48:A:PHE:HD2	3	0.19
(1,253)	1:40:A:SER:HA	1:41:A:THR:H	2	0.19
(1,236)	1:52:A:GLN:HB2	1:52:A:GLN:H	9	0.19
(1,214)	1:66:A:SER:HA	1:67:A:ARG:H	3	0.19
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	4	0.19
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	4	0.19
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	4	0.19
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	7	0.19
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	7	0.19
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	7	0.19
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	1	0.19
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	1	0.19
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	1	0.19
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	2	0.19
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	2	0.19
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	2	0.19
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	6	0.19
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	6	0.19
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	6	0.19
(1,146)	1:63:A:LEU:HB3	1:63:A:LEU:HG	10	0.19
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	5	0.19
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	5	0.19
(1,111)	1:64:A:GLU:HA	1:65:A:ALA:H	9	0.19
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	5	0.19
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	2	0.19
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE1	6	0.19
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE2	6	0.19
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	6	0.19
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	6	0.19
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	6	0.19
(1,41)	1:69:A:ALA:HB1	1:69:A:ALA:H	6	0.19
(1,41)	1:69:A:ALA:HB2	1:69:A:ALA:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:69:A:ALA:HB3	1:69:A:ALA:H	6	0.19
(1,36)	1:52:A:GLN:HB3	1:52:A:GLN:H	10	0.19
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	10	0.19
(1,22)	1:55:A:ALA:HA	1:55:A:ALA:H	5	0.19
(1,22)	1:55:A:ALA:HA	1:55:A:ALA:H	9	0.19
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	6	0.19
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	8	0.19
(1,14)	1:14:A:LEU:HA	1:14:A:LEU:H	1	0.19
(1,1)	1:15:A:ALA:HB1	1:16:A:PRO:HB2	9	0.19
(1,1)	1:15:A:ALA:HB2	1:16:A:PRO:HB2	9	0.19
(1,1)	1:15:A:ALA:HB3	1:16:A:PRO:HB2	9	0.19
(4,50)	1:25:A:ALA:N	1:21:A:PHE:O	6	0.18
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	2	0.18
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	4	0.18
(4,38)	1:14:A:LEU:N	1:39:A:ARG:O	2	0.18
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	4	0.18
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	1	0.18
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	3	0.18
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	7	0.18
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	9	0.18
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	10	0.18
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	6	0.18
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	1	0.18
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	10	0.18
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	2	0.18
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	4	0.18
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	9	0.18
(3,29)	1:47:A:ARG:HG2	1:47:A:ARG:HD2	8	0.18
(3,29)	1:47:A:ARG:HG3	1:47:A:ARG:HD2	8	0.18
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	8	0.18
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	8	0.18
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	5	0.18
(2,479)	1:76:A:GLN:H	1:76:A:GLN:HA	7	0.18
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD11	4	0.18
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD12	4	0.18
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD13	4	0.18
(2,420)	1:72:A:SER:H	1:72:A:SER:HB2	7	0.18
(2,420)	1:72:A:SER:H	1:72:A:SER:HB3	7	0.18
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	7	0.18
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	5	0.18
(2,378)	1:49:A:ASP:H	1:49:A:ASP:HB2	10	0.18
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	3	0.18
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	10	0.18
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	5	0.18
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	5	0.18
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	5	0.18
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	5	0.18
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	6	0.18
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	2	0.18
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	4	0.18
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	8	0.18
(2,250)	1:55:A:ALA:H	1:54:A:LEU:HG	6	0.18
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD11	5	0.18
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD12	5	0.18
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD13	5	0.18
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	2	0.18
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	5	0.18
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	6	0.18
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	7	0.18
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	2	0.18
(2,228)	1:60:A:GLY:H	1:60:A:GLY:HA2	5	0.18
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	4	0.18
(2,223)	1:28:A:LEU:H	1:27:A:ILE:HB	9	0.18
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	8	0.18
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	9	0.18
(2,207)	1:44:A:LEU:H	1:44:A:LEU:HG	9	0.18
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD21	3	0.18
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD22	3	0.18
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD23	3	0.18
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	6	0.18
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	1	0.18
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	8	0.18
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	1	0.18
(2,54)	1:38:A:GLY:H	1:39:A:ARG:HA	2	0.18
(2,53)	1:38:A:GLY:H	1:37:A:GLU:HG3	3	0.18
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	8	0.18
(2,10)	1:30:A:SER:H	1:74:A:SER:HA	5	0.18
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	6	0.18
(1,445)	1:74:A:SER:HA	1:30:A:SER:H	8	0.18
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	2	0.18
(1,418)	1:29:A:LEU:HB3	1:29:A:LEU:HA	2	0.18
(1,418)	1:29:A:LEU:HB3	1:29:A:LEU:HA	3	0.18
(1,418)	1:29:A:LEU:HB3	1:29:A:LEU:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	5	0.18
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	5	0.18
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	8	0.18
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	1	0.18
(1,343)	1:63:A:LEU:HD11	1:77:A:ALA:HA	1	0.18
(1,343)	1:63:A:LEU:HD12	1:77:A:ALA:HA	1	0.18
(1,343)	1:63:A:LEU:HD13	1:77:A:ALA:HA	1	0.18
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	4	0.18
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	4	0.18
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	4	0.18
(1,329)	1:72:A:SER:HB3	1:72:A:SER:HA	5	0.18
(1,329)	1:72:A:SER:HB3	1:72:A:SER:HA	8	0.18
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	1	0.18
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	1	0.18
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	3	0.18
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	3	0.18
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	8	0.18
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	8	0.18
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	1	0.18
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	1	0.18
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	1	0.18
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	10	0.18
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	10	0.18
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	10	0.18
(1,303)	1:78:A:SER:HA	1:78:A:SER:HB2	1	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	1	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	1	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	1	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	2	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	2	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	2	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	3	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	3	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	3	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	4	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	4	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	4	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	5	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	5	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	5	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	6	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	6	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	7	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	7	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	7	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	8	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	8	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	8	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	9	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	9	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	9	0.18
(1,281)	1:56:A:ILE:HD11	1:56:A:ILE:HG13	10	0.18
(1,281)	1:56:A:ILE:HD12	1:56:A:ILE:HG13	10	0.18
(1,281)	1:56:A:ILE:HD13	1:56:A:ILE:HG13	10	0.18
(1,265)	1:49:A:ASP:HA	1:4:A:GLN:HG2	3	0.18
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	4	0.18
(1,217)	1:27:A:ILE:HB	1:28:A:LEU:H	9	0.18
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.18
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.18
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.18
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	1	0.18
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	1	0.18
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	1	0.18
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	2	0.18
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	2	0.18
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	2	0.18
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	5	0.18
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	5	0.18
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	5	0.18
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	6	0.18
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	6	0.18
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	6	0.18
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	10	0.18
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	10	0.18
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	10	0.18
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	7	0.18
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	7	0.18
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	7	0.18
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	2	0.18
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	2	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	1	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	1	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	4	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	4	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	4	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	5	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	5	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	5	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	7	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	7	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	7	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB1	9	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB2	9	0.18
(1,148)	1:11:A:ALA:HA	1:11:A:ALA:HB3	9	0.18
(1,146)	1:63:A:LEU:HB3	1:63:A:LEU:HG	7	0.18
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	1	0.18
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	2	0.18
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	9	0.18
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	6	0.18
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	10	0.18
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	6	0.18
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	7	0.18
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	2	0.18
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	3	0.18
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	6	0.18
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE1	2	0.18
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE2	2	0.18
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	1	0.18
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	1	0.18
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	1	0.18
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	10	0.18
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	10	0.18
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	10	0.18
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD21	6	0.18
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD22	6	0.18
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD23	6	0.18
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD21	6	0.18
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD22	6	0.18
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD23	6	0.18
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD21	6	0.18
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD22	6	0.18
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD23	6	0.18
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	1	0.18
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:72:A:SER:HB2	1:72:A:SER:H	3	0.18
(1,47)	1:72:A:SER:HB3	1:72:A:SER:H	3	0.18
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB1	6	0.18
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB2	6	0.18
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB3	6	0.18
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	3	0.18
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	7	0.18
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	10	0.18
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	4	0.17
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	8	0.17
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	6	0.17
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	7	0.17
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	7	0.17
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	5	0.17
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	9	0.17
(4,1)	1:18:A:LEU:H	1:14:A:LEU:O	5	0.17
(2,489)	1:69:A:ALA:H	1:68:A:GLY:HA2	6	0.17
(2,468)	1:77:A:ALA:H	1:64:A:GLU:HG3	4	0.17
(2,466)	1:39:A:ARG:HE	1:39:A:ARG:HD2	10	0.17
(2,439)	1:66:A:SER:H	1:65:A:ALA:HB1	9	0.17
(2,439)	1:66:A:SER:H	1:65:A:ALA:HB2	9	0.17
(2,439)	1:66:A:SER:H	1:65:A:ALA:HB3	9	0.17
(2,422)	1:76:A:GLN:H	1:75:A:LEU:HA	10	0.17
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	4	0.17
(2,390)	1:5:A:ALA:H	1:4:A:GLN:HA	6	0.17
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	10	0.17
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	2	0.17
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	7	0.17
(2,379)	1:45:A:ALA:H	1:46:A:GLY:H	1	0.17
(2,376)	1:28:A:LEU:H	1:27:A:ILE:HG13	5	0.17
(2,368)	1:64:A:GLU:H	1:63:A:LEU:HA	1	0.17
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	6	0.17
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	6	0.17
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	6	0.17
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	8	0.17
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	8	0.17
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	8	0.17
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	8	0.17
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	6	0.17
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	9	0.17
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	5	0.17
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	5	0.17
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	10	0.17
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	10	0.17
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	10	0.17
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	4	0.17
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	4	0.17
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	3	0.17
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB1	4	0.17
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB2	4	0.17
(2,264)	1:20:A:HIS:H	1:19:A:ALA:HB3	4	0.17
(2,263)	1:42:A:SER:H	1:42:A:SER:HA	10	0.17
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	1	0.17
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	3	0.17
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	3	0.17
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	6	0.17
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	7	0.17
(2,228)	1:60:A:GLY:H	1:60:A:GLY:HA2	3	0.17
(2,228)	1:60:A:GLY:H	1:60:A:GLY:HA2	4	0.17
(2,228)	1:60:A:GLY:H	1:60:A:GLY:HA2	10	0.17
(2,227)	1:19:A:ALA:H	1:16:A:PRO:HB2	9	0.17
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	1	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	3	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	3	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	3	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	7	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	7	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	7	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	9	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	9	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	9	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	10	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	10	0.17
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	10	0.17
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	10	0.17
(2,172)	1:48:A:PHE:H	1:47:A:ARG:HG2	8	0.17
(2,126)	1:64:A:GLU:H	1:63:A:LEU:HD21	6	0.17
(2,126)	1:64:A:GLU:H	1:63:A:LEU:HD22	6	0.17
(2,126)	1:64:A:GLU:H	1:63:A:LEU:HD23	6	0.17
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	3	0.17
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	5	0.17
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	6	0.17
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD21	5	0.17
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD22	5	0.17
(2,98)	1:43:A:GLY:H	1:57:A:LEU:HD23	5	0.17
(2,38)	1:50:A:ILE:H	1:49:A:ASP:HB2	10	0.17
(2,31)	1:37:A:GLU:H	1:37:A:GLU:HG3	5	0.17
(2,29)	1:14:A:LEU:H	1:13:A:PRO:HB2	6	0.17
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	3	0.17
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	3	0.17
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	3	0.17
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	4	0.17
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	6	0.17
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	9	0.17
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	10	0.17
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	9	0.17
(1,483)	1:64:A:GLU:HB3	1:64:A:GLU:HA	3	0.17
(1,479)	1:18:A:LEU:HD11	1:18:A:LEU:HA	8	0.17
(1,479)	1:18:A:LEU:HD12	1:18:A:LEU:HA	8	0.17
(1,479)	1:18:A:LEU:HD13	1:18:A:LEU:HA	8	0.17
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	6	0.17
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	6	0.17
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	9	0.17
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	9	0.17
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	3	0.17
(1,448)	1:14:A:LEU:HD11	1:18:A:LEU:HG	6	0.17
(1,448)	1:14:A:LEU:HD12	1:18:A:LEU:HG	6	0.17
(1,448)	1:14:A:LEU:HD13	1:18:A:LEU:HG	6	0.17
(1,448)	1:14:A:LEU:HD11	1:18:A:LEU:HG	7	0.17
(1,448)	1:14:A:LEU:HD12	1:18:A:LEU:HG	7	0.17
(1,448)	1:14:A:LEU:HD13	1:18:A:LEU:HG	7	0.17
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	4	0.17
(1,442)	1:18:A:LEU:HA	1:18:A:LEU:HB3	9	0.17
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	9	0.17
(1,418)	1:29:A:LEU:HB3	1:29:A:LEU:HA	4	0.17
(1,418)	1:29:A:LEU:HB3	1:29:A:LEU:HA	6	0.17
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	10	0.17
(1,347)	1:65:A:ALA:HA	1:66:A:SER:H	9	0.17
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	1	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	1	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	1	0.17
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	3	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	3	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	5	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	5	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	5	0.17
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	6	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	6	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	6	0.17
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	7	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	7	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	7	0.17
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	8	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	8	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	8	0.17
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	9	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	9	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	9	0.17
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	10	0.17
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	10	0.17
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	10	0.17
(1,329)	1:72:A:SER:HB3	1:72:A:SER:HA	6	0.17
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	10	0.17
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	10	0.17
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	4	0.17
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	4	0.17
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	4	0.17
(1,304)	1:14:A:LEU:HD11	1:36:A:THR:HA	9	0.17
(1,304)	1:14:A:LEU:HD12	1:36:A:THR:HA	9	0.17
(1,304)	1:14:A:LEU:HD13	1:36:A:THR:HA	9	0.17
(1,300)	1:4:A:GLN:HA	1:5:A:ALA:H	6	0.17
(1,297)	1:37:A:GLU:HG3	1:37:A:GLU:H	5	0.17
(1,283)	1:39:A:ARG:HD3	1:39:A:ARG:HB3	1	0.17
(1,268)	1:13:A:PRO:HD3	1:13:A:PRO:HA	2	0.17
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	5	0.17
(1,253)	1:40:A:SER:HA	1:41:A:THR:H	4	0.17
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	9	0.17
(1,203)	1:49:A:ASP:HB2	1:49:A:ASP:HA	7	0.17
(1,186)	1:71:A:ALA:HB1	1:71:A:ALA:HA	8	0.17
(1,186)	1:71:A:ALA:HB2	1:71:A:ALA:HA	8	0.17
(1,186)	1:71:A:ALA:HB3	1:71:A:ALA:HA	8	0.17
(1,181)	1:75:A:LEU:HA	1:76:A:GLN:H	10	0.17
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	2	0.17
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	2	0.17
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:32:A:PRO:HD3	1:31:A:TYR:HA	8	0.17
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	7	0.17
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	7	0.17
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	7	0.17
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	4	0.17
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	10	0.17
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	3	0.17
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	10	0.17
(1,88)	1:63:A:LEU:HA	1:64:A:GLU:H	1	0.17
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	3	0.17
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	4	0.17
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	4	0.17
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	4	0.17
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB1	10	0.17
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB2	10	0.17
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB3	10	0.17
(1,22)	1:55:A:ALA:HA	1:55:A:ALA:H	4	0.17
(1,22)	1:55:A:ALA:HA	1:55:A:ALA:H	10	0.17
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	2	0.17
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	5	0.17
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	9	0.17
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	9	0.17
(1,1)	1:15:A:ALA:HB1	1:16:A:PRO:HB2	3	0.17
(1,1)	1:15:A:ALA:HB2	1:16:A:PRO:HB2	3	0.17
(1,1)	1:15:A:ALA:HB3	1:16:A:PRO:HB2	3	0.17
(4,44)	1:17:A:ALA:N	1:14:A:LEU:O	6	0.16
(4,42)	1:43:A:GLY:N	1:41:A:THR:OG1	7	0.16
(4,38)	1:14:A:LEU:N	1:39:A:ARG:O	3	0.16
(4,38)	1:14:A:LEU:N	1:39:A:ARG:O	10	0.16
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	4	0.16
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	7	0.16
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	2	0.16
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	4	0.16
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	5	0.16
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	10	0.16
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	5	0.16
(4,10)	1:55:A:ALA:N	1:51:A:ASP:O	1	0.16
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	7	0.16
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	6	0.16
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	6	0.16
(2,466)	1:39:A:ARG:HE	1:39:A:ARG:HD2	7	0.16
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:74:A:SER:H	1:73:A:TYR:HA	9	0.16
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	9	0.16
(2,277)	1:45:A:ALA:H	1:44:A:LEU:HB2	1	0.16
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	3	0.16
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	3	0.16
(2,250)	1:55:A:ALA:H	1:54:A:LEU:HG	1	0.16
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	4	0.16
(2,229)	1:53:A:GLY:H	1:52:A:GLN:H	1	0.16
(2,228)	1:60:A:GLY:H	1:60:A:GLY:HA2	1	0.16
(2,228)	1:60:A:GLY:H	1:60:A:GLY:HA2	2	0.16
(2,227)	1:19:A:ALA:H	1:16:A:PRO:HB2	6	0.16
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	8	0.16
(2,226)	1:19:A:ALA:H	1:18:A:LEU:HA	10	0.16
(2,224)	1:19:A:ALA:H	1:18:A:LEU:HB2	4	0.16
(2,219)	1:23:A:GLN:H	1:20:A:HIS:HA	5	0.16
(2,211)	1:58:A:LEU:H	1:59:A:ALA:H	9	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	1	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	1	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	1	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	2	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	2	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	2	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	4	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	4	0.16
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	4	0.16
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	8	0.16
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	1	0.16
(2,181)	1:67:A:ARG:H	1:66:A:SER:HA	8	0.16
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD21	7	0.16
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD22	7	0.16
(2,163)	1:65:A:ALA:H	1:75:A:LEU:HD23	7	0.16
(2,152)	1:12:A:GLY:H	1:40:A:SER:HB2	4	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	2	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	3	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	4	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	5	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	6	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	7	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	8	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	9	0.16
(2,133)	1:46:A:GLY:H	1:46:A:GLY:HA2	10	0.16
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,104)	1:43:A:GLY:H	1:41:A:THR:HG1	8	0.16
(2,92)	1:3:A:ALA:H	1:4:A:GLN:HA	6	0.16
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	3	0.16
(2,29)	1:14:A:LEU:H	1:13:A:PRO:HB2	2	0.16
(2,29)	1:14:A:LEU:H	1:13:A:PRO:HB2	3	0.16
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD11	9	0.16
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD12	9	0.16
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD13	9	0.16
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	1	0.16
(2,18)	1:78:A:SER:H	1:78:A:SER:HA	5	0.16
(2,16)	1:36:A:THR:H	1:35:A:LEU:H	10	0.16
(1,452)	1:66:A:SER:HA	1:66:A:SER:HB2	3	0.16
(1,452)	1:66:A:SER:HA	1:66:A:SER:HB2	10	0.16
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	2	0.16
(1,424)	1:40:A:SER:HB3	1:41:A:THR:H	2	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	1	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	1	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	2	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	2	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	4	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	4	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	7	0.16
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	7	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	2	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	3	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	4	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	5	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	6	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	7	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	8	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	9	0.16
(1,355)	1:46:A:GLY:HA2	1:46:A:GLY:H	10	0.16
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	8	0.16
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	10	0.16
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	5	0.16
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	5	0.16
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	5	0.16
(1,341)	1:34:A:ALA:HB1	1:34:A:ALA:HA	2	0.16
(1,341)	1:34:A:ALA:HB2	1:34:A:ALA:HA	2	0.16
(1,341)	1:34:A:ALA:HB3	1:34:A:ALA:HA	2	0.16
(1,340)	1:38:A:GLY:HA2	1:38:A:GLY:H	4	0.16
(1,338)	1:28:A:LEU:HB2	1:28:A:LEU:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	6	0.16
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	6	0.16
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	6	0.16
(1,277)	1:50:A:ILE:HD11	1:26:A:HIS:HB3	4	0.16
(1,277)	1:50:A:ILE:HD12	1:26:A:HIS:HB3	4	0.16
(1,277)	1:50:A:ILE:HD13	1:26:A:HIS:HB3	4	0.16
(1,274)	1:16:A:PRO:HD2	1:15:A:ALA:HB1	8	0.16
(1,274)	1:16:A:PRO:HD2	1:15:A:ALA:HB2	8	0.16
(1,274)	1:16:A:PRO:HD2	1:15:A:ALA:HB3	8	0.16
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG21	8	0.16
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG22	8	0.16
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG23	8	0.16
(1,240)	1:44:A:LEU:HD21	1:56:A:ILE:HB	1	0.16
(1,240)	1:44:A:LEU:HD22	1:56:A:ILE:HB	1	0.16
(1,240)	1:44:A:LEU:HD23	1:56:A:ILE:HB	1	0.16
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	1	0.16
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	3	0.16
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	1	0.16
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	1	0.16
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	1	0.16
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	2	0.16
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	2	0.16
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	2	0.16
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	3	0.16
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	3	0.16
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	3	0.16
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	6	0.16
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	6	0.16
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	6	0.16
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	7	0.16
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	7	0.16
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	7	0.16
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	8	0.16
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	8	0.16
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	8	0.16
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	10	0.16
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	10	0.16
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	10	0.16
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	7	0.16
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	7	0.16
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	7	0.16
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	9	0.16
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	9	0.16
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	3	0.16
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	3	0.16
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	3	0.16
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	4	0.16
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	4	0.16
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	4	0.16
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	6	0.16
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	6	0.16
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	6	0.16
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	8	0.16
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	8	0.16
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	8	0.16
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	9	0.16
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	9	0.16
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	9	0.16
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	10	0.16
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	10	0.16
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	10	0.16
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	9	0.16
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	9	0.16
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	9	0.16
(1,111)	1:64:A:GLU:HA	1:65:A:ALA:H	5	0.16
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	2	0.16
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	5	0.16
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	8	0.16
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	1	0.16
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	10	0.16
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE1	8	0.16
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE2	8	0.16
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB1	10	0.16
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB2	10	0.16
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB3	10	0.16
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB1	10	0.16
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB2	10	0.16
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB3	10	0.16
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB1	10	0.16
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB2	10	0.16
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB3	10	0.16
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	1	0.16
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:15:A:ALA:HB1	1:16:A:PRO:HB2	7	0.16
(1,1)	1:15:A:ALA:HB2	1:16:A:PRO:HB2	7	0.16
(1,1)	1:15:A:ALA:HB3	1:16:A:PRO:HB2	7	0.16
(4,38)	1:14:A:LEU:N	1:39:A:ARG:O	9	0.15
(4,37)	1:14:A:LEU:H	1:39:A:ARG:O	8	0.15
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	3	0.15
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	6	0.15
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	2	0.15
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	8	0.15
(4,16)	1:46:A:GLY:N	1:7:A:PHE:O	7	0.15
(2,473)	1:78:A:SER:H	1:63:A:LEU:HA	10	0.15
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD11	6	0.15
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD12	6	0.15
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD13	6	0.15
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	4	0.15
(2,419)	1:72:A:SER:H	1:70:A:ASN:HA	10	0.15
(2,418)	1:5:A:ALA:H	1:49:A:ASP:HA	1	0.15
(2,409)	1:21:A:PHE:H	1:18:A:LEU:HA	4	0.15
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	2	0.15
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	7	0.15
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	4	0.15
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	3	0.15
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	9	0.15
(2,382)	1:43:A:GLY:H	1:57:A:LEU:HA	9	0.15
(2,380)	1:52:A:GLN:H	1:52:A:GLN:HB3	2	0.15
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	1	0.15
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	1	0.15
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	1	0.15
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	7	0.15
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	7	0.15
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	7	0.15
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	4	0.15
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	1	0.15
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	2	0.15
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	6	0.15
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	6	0.15
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD11	7	0.15
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD12	7	0.15
(2,296)	1:8:A:ASP:H	1:9:A:ILE:HD13	7	0.15
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	2	0.15
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	2	0.15
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	6	0.15
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	6	0.15
(2,240)	1:72:A:SER:H	1:72:A:SER:HA	9	0.15
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	5	0.15
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	5	0.15
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	5	0.15
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD21	6	0.15
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD22	6	0.15
(2,210)	1:44:A:LEU:H	1:44:A:LEU:HD23	6	0.15
(2,188)	1:67:A:ARG:H	1:67:A:ARG:HB2	7	0.15
(2,185)	1:74:A:SER:H	1:67:A:ARG:HA	4	0.15
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	4	0.15
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD21	7	0.15
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD22	7	0.15
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD23	7	0.15
(2,135)	1:58:A:LEU:H	1:57:A:LEU:H	4	0.15
(2,121)	1:47:A:ARG:HE	1:47:A:ARG:HD2	4	0.15
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	5	0.15
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	9	0.15
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	2	0.15
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	3	0.15
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	4	0.15
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	6	0.15
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	2	0.15
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	4	0.15
(2,54)	1:38:A:GLY:H	1:39:A:ARG:HA	7	0.15
(1,452)	1:66:A:SER:HA	1:66:A:SER:HB2	4	0.15
(1,452)	1:66:A:SER:HA	1:66:A:SER:HB2	5	0.15
(1,452)	1:66:A:SER:HA	1:66:A:SER:HB2	7	0.15
(1,452)	1:66:A:SER:HA	1:66:A:SER:HB2	8	0.15
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	4	0.15
(1,441)	1:34:A:ALA:HA	1:34:A:ALA:H	7	0.15
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	3	0.15
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	5	0.15
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	6	0.15
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	7	0.15
(1,418)	1:29:A:LEU:HB3	1:29:A:LEU:HA	10	0.15
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	10	0.15
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	10	0.15
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	3	0.15
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	2	0.15
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	5	0.15
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	7	0.15
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	7	0.15
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	7	0.15
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	8	0.15
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	8	0.15
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	8	0.15
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	10	0.15
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	10	0.15
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	10	0.15
(1,320)	1:74:A:SER:HA	1:74:A:SER:HB2	5	0.15
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	2	0.15
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	2	0.15
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG21	2	0.15
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG22	2	0.15
(1,311)	1:41:A:THR:HB	1:61:A:THR:HG23	2	0.15
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	8	0.15
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	10	0.15
(1,304)	1:14:A:LEU:HD11	1:36:A:THR:HA	3	0.15
(1,304)	1:14:A:LEU:HD12	1:36:A:THR:HA	3	0.15
(1,304)	1:14:A:LEU:HD13	1:36:A:THR:HA	3	0.15
(1,296)	1:27:A:ILE:HG13	1:27:A:ILE:H	1	0.15
(1,268)	1:13:A:PRO:HD3	1:13:A:PRO:HA	6	0.15
(1,224)	1:27:A:ILE:HA	1:27:A:ILE:HG12	6	0.15
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	4	0.15
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	4	0.15
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	4	0.15
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	5	0.15
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	5	0.15
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	5	0.15
(1,219)	1:55:A:ALA:HB1	1:55:A:ALA:HA	9	0.15
(1,219)	1:55:A:ALA:HB2	1:55:A:ALA:HA	9	0.15
(1,219)	1:55:A:ALA:HB3	1:55:A:ALA:HA	9	0.15
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.15
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.15
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.15
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD11	1	0.15
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD12	1	0.15
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD13	1	0.15
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD11	1	0.15
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD12	1	0.15
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD13	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD11	1	0.15
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD12	1	0.15
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD13	1	0.15
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	5	0.15
(1,171)	1:55:A:ALA:HB1	1:55:A:ALA:H	5	0.15
(1,171)	1:55:A:ALA:HB2	1:55:A:ALA:H	5	0.15
(1,171)	1:55:A:ALA:HB3	1:55:A:ALA:H	5	0.15
(1,167)	1:54:A:LEU:HB3	1:51:A:ASP:HA	10	0.15
(1,133)	1:73:A:TYR:HA	1:74:A:SER:H	8	0.15
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	4	0.15
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	10	0.15
(1,100)	1:35:A:LEU:HA	1:35:A:LEU:H	3	0.15
(1,95)	1:63:A:LEU:HA	1:78:A:SER:H	10	0.15
(1,63)	1:35:A:LEU:HD11	1:35:A:LEU:HB2	7	0.15
(1,63)	1:35:A:LEU:HD12	1:35:A:LEU:HB2	7	0.15
(1,63)	1:35:A:LEU:HD13	1:35:A:LEU:HB2	7	0.15
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD21	8	0.15
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD22	8	0.15
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD23	8	0.15
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD21	8	0.15
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD22	8	0.15
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD23	8	0.15
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD21	8	0.15
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD22	8	0.15
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD23	8	0.15
(1,36)	1:52:A:GLN:HB3	1:52:A:GLN:H	2	0.15
(1,32)	1:67:A:ARG:HA	1:67:A:ARG:HB2	9	0.15
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	4	0.15
(1,22)	1:55:A:ALA:HA	1:55:A:ALA:H	7	0.15
(1,20)	1:5:A:ALA:HA	1:5:A:ALA:H	4	0.15
(4,38)	1:14:A:LEU:N	1:39:A:ARG:O	7	0.14
(4,36)	1:41:A:THR:N	1:12:A:GLY:O	8	0.14
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	2	0.14
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	3	0.14
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	1	0.14
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	2	0.14
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	8	0.14
(4,26)	1:48:A:PHE:N	1:5:A:ALA:O	6	0.14
(4,16)	1:46:A:GLY:N	1:7:A:PHE:O	10	0.14
(4,5)	1:27:A:ILE:H	1:22:A:GLY:O	5	0.14
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	8	0.14
(4,2)	1:18:A:LEU:N	1:14:A:LEU:O	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	1:29:A:LEU:HB3	1:31:A:TYR:HE2	6	0.14
(2,409)	1:21:A:PHE:H	1:18:A:LEU:HA	7	0.14
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	3	0.14
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	8	0.14
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	3	0.14
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	4	0.14
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	6	0.14
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	3	0.14
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	6	0.14
(2,385)	1:14:A:LEU:H	1:15:A:ALA:H	6	0.14
(2,382)	1:43:A:GLY:H	1:57:A:LEU:HA	3	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	3	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	3	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	3	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	10	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	10	0.14
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	10	0.14
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	6	0.14
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	9	0.14
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	3	0.14
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	4	0.14
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	8	0.14
(2,320)	1:71:A:ALA:H	1:70:A:ASN:HA	1	0.14
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	8	0.14
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	8	0.14
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	8	0.14
(2,224)	1:19:A:ALA:H	1:18:A:LEU:HB2	7	0.14
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD21	5	0.14
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD22	5	0.14
(2,193)	1:28:A:LEU:H	1:28:A:LEU:HD23	5	0.14
(2,184)	1:68:A:GLY:H	1:67:A:ARG:HA	3	0.14
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	4	0.14
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	8	0.14
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	3	0.14
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	6	0.14
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	7	0.14
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	8	0.14
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	9	0.14
(2,90)	1:49:A:ASP:H	1:51:A:ASP:HB2	7	0.14
(2,87)	1:4:A:GLN:H	1:3:A:ALA:HB1	9	0.14
(2,87)	1:4:A:GLN:H	1:3:A:ALA:HB2	9	0.14
(2,87)	1:4:A:GLN:H	1:3:A:ALA:HB3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	8	0.14
(2,81)	1:26:A:HIS:H	1:25:A:ALA:HB1	5	0.14
(2,81)	1:26:A:HIS:H	1:25:A:ALA:HB2	5	0.14
(2,81)	1:26:A:HIS:H	1:25:A:ALA:HB3	5	0.14
(2,48)	1:72:A:SER:H	1:70:A:ASN:HB3	9	0.14
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD11	4	0.14
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD12	4	0.14
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD13	4	0.14
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB2	9	0.14
(2,23)	1:7:A:PHE:H	1:7:A:PHE:HB3	9	0.14
(1,484)	1:29:A:LEU:HA	1:30:A:SER:H	7	0.14
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	8	0.14
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	8	0.14
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD1	10	0.14
(1,476)	1:31:A:TYR:HB2	1:31:A:TYR:HD2	10	0.14
(1,452)	1:66:A:SER:HA	1:66:A:SER:HB2	9	0.14
(1,447)	1:61:A:THR:HA	1:61:A:THR:HB	6	0.14
(1,447)	1:61:A:THR:HA	1:61:A:THR:HB	7	0.14
(1,447)	1:61:A:THR:HA	1:61:A:THR:HB	8	0.14
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	4	0.14
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	9	0.14
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	9	0.14
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD11	3	0.14
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD12	3	0.14
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD13	3	0.14
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD11	8	0.14
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD12	8	0.14
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD13	8	0.14
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	1	0.14
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD21	6	0.14
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD22	6	0.14
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD23	6	0.14
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	1	0.14
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	6	0.14
(1,350)	1:28:A:LEU:HA	1:29:A:LEU:H	7	0.14
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	2	0.14
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	2	0.14
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	2	0.14
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	3	0.14
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	3	0.14
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	3	0.14
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	4	0.14
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	4	0.14
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	6	0.14
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	6	0.14
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	6	0.14
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB2	4	0.14
(1,318)	1:23:A:GLN:HA	1:23:A:GLN:HB3	4	0.14
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	2	0.14
(1,253)	1:40:A:SER:HA	1:41:A:THR:H	7	0.14
(1,245)	1:70:A:ASN:HA	1:70:A:ASN:H	3	0.14
(1,233)	1:6:A:ASP:HB2	1:6:A:ASP:H	1	0.14
(1,231)	1:14:A:LEU:HB3	1:14:A:LEU:H	4	0.14
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD21	10	0.14
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD22	10	0.14
(1,227)	1:77:A:ALA:HB1	1:35:A:LEU:HD23	10	0.14
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD21	10	0.14
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD22	10	0.14
(1,227)	1:77:A:ALA:HB2	1:35:A:LEU:HD23	10	0.14
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD21	10	0.14
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD22	10	0.14
(1,227)	1:77:A:ALA:HB3	1:35:A:LEU:HD23	10	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	1	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	2	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	3	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	4	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	5	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	6	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	7	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	8	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	9	0.14
(1,205)	1:6:A:ASP:HB3	1:6:A:ASP:HB2	10	0.14
(1,113)	1:41:A:THR:HA	1:42:A:SER:H	7	0.14
(1,111)	1:64:A:GLU:HA	1:65:A:ALA:H	1	0.14
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD11	3	0.14
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD12	3	0.14
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD13	3	0.14
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD21	3	0.14
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD22	3	0.14
(1,105)	1:73:A:TYR:HB3	1:29:A:LEU:HD23	3	0.14
(1,87)	1:63:A:LEU:HD21	1:64:A:GLU:H	2	0.14
(1,87)	1:63:A:LEU:HD22	1:64:A:GLU:H	2	0.14
(1,87)	1:63:A:LEU:HD23	1:64:A:GLU:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:63:A:LEU:HD21	1:64:A:GLU:H	5	0.14
(1,87)	1:63:A:LEU:HD22	1:64:A:GLU:H	5	0.14
(1,87)	1:63:A:LEU:HD23	1:64:A:GLU:H	5	0.14
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	1	0.14
(1,84)	1:58:A:LEU:HA	1:58:A:LEU:H	10	0.14
(1,73)	1:76:A:GLN:HA	1:77:A:ALA:H	2	0.14
(1,71)	1:32:A:PRO:HD2	1:35:A:LEU:HB2	8	0.14
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE1	10	0.14
(1,65)	1:73:A:TYR:HB2	1:73:A:TYR:HE2	10	0.14
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD21	3	0.14
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD22	3	0.14
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD23	3	0.14
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD21	3	0.14
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD22	3	0.14
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD23	3	0.14
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD21	3	0.14
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD22	3	0.14
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD23	3	0.14
(1,49)	1:74:A:SER:HB2	1:75:A:LEU:H	7	0.14
(1,49)	1:74:A:SER:HB3	1:75:A:LEU:H	7	0.14
(1,46)	1:73:A:TYR:HA	1:68:A:GLY:H	2	0.14
(1,46)	1:73:A:TYR:HA	1:68:A:GLY:H	7	0.14
(1,24)	1:67:A:ARG:HA	1:68:A:GLY:H	3	0.14
(1,3)	1:79:A:ALA:HB1	1:79:A:ALA:H	6	0.14
(1,3)	1:79:A:ALA:HB2	1:79:A:ALA:H	6	0.14
(1,3)	1:79:A:ALA:HB3	1:79:A:ALA:H	6	0.14
(4,38)	1:14:A:LEU:N	1:39:A:ARG:O	4	0.13
(4,38)	1:14:A:LEU:N	1:39:A:ARG:O	8	0.13
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	2	0.13
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	2	0.13
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	3	0.13
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	4	0.13
(4,1)	1:18:A:LEU:H	1:14:A:LEU:O	10	0.13
(3,12)	1:32:A:PRO:HG2	1:32:A:PRO:HD2	8	0.13
(3,12)	1:32:A:PRO:HG3	1:32:A:PRO:HD2	8	0.13
(3,12)	1:32:A:PRO:HG2	1:32:A:PRO:HD2	9	0.13
(3,12)	1:32:A:PRO:HG3	1:32:A:PRO:HD2	9	0.13
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	5	0.13
(3,4)	1:30:A:SER:HB2	1:30:A:SER:H	5	0.13
(3,4)	1:30:A:SER:HB3	1:30:A:SER:H	5	0.13
(2,489)	1:69:A:ALA:H	1:68:A:GLY:HA2	7	0.13
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD11	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD12	4	0.13
(2,464)	1:66:A:SER:H	1:75:A:LEU:HD13	4	0.13
(2,459)	1:66:A:SER:H	1:73:A:TYR:HB2	2	0.13
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	2	0.13
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	7	0.13
(2,409)	1:21:A:PHE:H	1:18:A:LEU:HA	1	0.13
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	5	0.13
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	5	0.13
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	9	0.13
(2,382)	1:43:A:GLY:H	1:57:A:LEU:HA	8	0.13
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	2	0.13
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	2	0.13
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	2	0.13
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	9	0.13
(2,339)	1:8:A:ASP:H	1:7:A:PHE:HA	1	0.13
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	2	0.13
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	8	0.13
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	3	0.13
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	3	0.13
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	3	0.13
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	7	0.13
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	7	0.13
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	7	0.13
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB2	2	0.13
(2,273)	1:76:A:GLN:H	1:76:A:GLN:HB3	2	0.13
(2,185)	1:74:A:SER:H	1:67:A:ARG:HA	10	0.13
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD11	6	0.13
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD12	6	0.13
(2,182)	1:41:A:THR:H	1:14:A:LEU:HD13	6	0.13
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	2	0.13
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	4	0.13
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	5	0.13
(2,101)	1:43:A:GLY:H	1:43:A:GLY:HA3	10	0.13
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	7	0.13
(2,53)	1:38:A:GLY:H	1:37:A:GLU:HG3	2	0.13
(2,48)	1:72:A:SER:H	1:70:A:ASN:HB3	4	0.13
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD11	5	0.13
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD12	5	0.13
(2,25)	1:14:A:LEU:H	1:14:A:LEU:HD13	5	0.13
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD11	5	0.13
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD12	5	0.13
(2,20)	1:78:A:SER:H	1:63:A:LEU:HD13	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:7:A:PHE:HB2	1:7:A:PHE:H	4	0.13
(1,484)	1:29:A:LEU:HA	1:30:A:SER:H	2	0.13
(1,483)	1:64:A:GLU:HB3	1:64:A:GLU:HA	2	0.13
(1,455)	1:19:A:ALA:HB1	1:20:A:HIS:H	6	0.13
(1,455)	1:19:A:ALA:HB2	1:20:A:HIS:H	6	0.13
(1,455)	1:19:A:ALA:HB3	1:20:A:HIS:H	6	0.13
(1,437)	1:18:A:LEU:HA	1:18:A:LEU:H	1	0.13
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	7	0.13
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	3	0.13
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	3	0.13
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	6	0.13
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	6	0.13
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB2	8	0.13
(1,414)	1:76:A:GLN:HA	1:76:A:GLN:HB3	8	0.13
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD11	10	0.13
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD12	10	0.13
(1,394)	1:58:A:LEU:HG	1:14:A:LEU:HD13	10	0.13
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD11	2	0.13
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD12	2	0.13
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD13	2	0.13
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	4	0.13
(1,354)	1:75:A:LEU:HD11	1:75:A:LEU:HB3	8	0.13
(1,354)	1:75:A:LEU:HD12	1:75:A:LEU:HB3	8	0.13
(1,354)	1:75:A:LEU:HD13	1:75:A:LEU:HB3	8	0.13
(1,345)	1:19:A:ALA:HB1	1:19:A:ALA:H	9	0.13
(1,345)	1:19:A:ALA:HB2	1:19:A:ALA:H	9	0.13
(1,345)	1:19:A:ALA:HB3	1:19:A:ALA:H	9	0.13
(1,340)	1:38:A:GLY:HA2	1:38:A:GLY:H	1	0.13
(1,340)	1:38:A:GLY:HA2	1:38:A:GLY:H	3	0.13
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD21	5	0.13
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD22	5	0.13
(1,335)	1:32:A:PRO:HD2	1:35:A:LEU:HD23	5	0.13
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	1	0.13
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	2	0.13
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	4	0.13
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	5	0.13
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	2	0.13
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	2	0.13
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	2	0.13
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	7	0.13
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	7	0.13
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:65:A:ALA:HB1	1:65:A:ALA:H	8	0.13
(1,307)	1:65:A:ALA:HB2	1:65:A:ALA:H	8	0.13
(1,307)	1:65:A:ALA:HB3	1:65:A:ALA:H	8	0.13
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	7	0.13
(1,237)	1:75:A:LEU:HB3	1:75:A:LEU:H	1	0.13
(1,232)	1:57:A:LEU:HD21	1:44:A:LEU:HD21	8	0.13
(1,232)	1:57:A:LEU:HD21	1:44:A:LEU:HD22	8	0.13
(1,232)	1:57:A:LEU:HD21	1:44:A:LEU:HD23	8	0.13
(1,232)	1:57:A:LEU:HD22	1:44:A:LEU:HD21	8	0.13
(1,232)	1:57:A:LEU:HD22	1:44:A:LEU:HD22	8	0.13
(1,232)	1:57:A:LEU:HD22	1:44:A:LEU:HD23	8	0.13
(1,232)	1:57:A:LEU:HD23	1:44:A:LEU:HD21	8	0.13
(1,232)	1:57:A:LEU:HD23	1:44:A:LEU:HD22	8	0.13
(1,232)	1:57:A:LEU:HD23	1:44:A:LEU:HD23	8	0.13
(1,218)	1:40:A:SER:HB2	1:41:A:THR:H	4	0.13
(1,214)	1:66:A:SER:HA	1:67:A:ARG:H	9	0.13
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.13
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.13
(1,202)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.13
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD11	8	0.13
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD12	8	0.13
(1,197)	1:28:A:LEU:HA	1:28:A:LEU:HD13	8	0.13
(1,183)	1:70:A:ASN:HA	1:71:A:ALA:H	4	0.13
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	5	0.13
(1,111)	1:64:A:GLU:HA	1:65:A:ALA:H	4	0.13
(1,103)	1:37:A:GLU:HB2	1:37:A:GLU:H	8	0.13
(1,87)	1:63:A:LEU:HD21	1:64:A:GLU:H	1	0.13
(1,87)	1:63:A:LEU:HD22	1:64:A:GLU:H	1	0.13
(1,87)	1:63:A:LEU:HD23	1:64:A:GLU:H	1	0.13
(1,87)	1:63:A:LEU:HD21	1:64:A:GLU:H	4	0.13
(1,87)	1:63:A:LEU:HD22	1:64:A:GLU:H	4	0.13
(1,87)	1:63:A:LEU:HD23	1:64:A:GLU:H	4	0.13
(1,78)	1:57:A:LEU:HD21	1:57:A:LEU:HB3	3	0.13
(1,78)	1:57:A:LEU:HD22	1:57:A:LEU:HB3	3	0.13
(1,78)	1:57:A:LEU:HD23	1:57:A:LEU:HB3	3	0.13
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB1	4	0.13
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB2	4	0.13
(1,23)	1:27:A:ILE:HG13	1:25:A:ALA:HB3	4	0.13
(1,6)	1:54:A:LEU:HB3	1:55:A:ALA:H	10	0.13
(4,33)	1:21:A:PHE:H	1:17:A:ALA:O	10	0.12
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	1	0.12
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	1	0.12
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	8	0.12
(4,15)	1:46:A:GLY:H	1:7:A:PHE:O	5	0.12
(4,15)	1:46:A:GLY:H	1:7:A:PHE:O	8	0.12
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	6	0.12
(3,12)	1:32:A:PRO:HG2	1:32:A:PRO:HD2	7	0.12
(3,12)	1:32:A:PRO:HG3	1:32:A:PRO:HD2	7	0.12
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	4	0.12
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	9	0.12
(2,466)	1:39:A:ARG:HE	1:39:A:ARG:HD2	2	0.12
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	3	0.12
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	5	0.12
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	9	0.12
(2,422)	1:76:A:GLN:H	1:75:A:LEU:HA	2	0.12
(2,419)	1:72:A:SER:H	1:70:A:ASN:HA	4	0.12
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	1	0.12
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	8	0.12
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	10	0.12
(2,371)	1:74:A:SER:H	1:73:A:TYR:HB2	5	0.12
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	5	0.12
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	5	0.12
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	5	0.12
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	9	0.12
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	9	0.12
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	9	0.12
(2,341)	1:21:A:PHE:H	1:17:A:ALA:HA	3	0.12
(2,332)	1:42:A:SER:H	1:41:A:THR:HG1	9	0.12
(2,313)	1:58:A:LEU:H	1:54:A:LEU:HA	3	0.12
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB1	6	0.12
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB2	6	0.12
(2,286)	1:5:A:ALA:H	1:5:A:ALA:HB3	6	0.12
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD21	5	0.12
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD22	5	0.12
(2,201)	1:76:A:GLN:H	1:75:A:LEU:HD23	5	0.12
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD21	6	0.12
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD22	6	0.12
(2,138)	1:57:A:LEU:H	1:44:A:LEU:HD23	6	0.12
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	6	0.12
(2,118)	1:11:A:ALA:H	1:10:A:PRO:HB3	1	0.12
(2,105)	1:43:A:GLY:H	1:43:A:GLY:HA2	10	0.12
(2,103)	1:43:A:GLY:H	1:11:A:ALA:HA	4	0.12
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:3:A:ALA:H	1:2:A:SER:HA	10	0.12
(2,57)	1:49:A:ASP:H	1:52:A:GLN:HB2	5	0.12
(2,46)	1:55:A:ALA:H	1:54:A:LEU:H	3	0.12
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD11	7	0.12
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD12	7	0.12
(2,40)	1:54:A:LEU:H	1:44:A:LEU:HD13	7	0.12
(2,8)	1:30:A:SER:H	1:74:A:SER:HB3	9	0.12
(1,493)	1:7:A:PHE:HB2	1:7:A:PHE:H	2	0.12
(1,493)	1:7:A:PHE:HB2	1:7:A:PHE:H	6	0.12
(1,483)	1:64:A:GLU:HB3	1:64:A:GLU:HA	4	0.12
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	5	0.12
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	5	0.12
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	5	0.12
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	8	0.12
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	8	0.12
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	8	0.12
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	10	0.12
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	10	0.12
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	10	0.12
(1,455)	1:19:A:ALA:HB1	1:20:A:HIS:H	3	0.12
(1,455)	1:19:A:ALA:HB2	1:20:A:HIS:H	3	0.12
(1,455)	1:19:A:ALA:HB3	1:20:A:HIS:H	3	0.12
(1,453)	1:49:A:ASP:HB2	1:49:A:ASP:H	4	0.12
(1,448)	1:14:A:LEU:HD11	1:18:A:LEU:HG	3	0.12
(1,448)	1:14:A:LEU:HD12	1:18:A:LEU:HG	3	0.12
(1,448)	1:14:A:LEU:HD13	1:18:A:LEU:HG	3	0.12
(1,440)	1:18:A:LEU:HA	1:21:A:PHE:HB2	8	0.12
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	4	0.12
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	5	0.12
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD11	7	0.12
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD12	7	0.12
(1,403)	1:39:A:ARG:HD3	1:63:A:LEU:HD13	7	0.12
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	2	0.12
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	5	0.12
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	6	0.12
(1,378)	1:27:A:ILE:HA	1:28:A:LEU:H	5	0.12
(1,372)	1:40:A:SER:HA	1:40:A:SER:HB2	10	0.12
(1,354)	1:75:A:LEU:HD11	1:75:A:LEU:HB3	2	0.12
(1,354)	1:75:A:LEU:HD12	1:75:A:LEU:HB3	2	0.12
(1,354)	1:75:A:LEU:HD13	1:75:A:LEU:HB3	2	0.12
(1,340)	1:38:A:GLY:HA2	1:38:A:GLY:H	9	0.12
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	6	0.12
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	7	0.12
(1,309)	1:17:A:ALA:HA	1:17:A:ALA:H	9	0.12
(1,303)	1:78:A:SER:HA	1:78:A:SER:HB2	8	0.12
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG21	3	0.12
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG22	3	0.12
(1,258)	1:41:A:THR:HA	1:61:A:THR:HG23	3	0.12
(1,253)	1:40:A:SER:HA	1:41:A:THR:H	3	0.12
(1,228)	1:39:A:ARG:HD3	1:38:A:GLY:HA3	3	0.12
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD11	5	0.12
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD12	5	0.12
(1,210)	1:41:A:THR:HB	1:14:A:LEU:HD13	5	0.12
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD11	6	0.12
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD12	6	0.12
(1,192)	1:17:A:ALA:HB1	1:14:A:LEU:HD13	6	0.12
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD11	6	0.12
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD12	6	0.12
(1,192)	1:17:A:ALA:HB2	1:14:A:LEU:HD13	6	0.12
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD11	6	0.12
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD12	6	0.12
(1,192)	1:17:A:ALA:HB3	1:14:A:LEU:HD13	6	0.12
(1,181)	1:75:A:LEU:HA	1:76:A:GLN:H	2	0.12
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB2	9	0.12
(1,152)	1:72:A:SER:HA	1:72:A:SER:HB3	9	0.12
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	1	0.12
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	1	0.12
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	1	0.12
(1,116)	1:41:A:THR:HA	1:41:A:THR:HB	10	0.12
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	8	0.12
(1,46)	1:73:A:TYR:HA	1:68:A:GLY:H	10	0.12
(1,3)	1:79:A:ALA:HB1	1:79:A:ALA:H	5	0.12
(1,3)	1:79:A:ALA:HB2	1:79:A:ALA:H	5	0.12
(1,3)	1:79:A:ALA:HB3	1:79:A:ALA:H	5	0.12
(1,1)	1:15:A:ALA:HB1	1:16:A:PRO:HB2	2	0.12
(1,1)	1:15:A:ALA:HB2	1:16:A:PRO:HB2	2	0.12
(1,1)	1:15:A:ALA:HB3	1:16:A:PRO:HB2	2	0.12
(4,47)	1:76:A:GLN:H	1:64:A:GLU:O	7	0.11
(4,39)	1:12:A:GLY:H	1:41:A:THR:O	6	0.11
(4,35)	1:41:A:THR:H	1:12:A:GLY:O	5	0.11
(4,32)	1:57:A:LEU:N	1:53:A:GLY:O	5	0.11
(4,30)	1:44:A:LEU:N	1:9:A:ILE:O	8	0.11
(4,27)	1:9:A:ILE:H	1:44:A:LEU:O	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,21)	1:59:A:ALA:H	1:56:A:ILE:O	1	0.11
(4,19)	1:58:A:LEU:H	1:54:A:LEU:O	3	0.11
(4,17)	1:54:A:LEU:H	1:50:A:ILE:O	5	0.11
(4,16)	1:46:A:GLY:N	1:7:A:PHE:O	5	0.11
(4,16)	1:46:A:GLY:N	1:7:A:PHE:O	6	0.11
(4,16)	1:46:A:GLY:N	1:7:A:PHE:O	9	0.11
(4,15)	1:46:A:GLY:H	1:7:A:PHE:O	7	0.11
(4,15)	1:46:A:GLY:H	1:7:A:PHE:O	9	0.11
(4,15)	1:46:A:GLY:H	1:7:A:PHE:O	10	0.11
(4,4)	1:53:A:GLY:N	1:49:A:ASP:O	7	0.11
(4,1)	1:18:A:LEU:H	1:14:A:LEU:O	8	0.11
(4,1)	1:18:A:LEU:H	1:14:A:LEU:O	9	0.11
(3,12)	1:32:A:PRO:HG2	1:32:A:PRO:HD2	2	0.11
(3,12)	1:32:A:PRO:HG3	1:32:A:PRO:HD2	2	0.11
(3,11)	1:78:A:SER:HB2	1:78:A:SER:H	3	0.11
(3,11)	1:78:A:SER:HB3	1:78:A:SER:H	3	0.11
(3,10)	1:30:A:SER:HB2	1:30:A:SER:H	8	0.11
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	3	0.11
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	6	0.11
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	8	0.11
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD11	5	0.11
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD12	5	0.11
(2,462)	1:22:A:GLY:H	1:18:A:LEU:HD13	5	0.11
(2,436)	1:66:A:SER:H	1:74:A:SER:HB2	9	0.11
(2,432)	1:19:A:ALA:H	1:19:A:ALA:HA	6	0.11
(2,422)	1:76:A:GLN:H	1:75:A:LEU:HA	4	0.11
(2,422)	1:76:A:GLN:H	1:75:A:LEU:HA	8	0.11
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD11	9	0.11
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD12	9	0.11
(2,421)	1:35:A:LEU:H	1:35:A:LEU:HD13	9	0.11
(2,397)	1:21:A:PHE:H	1:20:A:HIS:HB3	6	0.11
(2,395)	1:36:A:THR:H	1:33:A:THR:HA	7	0.11
(2,389)	1:23:A:GLN:H	1:24:A:SER:H	1	0.11
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	2	0.11
(2,388)	1:39:A:ARG:H	1:38:A:GLY:HA2	7	0.11
(2,377)	1:74:A:SER:H	1:66:A:SER:HB2	1	0.11
(2,377)	1:74:A:SER:H	1:66:A:SER:HB3	1	0.11
(2,356)	1:39:A:ARG:HE	1:39:A:ARG:H	3	0.11
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD1	4	0.11
(2,306)	1:73:A:TYR:H	1:73:A:TYR:HD2	4	0.11
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	1	0.11
(2,297)	1:48:A:PHE:H	1:6:A:ASP:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,157)	1:53:A:GLY:H	1:48:A:PHE:HB3	1	0.11
(2,130)	1:9:A:ILE:H	1:9:A:ILE:HB	2	0.11
(2,46)	1:55:A:ALA:H	1:54:A:LEU:H	1	0.11
(1,486)	1:77:A:ALA:HA	1:78:A:SER:H	2	0.11
(1,478)	1:55:A:ALA:HA	1:58:A:LEU:HB2	7	0.11
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	3	0.11
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	3	0.11
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	3	0.11
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	6	0.11
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	6	0.11
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	6	0.11
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	7	0.11
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	7	0.11
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	7	0.11
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	9	0.11
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	9	0.11
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	9	0.11
(1,448)	1:14:A:LEU:HD11	1:18:A:LEU:HG	9	0.11
(1,448)	1:14:A:LEU:HD12	1:18:A:LEU:HG	9	0.11
(1,448)	1:14:A:LEU:HD13	1:18:A:LEU:HG	9	0.11
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	6	0.11
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	8	0.11
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	9	0.11
(1,425)	1:71:A:ALA:HB1	1:71:A:ALA:H	7	0.11
(1,425)	1:71:A:ALA:HB2	1:71:A:ALA:H	7	0.11
(1,425)	1:71:A:ALA:HB3	1:71:A:ALA:H	7	0.11
(1,412)	1:42:A:SER:HA	1:42:A:SER:H	9	0.11
(1,393)	1:72:A:SER:HA	1:28:A:LEU:HB2	4	0.11
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD11	6	0.11
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD12	6	0.11
(1,392)	1:58:A:LEU:HG	1:54:A:LEU:HD13	6	0.11
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD11	5	0.11
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD12	5	0.11
(1,391)	1:35:A:LEU:HB2	1:63:A:LEU:HD13	5	0.11
(1,386)	1:13:A:PRO:HA	1:14:A:LEU:H	9	0.11
(1,372)	1:40:A:SER:HA	1:40:A:SER:HB2	5	0.11
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD21	1	0.11
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD22	1	0.11
(1,367)	1:53:A:GLY:HA3	1:44:A:LEU:HD23	1	0.11
(1,303)	1:78:A:SER:HA	1:78:A:SER:HB2	2	0.11
(1,303)	1:78:A:SER:HA	1:78:A:SER:HB2	3	0.11
(1,283)	1:39:A:ARG:HD3	1:39:A:ARG:HB3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:16:A:PRO:HD2	1:15:A:ALA:H	3	0.11
(1,240)	1:44:A:LEU:HD21	1:56:A:ILE:HB	3	0.11
(1,240)	1:44:A:LEU:HD22	1:56:A:ILE:HB	3	0.11
(1,240)	1:44:A:LEU:HD23	1:56:A:ILE:HB	3	0.11
(1,240)	1:44:A:LEU:HD21	1:56:A:ILE:HB	5	0.11
(1,240)	1:44:A:LEU:HD22	1:56:A:ILE:HB	5	0.11
(1,240)	1:44:A:LEU:HD23	1:56:A:ILE:HB	5	0.11
(1,231)	1:14:A:LEU:HB3	1:14:A:LEU:H	3	0.11
(1,231)	1:14:A:LEU:HB3	1:14:A:LEU:H	9	0.11
(1,181)	1:75:A:LEU:HA	1:76:A:GLN:H	4	0.11
(1,181)	1:75:A:LEU:HA	1:76:A:GLN:H	8	0.11
(1,150)	1:57:A:LEU:HD11	1:57:A:LEU:HB2	5	0.11
(1,150)	1:57:A:LEU:HD12	1:57:A:LEU:HB2	5	0.11
(1,150)	1:57:A:LEU:HD13	1:57:A:LEU:HB2	5	0.11
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD11	8	0.11
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD12	8	0.11
(1,129)	1:41:A:THR:HA	1:14:A:LEU:HD13	8	0.11
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	2	0.11
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	2	0.11
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	2	0.11
(1,111)	1:64:A:GLU:HA	1:65:A:ALA:H	7	0.11
(1,80)	1:54:A:LEU:HB3	1:54:A:LEU:HD11	9	0.11
(1,80)	1:54:A:LEU:HB3	1:54:A:LEU:HD12	9	0.11
(1,80)	1:54:A:LEU:HB3	1:54:A:LEU:HD13	9	0.11
(1,78)	1:57:A:LEU:HD21	1:57:A:LEU:HB3	1	0.11
(1,78)	1:57:A:LEU:HD22	1:57:A:LEU:HB3	1	0.11
(1,78)	1:57:A:LEU:HD23	1:57:A:LEU:HB3	1	0.11
(1,66)	1:49:A:ASP:HA	1:50:A:ILE:H	5	0.11
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB1	8	0.11
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB2	8	0.11
(1,44)	1:25:A:ALA:HB1	1:5:A:ALA:HB3	8	0.11
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB1	8	0.11
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB2	8	0.11
(1,44)	1:25:A:ALA:HB2	1:5:A:ALA:HB3	8	0.11
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB1	8	0.11
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB2	8	0.11
(1,44)	1:25:A:ALA:HB3	1:5:A:ALA:HB3	8	0.11
(1,3)	1:79:A:ALA:HB1	1:79:A:ALA:H	2	0.11
(1,3)	1:79:A:ALA:HB2	1:79:A:ALA:H	2	0.11
(1,3)	1:79:A:ALA:HB3	1:79:A:ALA:H	2	0.11
(1,1)	1:15:A:ALA:HB1	1:16:A:PRO:HB2	6	0.11
(1,1)	1:15:A:ALA:HB2	1:16:A:PRO:HB2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:15:A:ALA:HB3	1:16:A:PRO:HB2	6	0.11
(4,37)	1:14:A:LEU:H	1:39:A:ARG:O	2	0.1
(4,1)	1:18:A:LEU:H	1:14:A:LEU:O	2	0.1
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	1	0.1
(3,6)	1:51:A:ASP:HA	1:51:A:ASP:H	2	0.1
(2,371)	1:74:A:SER:H	1:73:A:TYR:HB2	1	0.1
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB1	4	0.1
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB2	4	0.1
(2,357)	1:59:A:ALA:H	1:59:A:ALA:HB3	4	0.1
(2,275)	1:43:A:GLY:H	1:44:A:LEU:HB2	1	0.1
(2,269)	1:51:A:ASP:H	1:50:A:ILE:HB	2	0.1
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD11	1	0.1
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD12	1	0.1
(2,242)	1:18:A:LEU:H	1:18:A:LEU:HD13	1	0.1
(2,170)	1:9:A:ILE:H	1:8:A:ASP:H	1	0.1
(2,97)	1:55:A:ALA:H	1:52:A:GLN:HA	3	0.1
(1,484)	1:29:A:LEU:HA	1:30:A:SER:H	3	0.1
(1,484)	1:29:A:LEU:HA	1:30:A:SER:H	8	0.1
(1,467)	1:5:A:ALA:HB1	1:5:A:ALA:H	4	0.1
(1,467)	1:5:A:ALA:HB2	1:5:A:ALA:H	4	0.1
(1,467)	1:5:A:ALA:HB3	1:5:A:ALA:H	4	0.1
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	2	0.1
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	2	0.1
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	2	0.1
(1,465)	1:45:A:ALA:HB1	1:45:A:ALA:H	4	0.1
(1,465)	1:45:A:ALA:HB2	1:45:A:ALA:H	4	0.1
(1,465)	1:45:A:ALA:HB3	1:45:A:ALA:H	4	0.1
(1,460)	1:50:A:ILE:HB	1:51:A:ASP:H	2	0.1
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	1	0.1
(1,426)	1:61:A:THR:HA	1:61:A:THR:H	3	0.1
(1,412)	1:42:A:SER:HA	1:42:A:SER:H	5	0.1
(1,412)	1:42:A:SER:HA	1:42:A:SER:H	7	0.1
(1,294)	1:15:A:ALA:HB1	1:15:A:ALA:HA	9	0.1
(1,294)	1:15:A:ALA:HB2	1:15:A:ALA:HA	9	0.1
(1,294)	1:15:A:ALA:HB3	1:15:A:ALA:HA	9	0.1
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB1	4	0.1
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB2	4	0.1
(1,290)	1:14:A:LEU:HA	1:17:A:ALA:HB3	4	0.1
(1,145)	1:11:A:ALA:HA	1:12:A:GLY:H	7	0.1
(1,143)	1:75:A:LEU:HA	1:75:A:LEU:HB3	1	0.1
(1,138)	1:52:A:GLN:HA	1:52:A:GLN:H	7	0.1
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG21	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG22	7	0.1
(1,120)	1:50:A:ILE:HA	1:27:A:ILE:HG23	7	0.1
(1,111)	1:64:A:GLU:HA	1:65:A:ALA:H	10	0.1
(1,103)	1:37:A:GLU:HB2	1:37:A:GLU:H	7	0.1
(1,61)	1:44:A:LEU:HD21	1:56:A:ILE:HG13	1	0.1
(1,61)	1:44:A:LEU:HD22	1:56:A:ILE:HG13	1	0.1
(1,61)	1:44:A:LEU:HD23	1:56:A:ILE:HG13	1	0.1
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD21	1	0.1
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD22	1	0.1
(1,55)	1:9:A:ILE:HG21	1:57:A:LEU:HD23	1	0.1
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD21	1	0.1
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD22	1	0.1
(1,55)	1:9:A:ILE:HG22	1:57:A:LEU:HD23	1	0.1
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD21	1	0.1
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD22	1	0.1
(1,55)	1:9:A:ILE:HG23	1:57:A:LEU:HD23	1	0.1
(1,22)	1:55:A:ALA:HA	1:55:A:ALA:H	1	0.1
(1,22)	1:55:A:ALA:HA	1:55:A:ALA:H	8	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found