Full wwPDB NMR Structure Validation Report

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PDB ID	:	6CMY / pdb_00006cmy
BMRB ID	:	30101
Title	:	Solution NMR Structure Determination of Mouse Melanoregulin
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Deposited on	:	2018-03-06

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:

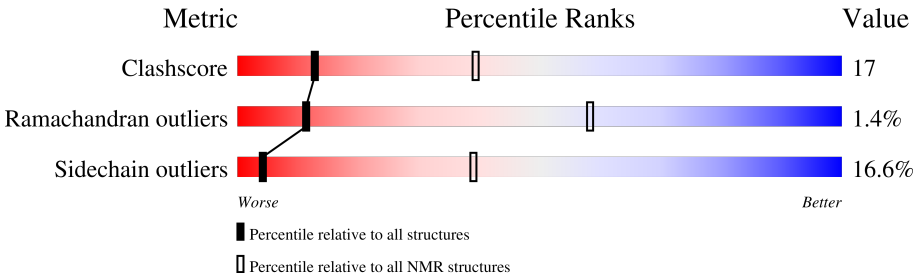
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 58%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	182	45% 21% 7% • 26%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest outliers*.

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:59-A:192 (134)	0.52	8

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

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

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

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2993 atoms, of which 1491 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Melanoregulin.

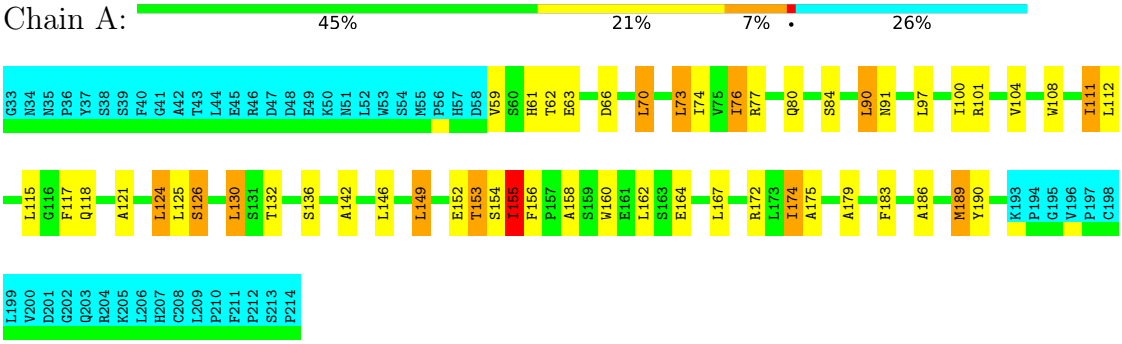
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	182	2993	943	1491	268	285	6	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Melanoregulin

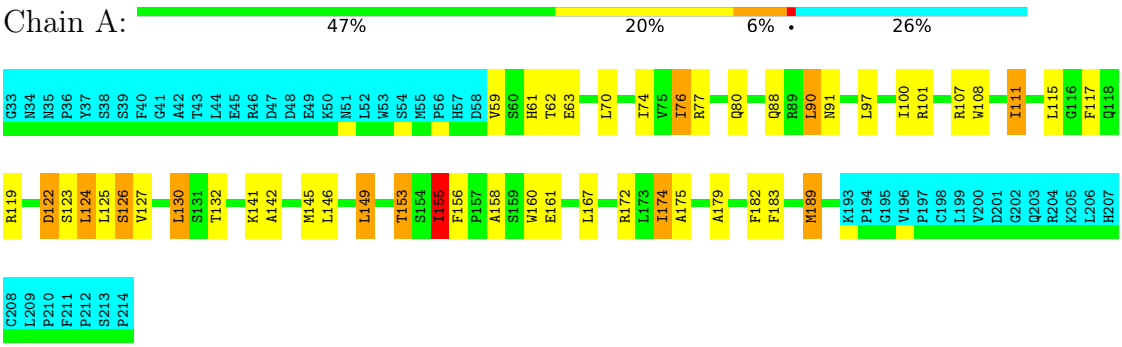


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

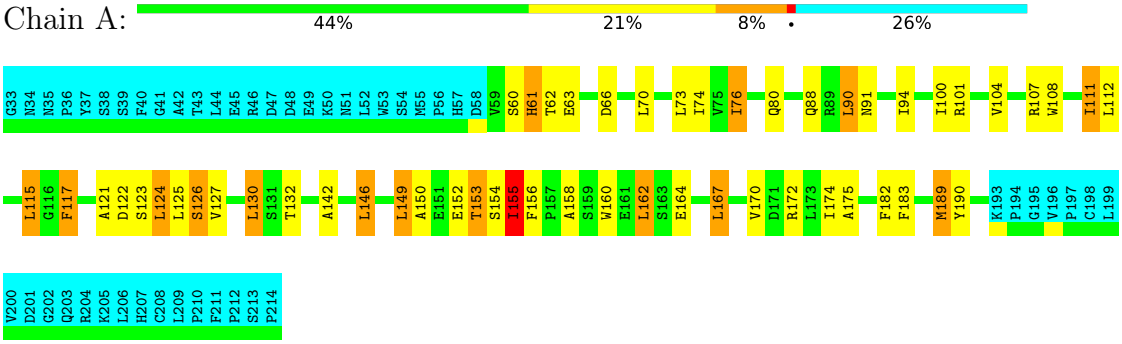
• Molecule 1: Melanoregulin



4.2.2 Score per residue for model 2

• Molecule 1: Melanoregulin

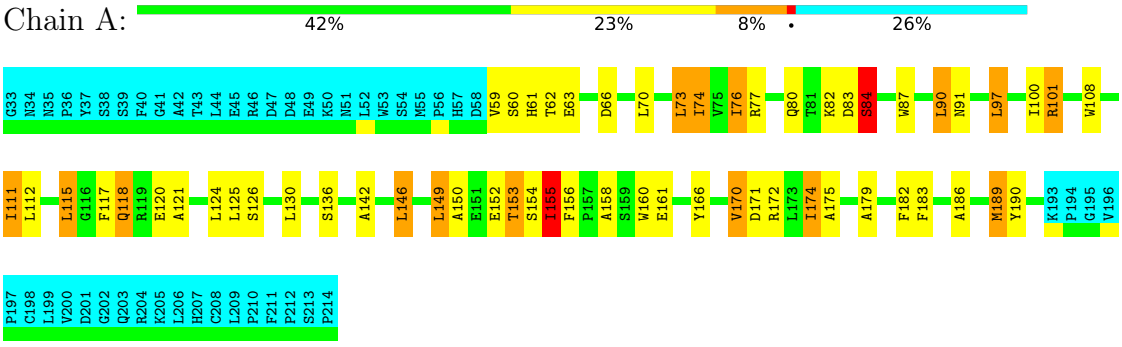
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Melanoregulin

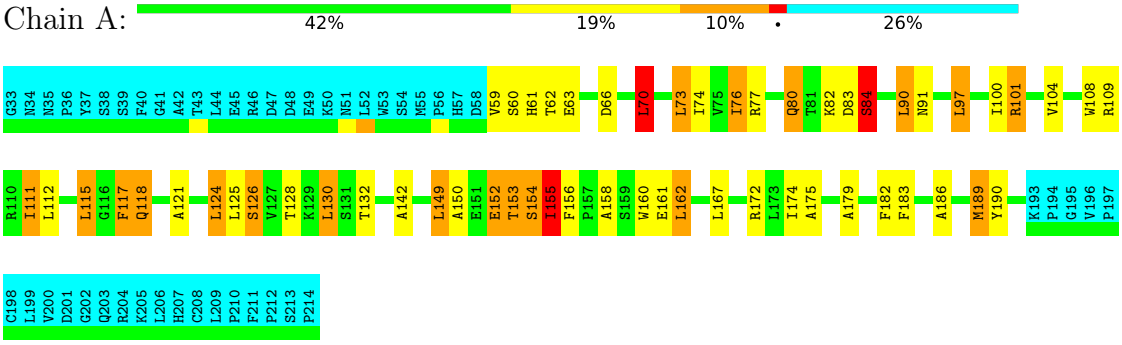
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Melanoregulin

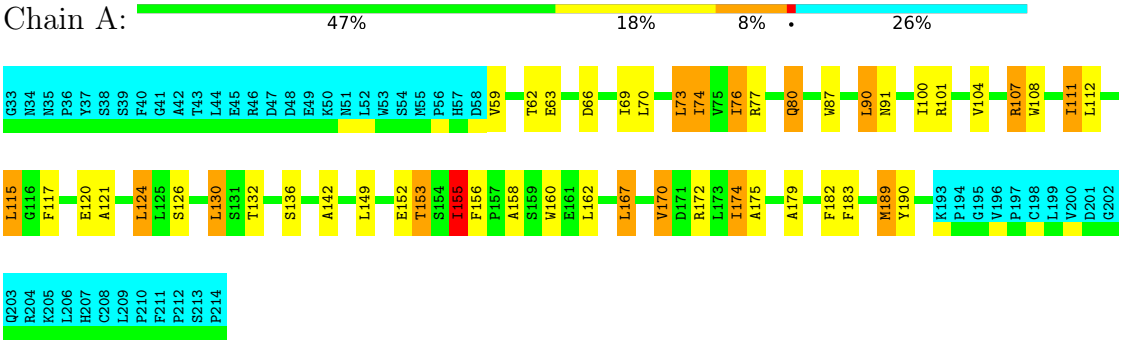
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Melanoregulin

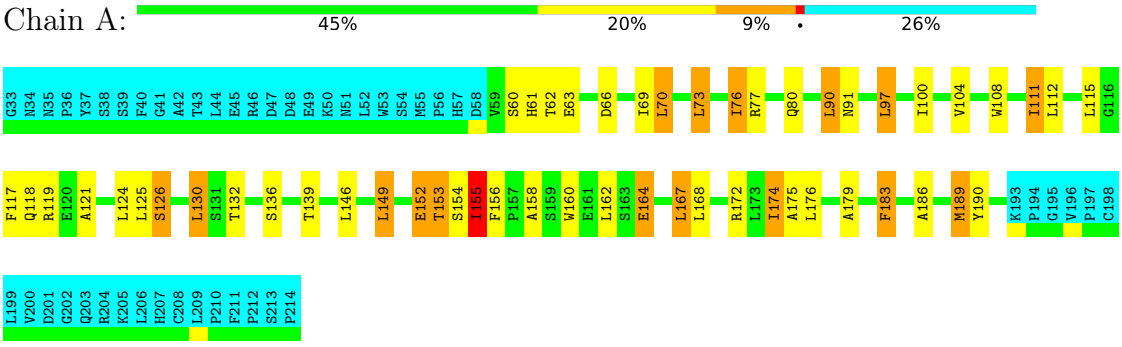
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Melanoregulin

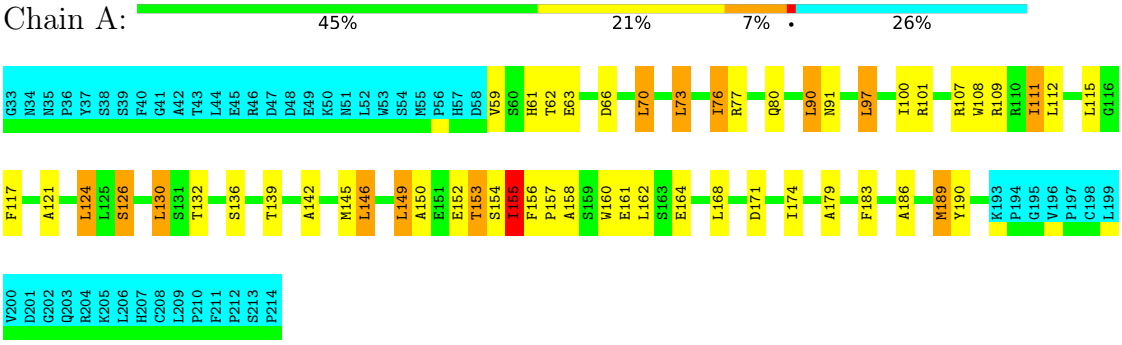
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Melanoregulin

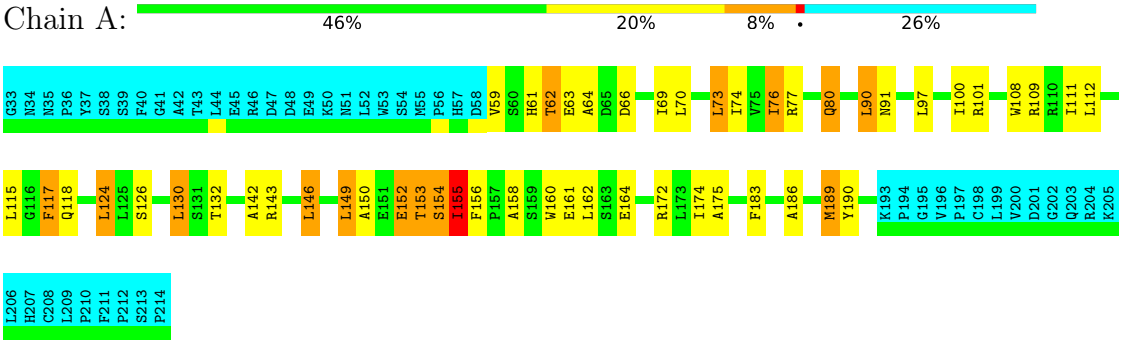
Chain A:



4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: Melanoregulin

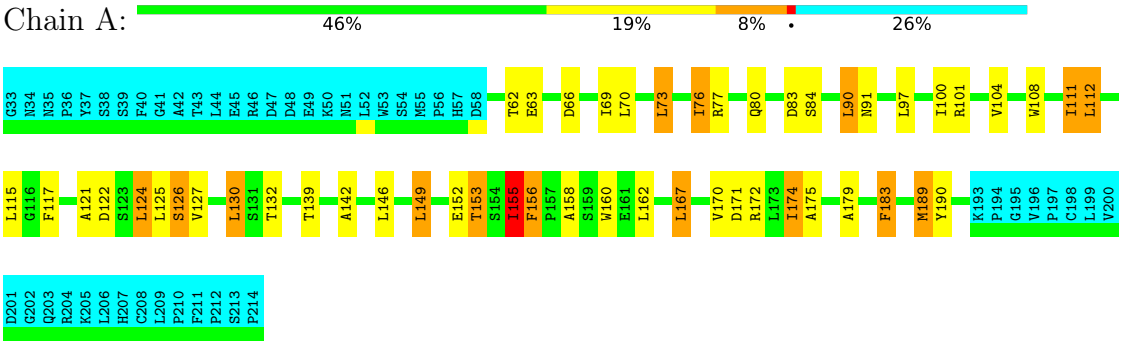
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Melanoregulin

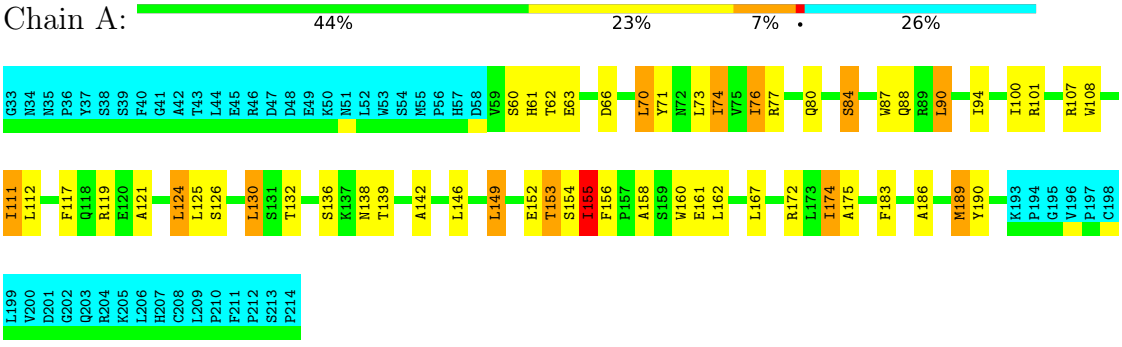
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Melanoregulin

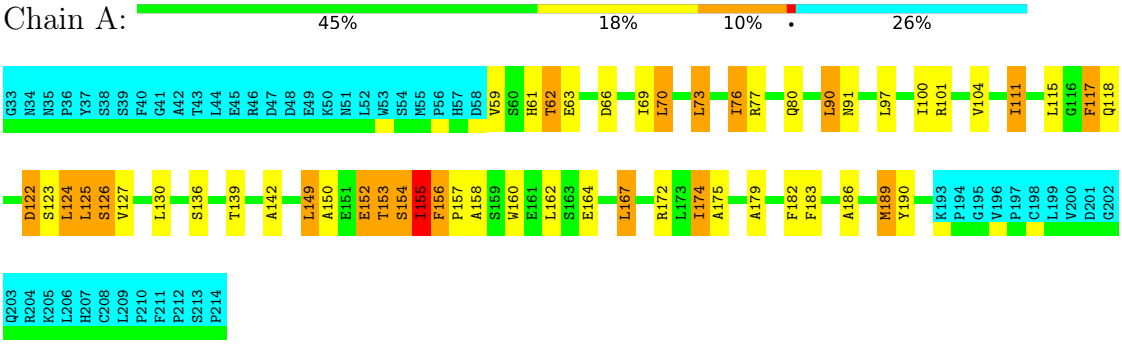
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Melanoregulin

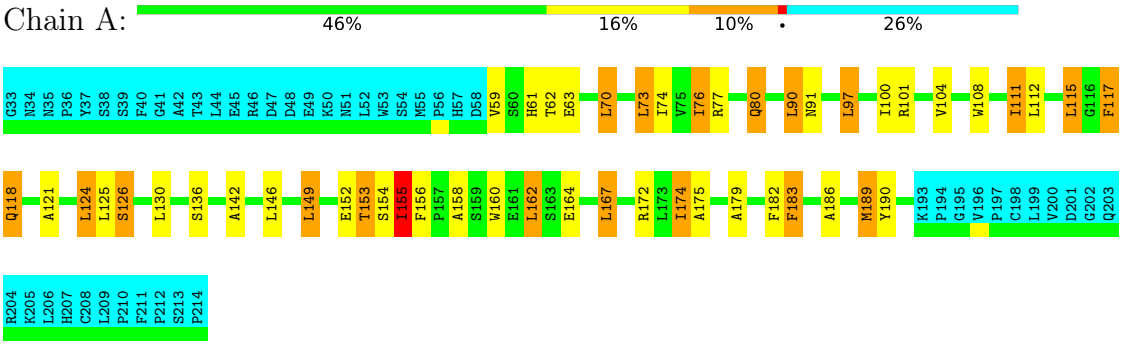
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Melanoregulin

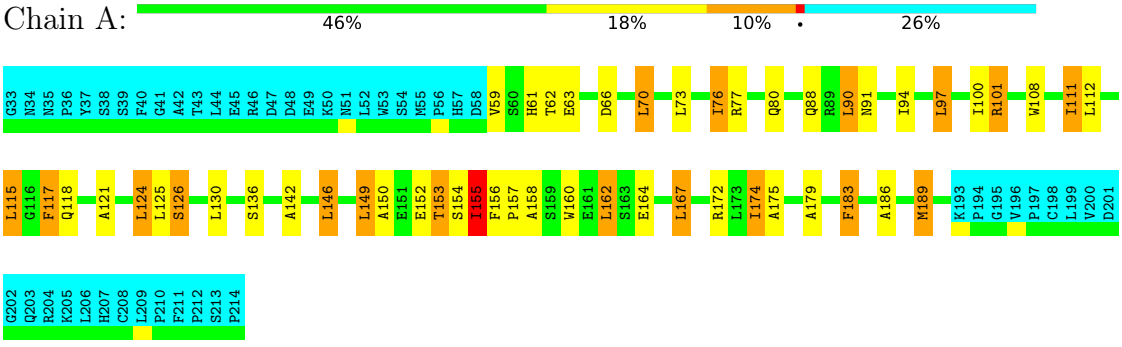
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Melanoregulin

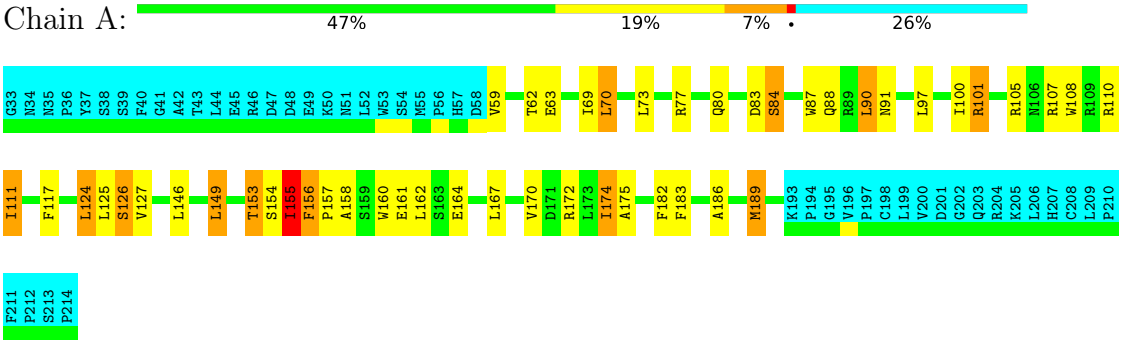
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Melanoregulin

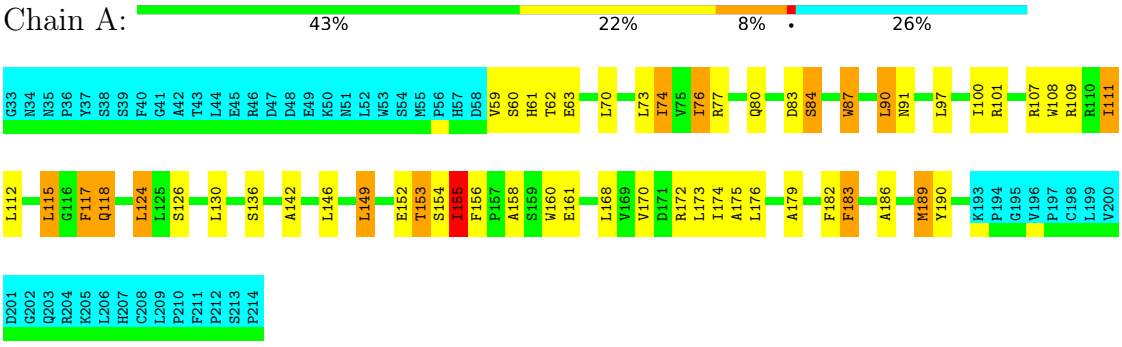
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Melanoregulin

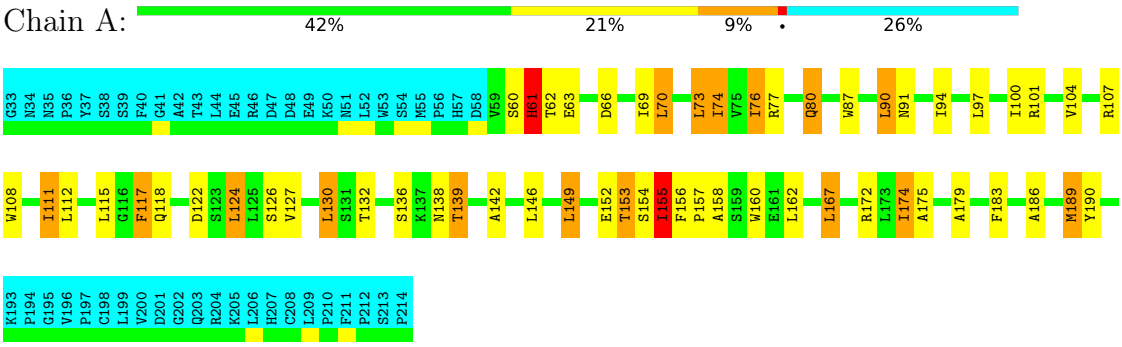
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Melanoregulin

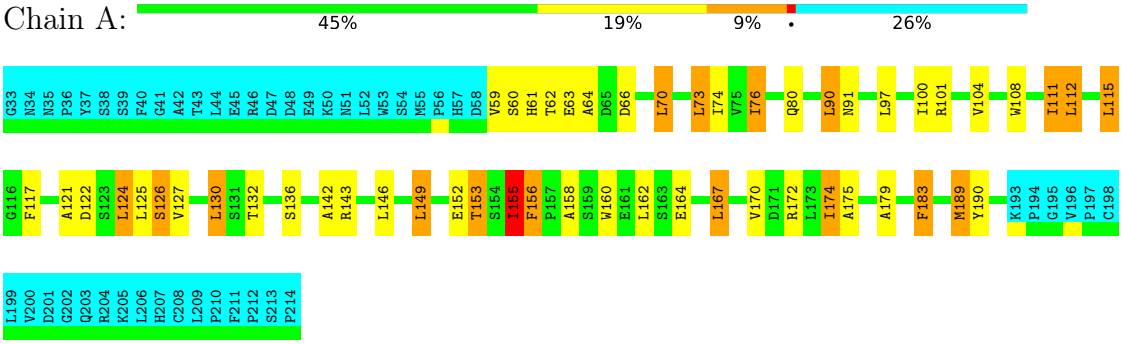
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Melanoregulin

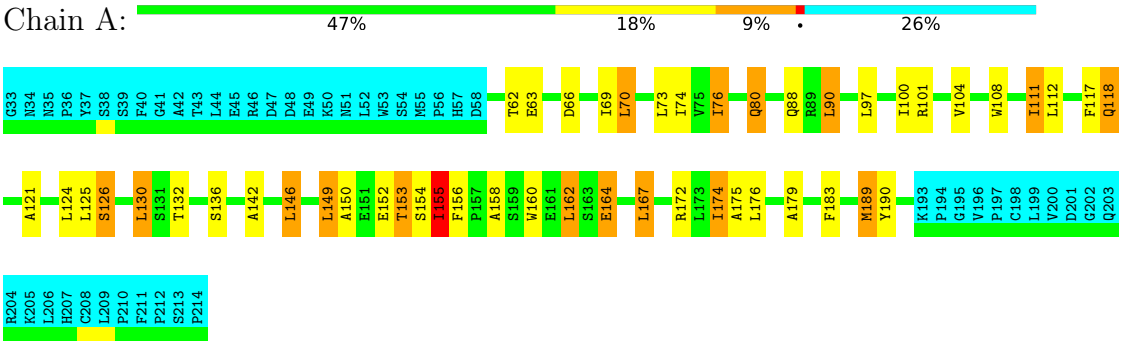
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Melanoregulin

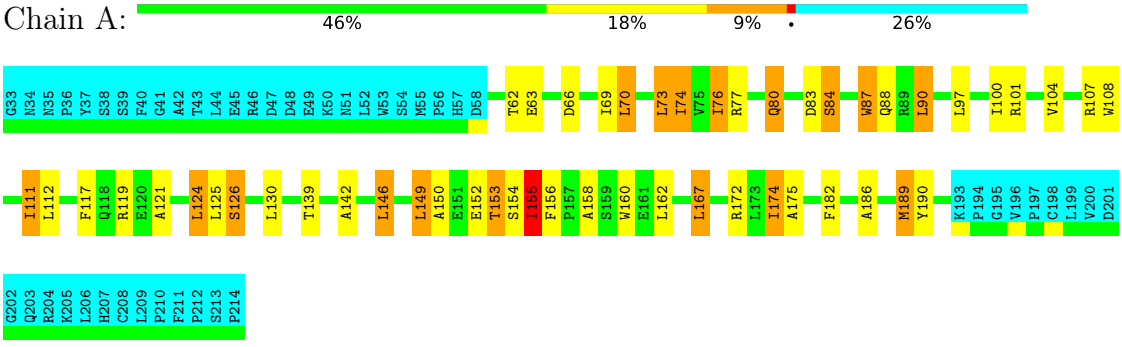
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Melanoregulin

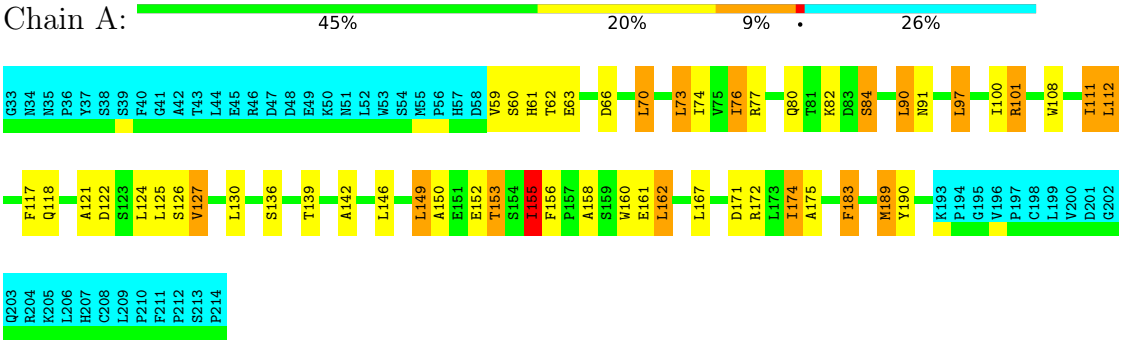
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Melanoregulin

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 125 calculated structures, 20 were deposited, based on the following criterion: *20 structures with lowest energy.*

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

Software name	Classification	Version
XPLOR-NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1381
Number of shifts mapped to atoms	1381
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

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	0.81±0.01	0±0/1144 (0.0± 0.0%)	1.24±0.01	3±1/1543 (0.2± 0.1%)
All	All	0.81	0/22880 (0.0%)	1.24	66/30860 (0.2%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	155	ILE	N-CA-C	-8.67	102.85	110.74	18	20
1	A	118	GLN	N-CA-C	6.36	119.03	111.71	18	6
1	A	61	HIS	CA-CB-CG	-6.33	107.47	113.80	3	10
1	A	61	HIS	N-CA-C	6.04	118.57	110.35	16	1
1	A	88	GLN	N-CA-C	-5.91	104.75	111.07	10	7
1	A	154	SER	CA-C-N	-5.38	114.15	120.72	11	5
1	A	154	SER	C-N-CA	-5.38	114.15	120.72	11	5
1	A	119	ARG	N-CA-C	5.37	116.82	111.07	1	4
1	A	156	PHE	N-CA-C	-5.20	102.59	110.39	9	4
1	A	70	LEU	N-CA-C	-5.19	105.52	111.07	4	1
1	A	183	PHE	CA-CB-CG	-5.17	108.62	113.80	14	2
1	A	110	ARG	N-CA-C	5.02	116.83	111.36	14	1

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	1126	1132	1131	37±5
All	All	22520	22640	22620	748

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:LEU:HD21	1:A:121:ALA:HB3	1.01	1.28	6	1
1:A:124:LEU:HD13	1:A:149:LEU:HD12	0.93	1.37	6	6
1:A:124:LEU:HD22	1:A:153:THR:OG1	0.89	1.68	2	9
1:A:149:LEU:HD11	1:A:162:LEU:HD22	0.85	1.45	20	5
1:A:108:TRP:CZ3	1:A:124:LEU:HD11	0.80	2.12	6	3
1:A:158:ALA:HB2	1:A:189:MET:SD	0.79	2.18	3	20
1:A:124:LEU:HD12	1:A:125:LEU:N	0.75	1.96	6	7
1:A:115:LEU:HD22	1:A:179:ALA:HB3	0.75	1.56	3	1
1:A:108:TRP:CE3	1:A:121:ALA:HB1	0.75	2.17	18	5
1:A:100:ILE:HD12	1:A:101:ARG:N	0.74	1.98	18	8
1:A:149:LEU:HD23	1:A:150:ALA:N	0.73	1.98	18	9
1:A:162:LEU:HD23	1:A:167:LEU:HD11	0.72	1.60	4	2
1:A:149:LEU:HD21	1:A:162:LEU:HD21	0.72	1.61	13	2
1:A:146:LEU:HD13	1:A:149:LEU:HD22	0.71	1.62	15	9
1:A:111:ILE:HD12	1:A:174:ILE:HG21	0.71	1.62	1	7
1:A:149:LEU:C	1:A:149:LEU:HD22	0.70	2.11	11	1
1:A:146:LEU:CD2	1:A:149:LEU:HD22	0.70	2.17	2	7
1:A:90:LEU:O	1:A:90:LEU:HD22	0.68	1.89	13	3
1:A:124:LEU:HD13	1:A:153:THR:HB	0.68	1.66	2	2
1:A:100:ILE:HD13	1:A:164:GLU:OE1	0.67	1.89	18	2
1:A:149:LEU:HD11	1:A:162:LEU:HD11	0.67	1.66	6	1
1:A:111:ILE:HD12	1:A:174:ILE:CG2	0.66	2.19	11	9
1:A:104:VAL:HG13	1:A:167:LEU:CD1	0.66	2.19	2	4
1:A:108:TRP:CZ2	1:A:167:LEU:HD11	0.66	2.25	13	2
1:A:90:LEU:HD23	1:A:91:ASN:N	0.66	2.06	14	13
1:A:108:TRP:NE1	1:A:167:LEU:HD11	0.66	2.06	2	4
1:A:149:LEU:HD13	1:A:150:ALA:N	0.66	2.05	11	1
1:A:130:LEU:HD22	1:A:130:LEU:O	0.66	1.91	6	1
1:A:107:ARG:O	1:A:111:ILE:HG22	0.65	1.91	16	7
1:A:90:LEU:HD13	1:A:91:ASN:N	0.65	2.07	1	4
1:A:124:LEU:HD23	1:A:153:THR:HB	0.64	1.67	1	9
1:A:149:LEU:HD22	1:A:149:LEU:O	0.64	1.92	11	1
1:A:101:ARG:CZ	1:A:125:LEU:HD21	0.64	2.21	14	1
1:A:108:TRP:CZ3	1:A:121:ALA:HB1	0.63	2.27	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:LEU:HD11	1:A:162:LEU:HD21	0.63	1.70	11	1
1:A:112:LEU:CD2	1:A:121:ALA:HB3	0.63	2.16	6	6
1:A:146:LEU:HD22	1:A:149:LEU:HD22	0.62	1.71	8	5
1:A:115:LEU:CD1	1:A:179:ALA:HB3	0.61	2.25	17	1
1:A:84:SER:HG	1:A:87:TRP:CD1	0.61	2.13	14	1
1:A:104:VAL:HG13	1:A:167:LEU:HD12	0.61	1.73	2	1
1:A:108:TRP:CD1	1:A:167:LEU:HD11	0.61	2.30	2	1
1:A:117:PHE:CZ	1:A:179:ALA:HB1	0.61	2.30	3	5
1:A:66:ASP:O	1:A:70:LEU:HD13	0.61	1.96	5	13
1:A:146:LEU:HD23	1:A:149:LEU:HD22	0.60	1.71	2	1
1:A:115:LEU:HD13	1:A:179:ALA:HB3	0.60	1.74	13	4
1:A:124:LEU:HD23	1:A:124:LEU:N	0.60	2.12	5	9
1:A:101:ARG:HB2	1:A:142:ALA:HB1	0.59	1.75	2	9
1:A:108:TRP:HE1	1:A:167:LEU:HD12	0.59	1.58	14	2
1:A:108:TRP:CZ3	1:A:124:LEU:HD12	0.58	2.32	2	1
1:A:112:LEU:HD21	1:A:121:ALA:CB	0.58	2.19	6	1
1:A:124:LEU:HD13	1:A:149:LEU:HG	0.58	1.75	18	2
1:A:100:ILE:HD13	1:A:164:GLU:CD	0.58	2.22	18	2
1:A:108:TRP:CZ2	1:A:167:LEU:HD21	0.58	2.34	9	2
1:A:125:LEU:HD23	1:A:126:SER:OG	0.58	1.98	14	6
1:A:77:ARG:O	1:A:80:GLN:O	0.56	2.23	14	17
1:A:124:LEU:HD13	1:A:149:LEU:CG	0.56	2.30	18	2
1:A:112:LEU:HD13	1:A:121:ALA:HB3	0.56	1.77	7	4
1:A:172:ARG:O	1:A:175:ALA:HB3	0.56	2.00	14	19
1:A:108:TRP:CZ3	1:A:125:LEU:HD12	0.56	2.35	12	5
1:A:162:LEU:HD12	1:A:167:LEU:CD1	0.56	2.31	6	2
1:A:108:TRP:HE1	1:A:167:LEU:HD22	0.56	1.61	20	1
1:A:76:ILE:HD12	1:A:80:GLN:HB2	0.55	1.77	19	2
1:A:90:LEU:C	1:A:90:LEU:HD13	0.55	2.26	18	3
1:A:149:LEU:O	1:A:153:THR:O	0.55	2.25	13	10
1:A:66:ASP:O	1:A:70:LEU:HD23	0.55	2.02	2	3
1:A:104:VAL:HG13	1:A:167:LEU:HD13	0.55	1.78	5	5
1:A:70:LEU:HB3	1:A:90:LEU:HD23	0.55	1.77	13	3
1:A:90:LEU:HD13	1:A:90:LEU:C	0.55	2.27	2	4
1:A:90:LEU:HD22	1:A:90:LEU:C	0.54	2.27	15	3
1:A:155:ILE:HD12	1:A:182:PHE:HD2	0.54	1.61	12	5
1:A:115:LEU:HD12	1:A:117:PHE:CZ	0.54	2.38	2	1
1:A:101:ARG:HH22	1:A:104:VAL:HG11	0.54	1.63	2	1
1:A:162:LEU:HD12	1:A:167:LEU:HD12	0.54	1.79	5	2
1:A:64:ALA:HB3	1:A:143:ARG:NH2	0.54	2.17	17	2
1:A:170:VAL:HG12	1:A:182:PHE:CZ	0.53	2.37	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ILE:HA	1:A:174:ILE:HD13	0.53	1.78	13	1
1:A:149:LEU:HD21	1:A:162:LEU:HB2	0.53	1.79	7	1
1:A:124:LEU:CD1	1:A:149:LEU:HD12	0.53	2.24	6	4
1:A:156:PHE:HB2	1:A:160:TRP:CG	0.53	2.38	5	19
1:A:76:ILE:O	1:A:80:GLN:N	0.52	2.42	2	19
1:A:115:LEU:HG	1:A:179:ALA:HB3	0.52	1.81	7	3
1:A:111:ILE:HD12	1:A:182:PHE:CE1	0.52	2.40	15	2
1:A:108:TRP:NE1	1:A:167:LEU:HD22	0.52	2.20	20	1
1:A:101:ARG:NH2	1:A:104:VAL:HG11	0.52	2.20	2	1
1:A:112:LEU:HD23	1:A:118:GLN:HA	0.52	1.81	6	1
1:A:130:LEU:HD21	1:A:132:THR:OG1	0.51	2.05	2	11
1:A:115:LEU:CD2	1:A:179:ALA:HB3	0.51	2.34	3	1
1:A:108:TRP:CE2	1:A:167:LEU:HD21	0.51	2.41	9	2
1:A:174:ILE:HD13	1:A:175:ALA:N	0.51	2.21	10	1
1:A:120:GLU:OE2	1:A:153:THR:HG21	0.51	2.06	3	2
1:A:115:LEU:HD13	1:A:179:ALA:CB	0.51	2.36	5	3
1:A:108:TRP:CE2	1:A:167:LEU:HD11	0.50	2.41	12	1
1:A:149:LEU:C	1:A:149:LEU:CD2	0.50	2.83	11	1
1:A:152:GLU:O	1:A:190:TYR:CG	0.49	2.65	15	17
1:A:155:ILE:HG22	1:A:156:PHE:N	0.49	2.21	9	20
1:A:101:ARG:CB	1:A:142:ALA:HB1	0.49	2.36	2	11
1:A:70:LEU:O	1:A:90:LEU:CD1	0.49	2.61	8	13
1:A:130:LEU:HD22	1:A:130:LEU:C	0.49	2.32	6	1
1:A:74:ILE:HD13	1:A:87:TRP:CD1	0.49	2.42	19	6
1:A:117:PHE:HZ	1:A:179:ALA:HB1	0.49	1.67	11	5
1:A:108:TRP:CE3	1:A:111:ILE:HG21	0.49	2.42	20	3
1:A:154:SER:O	1:A:186:ALA:HA	0.48	2.08	11	13
1:A:174:ILE:HG22	1:A:182:PHE:CE1	0.48	2.43	14	2
1:A:160:TRP:CD1	1:A:161:GLU:O	0.48	2.67	7	9
1:A:111:ILE:HD12	1:A:174:ILE:HG22	0.48	1.84	13	3
1:A:108:TRP:O	1:A:112:LEU:HD12	0.48	2.09	15	4
1:A:122:ASP:HB3	1:A:127:VAL:O	0.48	2.09	17	4
1:A:183:PHE:N	1:A:183:PHE:CD2	0.47	2.81	20	4
1:A:108:TRP:HE1	1:A:167:LEU:HD11	0.47	1.69	18	3
1:A:112:LEU:CD1	1:A:121:ALA:HB3	0.47	2.39	7	4
1:A:111:ILE:HD11	1:A:182:PHE:CD1	0.47	2.44	19	2
1:A:108:TRP:CH2	1:A:149:LEU:HD11	0.47	2.45	2	1
1:A:97:LEU:O	1:A:100:ILE:HG13	0.47	2.09	8	9
1:A:162:LEU:N	1:A:162:LEU:HD23	0.47	2.24	6	1
1:A:105:ARG:HD2	1:A:125:LEU:HD22	0.47	1.86	14	1
1:A:108:TRP:CH2	1:A:124:LEU:HD11	0.47	2.44	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:LEU:HB3	1:A:118:GLN:HA	0.47	1.87	16	6
1:A:108:TRP:HA	1:A:111:ILE:HG22	0.47	1.87	3	1
1:A:104:VAL:HG22	1:A:167:LEU:HD13	0.47	1.87	17	2
1:A:138:ASN:C	1:A:139:THR:HG1	0.47	2.17	16	2
1:A:146:LEU:CD1	1:A:149:LEU:HD22	0.47	2.37	15	1
1:A:107:ARG:O	1:A:111:ILE:HG23	0.47	2.09	7	2
1:A:117:PHE:CD2	1:A:117:PHE:N	0.46	2.81	5	3
1:A:167:LEU:HD23	1:A:170:VAL:HB	0.46	1.88	17	2
1:A:122:ASP:OD1	1:A:122:ASP:C	0.46	2.58	11	2
1:A:152:GLU:O	1:A:190:TYR:CD1	0.46	2.68	2	6
1:A:70:LEU:O	1:A:73:LEU:N	0.46	2.48	9	13
1:A:101:ARG:NE	1:A:125:LEU:HD21	0.46	2.25	12	1
1:A:73:LEU:O	1:A:76:ILE:HG13	0.46	2.11	19	2
1:A:124:LEU:HD22	1:A:153:THR:HG1	0.45	1.69	19	2
1:A:111:ILE:HG23	1:A:112:LEU:N	0.45	2.27	3	1
1:A:108:TRP:HZ2	1:A:162:LEU:HD23	0.45	1.71	10	2
1:A:83:ASP:O	1:A:84:SER:C	0.45	2.60	14	6
1:A:124:LEU:HD12	1:A:124:LEU:C	0.45	2.35	3	2
1:A:104:VAL:CG1	1:A:167:LEU:HD13	0.45	2.41	4	1
1:A:62:THR:HG22	1:A:63:GLU:N	0.45	2.27	16	12
1:A:108:TRP:CZ2	1:A:162:LEU:HD23	0.45	2.47	10	1
1:A:189:MET:SD	1:A:189:MET:O	0.45	2.75	13	20
1:A:107:ARG:NE	1:A:168:LEU:HD12	0.45	2.27	15	1
1:A:122:ASP:OD1	1:A:127:VAL:HG21	0.44	2.12	2	1
1:A:126:SER:CB	1:A:145:MET:HE3	0.44	2.42	7	1
1:A:111:ILE:HG23	1:A:112:LEU:HD12	0.44	1.89	2	2
1:A:125:LEU:O	1:A:126:SER:CB	0.44	2.65	11	6
1:A:160:TRP:CD1	1:A:160:TRP:C	0.44	2.96	5	7
1:A:112:LEU:HD22	1:A:118:GLN:HA	0.44	1.90	3	2
1:A:126:SER:O	1:A:130:LEU:HD11	0.44	2.12	6	1
1:A:164:GLU:OE1	1:A:168:LEU:HD11	0.44	2.12	6	1
1:A:160:TRP:C	1:A:160:TRP:CD1	0.44	2.95	11	4
1:A:162:LEU:HD13	1:A:167:LEU:HG	0.44	1.89	2	2
1:A:170:VAL:O	1:A:174:ILE:HG23	0.44	2.11	14	2
1:A:108:TRP:HA	1:A:111:ILE:HG23	0.44	1.89	10	1
1:A:87:TRP:CD2	1:A:87:TRP:N	0.44	2.85	14	1
1:A:104:VAL:CG2	1:A:167:LEU:HD13	0.44	2.43	9	1
1:A:108:TRP:HZ3	1:A:111:ILE:HD13	0.44	1.71	17	1
1:A:76:ILE:HD12	1:A:80:GLN:CB	0.43	2.43	19	1
1:A:125:LEU:C	1:A:125:LEU:HD23	0.43	2.39	18	2
1:A:122:ASP:CG	1:A:123:SER:N	0.43	2.76	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:SER:OG	1:A:145:MET:HE3	0.43	2.13	7	1
1:A:174:ILE:HD12	1:A:174:ILE:O	0.43	2.13	19	1
1:A:124:LEU:N	1:A:124:LEU:CD2	0.43	2.80	4	3
1:A:100:ILE:HG22	1:A:164:GLU:CD	0.43	2.37	14	1
1:A:157:PRO:O	1:A:160:TRP:HB3	0.43	2.13	14	5
1:A:73:LEU:O	1:A:76:ILE:HG12	0.43	2.14	11	3
1:A:146:LEU:O	1:A:149:LEU:HD23	0.43	2.13	14	1
1:A:115:LEU:HD12	1:A:179:ALA:HB3	0.42	1.89	17	1
1:A:62:THR:CG2	1:A:63:GLU:N	0.42	2.82	8	11
1:A:117:PHE:CE1	1:A:183:PHE:CD1	0.42	3.08	8	1
1:A:155:ILE:CG2	1:A:156:PHE:N	0.42	2.82	20	1
1:A:155:ILE:HD12	1:A:182:PHE:CD2	0.42	2.47	12	1
1:A:162:LEU:O	1:A:162:LEU:HG	0.42	2.15	12	1
1:A:130:LEU:HD12	1:A:130:LEU:O	0.42	2.14	20	1
1:A:117:PHE:CD1	1:A:183:PHE:CD1	0.42	3.08	13	2
1:A:156:PHE:CE1	1:A:170:VAL:HG22	0.42	2.50	17	1
1:A:173:LEU:HD12	1:A:176:LEU:HD12	0.41	1.92	15	1
1:A:130:LEU:HD23	1:A:132:THR:OG1	0.41	2.15	6	1
1:A:166:TYR:O	1:A:170:VAL:HG23	0.41	2.15	3	1
1:A:108:TRP:O	1:A:109:ARG:C	0.41	2.63	4	4
1:A:117:PHE:CD2	1:A:183:PHE:CE2	0.41	3.09	6	1
1:A:117:PHE:CE2	1:A:183:PHE:CE2	0.41	3.09	9	2
1:A:111:ILE:CG1	1:A:112:LEU:N	0.41	2.83	7	1
1:A:171:ASP:O	1:A:174:ILE:HG12	0.41	2.15	9	2
1:A:122:ASP:CG	1:A:127:VAL:HG21	0.41	2.41	2	1
1:A:154:SER:CB	1:A:156:PHE:O	0.41	2.68	11	4
1:A:117:PHE:CE1	1:A:183:PHE:CD2	0.41	3.09	20	1
1:A:168:LEU:HD12	1:A:171:ASP:OD2	0.41	2.16	7	1
1:A:149:LEU:HD11	1:A:162:LEU:CD2	0.41	2.32	20	1
1:A:141:LYS:NZ	1:A:145:MET:HE3	0.41	2.31	1	1
1:A:171:ASP:O	1:A:174:ILE:N	0.41	2.54	3	1
1:A:174:ILE:O	1:A:174:ILE:HD13	0.41	2.16	3	1
1:A:108:TRP:N	1:A:108:TRP:CD1	0.41	2.88	6	1
1:A:90:LEU:HD22	1:A:90:LEU:O	0.41	2.16	2	1
1:A:171:ASP:O	1:A:174:ILE:HG22	0.41	2.16	3	1
1:A:87:TRP:N	1:A:87:TRP:CE3	0.41	2.89	14	1
1:A:176:LEU:HD12	1:A:176:LEU:N	0.40	2.31	6	2
1:A:61:HIS:O	1:A:61:HIS:ND1	0.40	2.54	16	1
1:A:108:TRP:HE1	1:A:167:LEU:HD21	0.40	1.76	2	1
1:A:117:PHE:CZ	1:A:183:PHE:CE2	0.40	3.09	17	1
1:A:125:LEU:HD23	1:A:125:LEU:C	0.40	2.42	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:ILE:HD12	1:A:100:ILE:C	0.40	2.42	8	1
1:A:108:TRP:CZ3	1:A:111:ILE:HD13	0.40	2.51	17	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	134/182 (74%)	128±1 (95±1%)	4±1 (3±1%)	2±1 (1±1%)	11	58
All	All	2680/3640 (74%)	2559 (95%)	83 (3%)	38 (1%)	11	58

All 5 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	126	SER	20
1	A	139	THR	7
1	A	84	SER	6
1	A	82	LYS	3
1	A	127	VAL	2

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	124/167 (74%)	103±3 (83±3%)	21±3 (17±3%)	4	39
All	All	2480/3340 (74%)	2068 (83%)	412 (17%)	4	39

All 43 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	90	LEU	20
1	A	111	ILE	20
1	A	149	LEU	20
1	A	153	THR	20
1	A	155	ILE	20
1	A	174	ILE	20
1	A	189	MET	20
1	A	76	ILE	19
1	A	130	LEU	18
1	A	183	PHE	17
1	A	124	LEU	16
1	A	73	LEU	16
1	A	97	LEU	15
1	A	74	ILE	14
1	A	136	SER	13
1	A	70	LEU	13
1	A	115	LEU	11
1	A	117	PHE	11
1	A	167	LEU	11
1	A	162	LEU	10
1	A	60	SER	9
1	A	100	ILE	8
1	A	164	GLU	8
1	A	146	LEU	7
1	A	80	GLN	7
1	A	61	HIS	5
1	A	84	SER	5
1	A	101	ARG	5
1	A	152	GLU	5
1	A	94	ILE	4
1	A	170	VAL	4
1	A	69	ILE	4
1	A	112	LEU	3
1	A	122	ASP	2
1	A	62	THR	2
1	A	127	VAL	2
1	A	87	TRP	2
1	A	123	SER	1
1	A	128	THR	1
1	A	107	ARG	1
1	A	71	TYR	1
1	A	125	LEU	1
1	A	118	GLN	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

The completeness of assignment taking into account all chemical shift lists is 58% for the well-defined parts and 53% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *MregChemicalShiftBmrb.tbl*

7.1.1 Bookkeeping

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

Total number of shifts	1381
Number of shifts mapped to atoms	1381
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	165	-0.30 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	161	1.34 ± 0.07	Should be checked
$^{13}C'$	153	-0.44 ± 0.13	None needed (< 0.5 ppm)
^{15}N	151	0.72 ± 0.21	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 58%, i.e. 1151 atoms were assigned a chemical shift out of a possible 1976. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	643/667 (96%)	259/267 (97%)	258/268 (96%)	126/132 (95%)
Sidechain	505/1180 (43%)	325/759 (43%)	180/358 (50%)	0/63 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	3/129 (2%)	3/62 (5%)	0/62 (0%)	0/5 (0%)
Overall	1151/1976 (58%)	587/1088 (54%)	438/688 (64%)	126/200 (63%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 53%, i.e. 1381 atoms were assigned a chemical shift out of a possible 2603. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	788/897 (88%)	319/360 (89%)	318/364 (87%)	151/173 (87%)
Sidechain	590/1520 (39%)	375/978 (38%)	215/466 (46%)	0/76 (0%)
Aromatic	3/186 (2%)	3/90 (3%)	0/86 (0%)	0/10 (0%)
Overall	1381/2603 (53%)	697/1428 (49%)	533/916 (58%)	151/259 (58%)

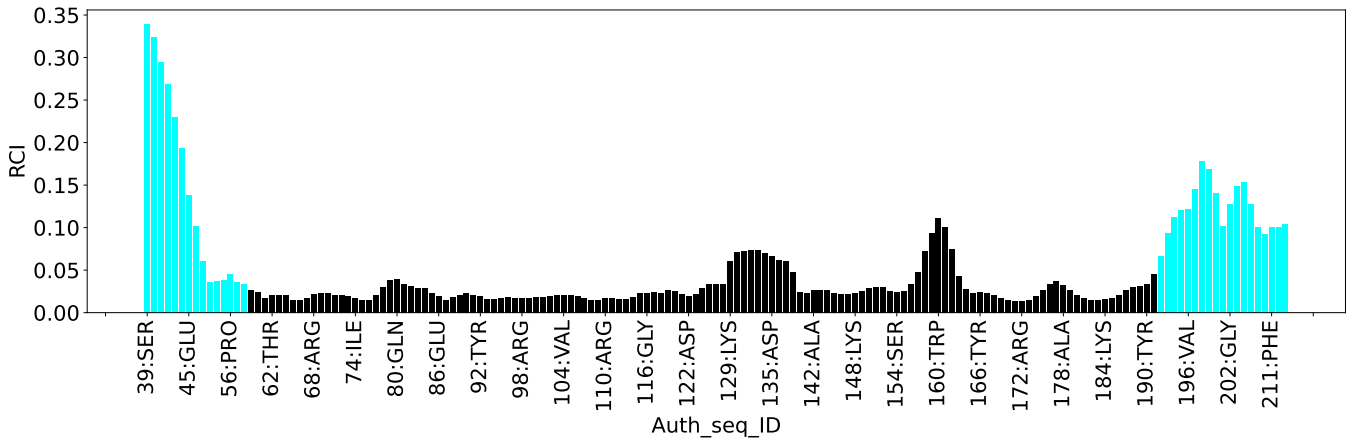
7.1.4 Statistically unusual chemical shifts (i)

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	1460
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	363
Medium range (|i-j|>1 and |i-j|<5)	244
Long range (|i-j|≥5)	671
Inter-chain	0
Hydrogen bond restraints	182
Disulfide bond restraints	0
Total dihedral-angle restraints	330
Number of unmapped restraints	0
Number of restraints per residue	9.8
Number of long range restraints per residue[1]	4.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	77.3	0.2
0.2-0.5 (Medium)	34.0	0.5
>0.5 (Large)	238.2	62.31

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	50.2	5.22
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

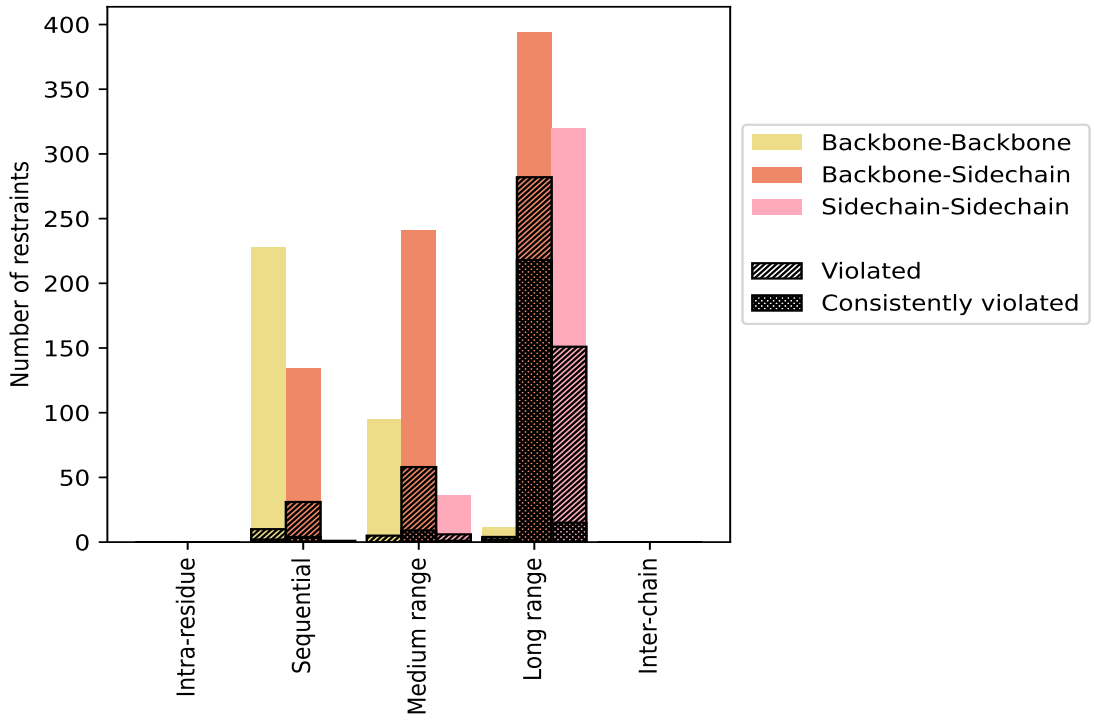
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	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
Sequential (|i-j|=1)	363	24.9	42	11.6	2.9	6	1.7	0.4
Backbone-Backbone	228	15.6	10	4.4	0.7	2	0.9	0.1
Backbone-Sidechain	134	9.2	31	23.1	2.1	4	3.0	0.3
Sidechain-Sidechain	1	0.1	1	100.0	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	244	16.7	29	11.9	2.0	5	2.0	0.3
Backbone-Backbone	95	6.5	5	5.3	0.3	0	0.0	0.0
Backbone-Sidechain	113	7.7	18	15.9	1.2	4	3.5	0.3
Sidechain-Sidechain	36	2.5	6	16.7	0.4	1	2.8	0.1
Long range (|i-j|≥5)	671	46.0	383	57.1	26.2	181	27.0	12.4
Backbone-Backbone	11	0.8	4	36.4	0.3	2	18.2	0.1
Backbone-Sidechain	340	23.3	228	67.1	15.6	164	48.2	11.2
Sidechain-Sidechain	320	21.9	151	47.2	10.3	15	4.7	1.0
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	182	12.5	94	51.6	6.4	59	32.4	4.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1460	100.0	548	37.5	37.5	251	17.2	17.2
Backbone-Backbone	334	22.9	19	5.7	1.3	4	1.2	0.3
Backbone-Sidechain	769	52.7	371	48.2	25.4	231	30.0	15.8
Sidechain-Sidechain	357	24.5	158	44.3	10.8	16	4.5	1.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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	0	22	31	303	0	356	14.41	58.19	14.74	11.44
2	0	26	35	308	0	369	13.93	58.15	14.77	10.7
3	0	21	27	300	0	348	15.51	58.07	15.58	12.94
4	0	24	30	299	0	353	13.24	61.61	13.59	11.22
5	0	24	30	308	0	362	14.2	59.68	14.8	11.04
6	0	27	29	301	0	357	14.39	58.27	14.67	11.52
7	0	23	34	301	0	358	13.53	59.52	13.95	11.22
8	0	23	32	296	0	351	13.55	62.31	13.78	11.36
9	0	22	26	307	0	355	13.22	62.05	13.33	11.12
10	0	25	33	305	0	363	14.78	58.04	15.41	11.26

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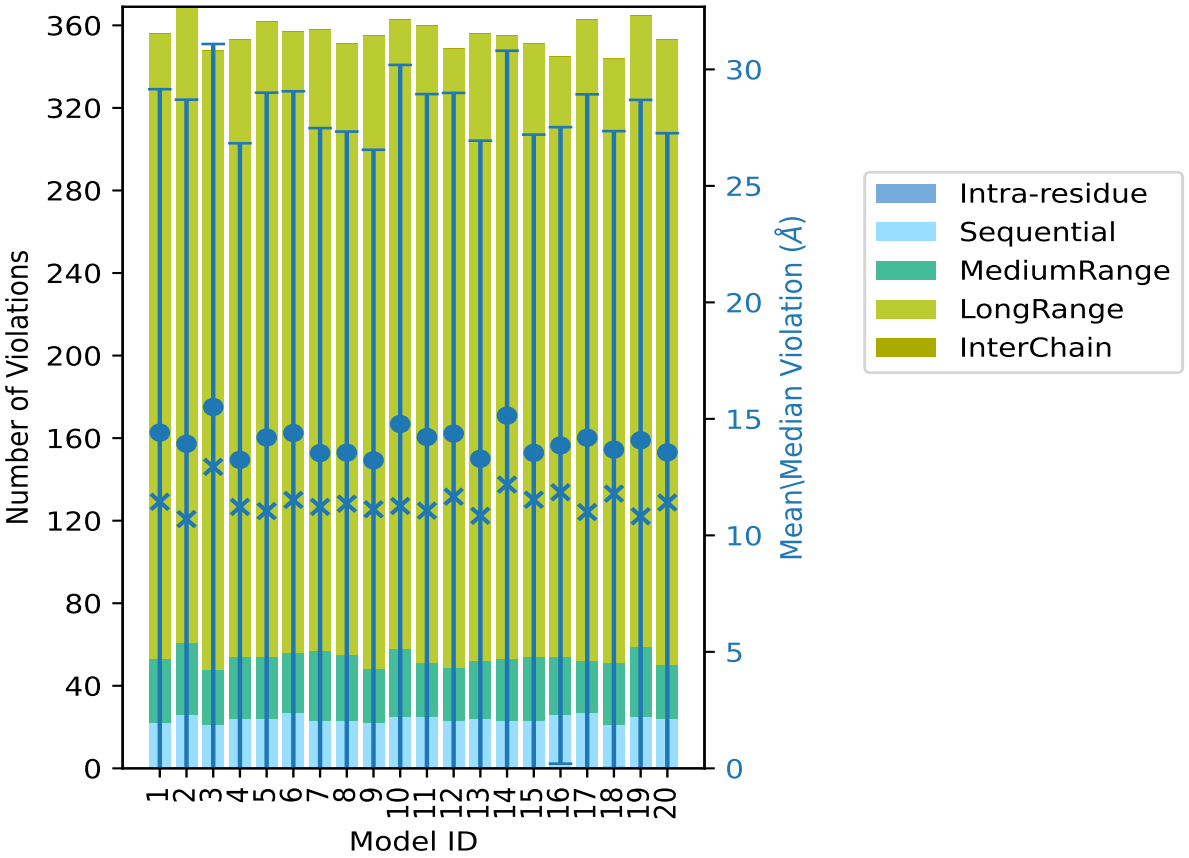
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	25	26	309	0	360	14.22	58.37	14.72	11.06
12	0	23	26	300	0	349	14.37	59.14	14.62	11.66
13	0	24	28	304	0	356	13.29	59.97	13.65	10.84
14	0	23	30	302	0	355	15.14	58.31	15.66	12.18
15	0	23	31	297	0	351	13.54	59.62	13.66	11.53
16	0	26	28	291	0	345	13.86	61.94	13.66	11.85
17	0	27	25	311	0	363	14.19	58.13	14.74	11.0
18	0	21	30	293	0	344	13.68	61.12	13.67	11.79
19	0	25	34	306	0	365	14.08	58.24	14.61	10.82
20	0	24	26	303	0	353	13.56	59.49	13.7	11.41

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

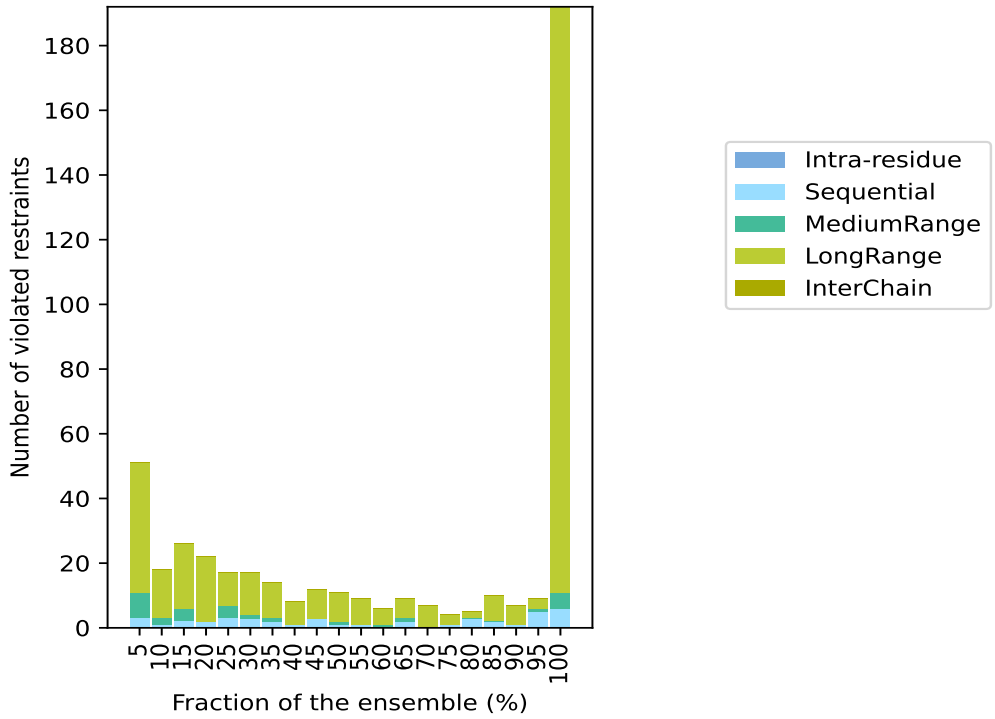
9.3 Distance violation statistics for the ensemble (i)

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, 824(IR:0, SQ:321, MR:215, LR:288, 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]	%
0	3	8	40	0	51	1	5.0
0	1	2	15	0	18	2	10.0
0	2	4	20	0	26	3	15.0
0	2	0	20	0	22	4	20.0
0	3	4	10	0	17	5	25.0
0	3	1	13	0	17	6	30.0
0	2	1	11	0	14	7	35.0
0	1	0	7	0	8	8	40.0
0	3	0	9	0	12	9	45.0
0	1	1	9	0	11	10	50.0
0	1	0	8	0	9	11	55.0
0	0	1	5	0	6	12	60.0
0	2	1	6	0	9	13	65.0
0	0	0	7	0	7	14	70.0
0	1	0	3	0	4	15	75.0
0	3	0	2	0	5	16	80.0
0	2	0	8	0	10	17	85.0
0	1	0	6	0	7	18	90.0
0	5	1	3	0	9	19	95.0
0	6	5	181	0	192	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

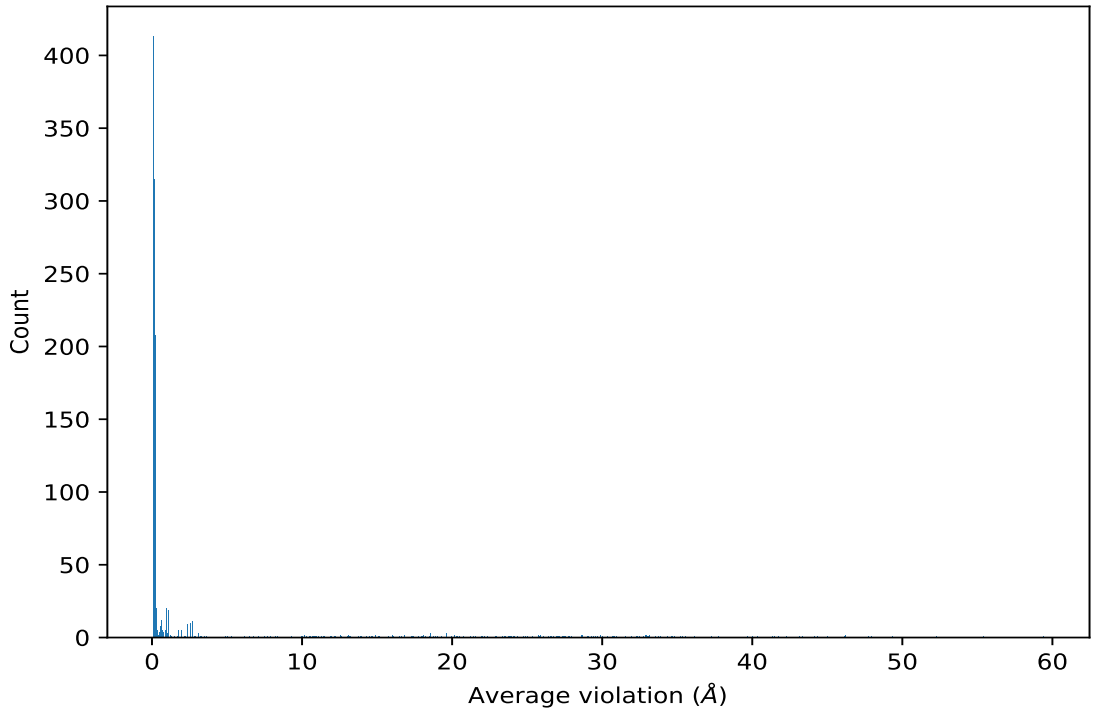
9.3.1 Bar graph : Distance violation statistics for the ensemble



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

The following table provides the mean and the standard deviation of theviolation 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)
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	20	59.44	1.5	58.76
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	20	55.39	0.23	55.36
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	20	52.26	0.41	52.34
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	20	49.35	7.59	50.18
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	20	47.99	0.22	48.01
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	20	47.78	8.22	49.78
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	20	46.24	3.13	47.09
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	20	46.21	2.88	47.45
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	20	46.14	3.04	47.53
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	20	45.0	3.02	46.45
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	20	44.39	6.25	45.29
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	20	44.19	0.2	44.2
(2,130)	1:43:A:THR:H	1:136:A:SER:O	20	43.37	6.42	43.87
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	20	43.16	3.02	44.56
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	20	42.3	3.15	43.42
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	20	41.8	0.19	41.84

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	20	41.47	0.14	41.5
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	20	41.39	2.67	42.8
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	20	40.32	2.79	41.8
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	20	40.0	2.73	41.34
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	20	39.67	3.14	40.94
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	20	37.76	3.26	38.83
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	20	37.28	3.35	38.18
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	20	36.15	2.19	35.19
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	20	35.57	4.37	35.69
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	20	35.39	2.63	35.52
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	20	35.21	3.42	35.96
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	20	34.81	5.9	32.66
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	20	34.65	3.46	35.38
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	20	34.62	2.58	35.41
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	20	34.38	2.75	35.03
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	20	33.85	1.44	33.44
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	20	33.74	9.28	37.2
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	20	33.59	3.62	34.05
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	20	33.55	6.57	31.64
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	20	33.19	7.17	32.88
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	20	33.13	2.46	33.11
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	20	33.13	2.58	33.58
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	20	33.07	3.21	32.86
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	20	33.04	2.79	33.78
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	20	32.92	0.52	32.76
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	20	32.9	2.46	33.03
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	20	32.89	3.25	32.64
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	20	32.89	7.43	32.86
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	20	32.76	0.67	32.7
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	20	32.47	6.96	32.14
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	20	32.34	6.51	33.25
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	20	32.28	2.29	32.22
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	20	31.93	3.38	32.7
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	20	31.58	2.88	33.36
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	20	30.97	3.66	31.18
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	20	30.83	0.62	30.69
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	20	30.75	0.33	30.68
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	20	30.68	0.63	30.58
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	20	30.4	3.01	32.29
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	20	30.0	2.87	31.76
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	20	29.86	2.72	31.02
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	20	29.86	2.78	31.1

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	20	29.66	3.0	31.15
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	20	29.5	0.2	29.48
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	20	29.45	0.66	29.38
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	20	29.28	0.35	29.36
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	20	29.05	8.48	30.3
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	20	29.04	3.53	29.22
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	20	28.68	3.06	29.8
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	20	28.66	3.09	28.3
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	20	28.65	0.52	28.64
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	20	28.63	3.33	28.88
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	20	27.96	2.78	29.87
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	20	27.83	0.17	27.85
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	20	27.71	0.35	27.67
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	20	27.59	2.2	27.58
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	20	27.49	3.69	27.76
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	20	27.45	2.98	29.58
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	20	27.36	4.16	27.66
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	20	27.13	0.43	27.21
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	20	27.09	0.45	27.19
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	20	27.0	0.63	26.9
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	20	26.99	7.21	27.71
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	20	26.76	0.48	26.66
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	20	26.72	3.77	26.89
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	20	26.6	0.3	26.58
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	20	26.54	3.12	26.18
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	20	26.45	0.65	26.36
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	20	26.09	0.7	25.98
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	20	25.88	2.85	27.27
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	20	25.85	3.07	27.26
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	20	25.82	3.63	25.63
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	20	25.79	2.92	27.97
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	20	25.79	3.0	26.8
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	20	25.73	3.75	26.06
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	20	25.3	0.53	25.12
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	20	25.04	3.36	25.44
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	20	24.9	2.17	25.17
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	20	24.74	0.44	24.76
(2,138)	1:154:A:SER:H	1:136:A:SER:O	20	24.37	0.34	24.32
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	20	24.14	3.05	25.76
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	20	24.05	0.65	24.02
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	20	23.99	2.68	22.32
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	20	23.89	3.46	23.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	20	23.8	0.53	23.76
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	20	23.78	0.3	23.74
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	20	23.56	0.52	23.43
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	20	23.49	0.41	23.47
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	20	23.31	0.69	23.22
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	20	22.98	4.91	22.56
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	20	22.85	0.45	22.91
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	20	22.33	0.68	22.16
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	20	22.11	0.5	21.97
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	20	22.03	0.45	21.97
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	20	21.93	0.65	21.84
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	20	21.55	2.23	21.58
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	20	21.41	0.44	21.46
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	20	21.23	0.32	21.22
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	20	20.76	0.47	20.68
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	20	20.73	0.31	20.73
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	20	20.46	0.69	20.4
(3,169)	1:187:A:SER:H	1:60:A:SER:O	20	20.39	0.61	20.29
(3,140)	1:123:A:SER:H	1:60:A:SER:O	20	20.32	0.45	20.24
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	20	20.26	0.49	20.26
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	20	20.16	1.9	20.45
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	20	20.16	0.46	20.1
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	20	19.95	0.37	20.04
(3,38)	1:153:A:THR:H	1:136:A:SER:O	20	19.61	0.35	19.6
(3,171)	1:189:A:MET:H	1:60:A:SER:O	20	19.61	0.6	19.48
(3,33)	1:132:A:THR:H	1:136:A:SER:O	20	19.6	0.12	19.58
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	20	19.27	3.5	20.02
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	20	19.02	0.45	18.89
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	20	18.88	0.34	18.88
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	20	18.75	0.24	18.77
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	20	18.59	0.64	18.52
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	20	18.59	0.23	18.59
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	20	18.58	2.0	19.39
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	20	18.45	0.19	18.46
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	20	18.2	2.19	19.08
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	20	18.12	0.3	18.14
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	20	18.11	0.15	18.12
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	20	18.04	0.28	18.04
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	20	17.97	0.43	17.85
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	20	17.77	0.31	17.77
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	20	17.44	0.49	17.39
(3,11)	1:81:A:THR:H	1:136:A:SER:O	20	17.35	0.32	17.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	20	17.34	3.76	17.76
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	20	16.82	0.61	16.7
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	20	16.81	0.53	16.93
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	20	16.6	0.3	16.51
(3,29)	1:123:A:SER:H	1:136:A:SER:O	20	16.54	0.43	16.49
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	20	16.13	0.25	16.19
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	20	16.01	2.71	17.32
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	20	16.01	0.44	15.94
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	20	15.75	0.25	15.8
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	20	15.16	0.22	15.14
(3,151)	1:154:A:SER:H	1:60:A:SER:O	20	15.1	0.56	14.97
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	20	14.92	4.04	14.69
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	20	14.92	0.24	14.92
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	20	14.74	0.45	14.8
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	20	14.64	0.68	14.54
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	20	14.54	0.29	14.5
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	20	14.35	0.24	14.3
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	20	14.27	0.46	14.44
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	20	13.98	0.38	13.97
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	20	13.87	2.84	14.24
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	20	13.75	0.19	13.7
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	20	13.24	0.4	13.16
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	20	13.17	0.28	13.17
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	20	13.14	0.24	13.18
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	20	13.14	0.65	13.07
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	20	13.01	0.21	13.03
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	20	12.64	3.06	11.25
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	20	12.6	0.26	12.6
(3,142)	1:126:A:SER:H	1:60:A:SER:O	20	12.56	0.41	12.49
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	20	12.23	0.71	12.16
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	20	12.17	2.88	14.08
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	20	11.99	0.3	11.96
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	20	11.92	0.24	11.86
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	20	11.52	0.28	11.48
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	20	11.41	0.68	11.34
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	20	11.3	0.17	11.28
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	20	11.12	0.37	11.19
(3,119)	1:81:A:THR:H	1:60:A:SER:O	20	11.07	0.4	11.17
(3,31)	1:126:A:SER:H	1:136:A:SER:O	20	10.98	0.37	10.92
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	20	10.88	2.56	12.34
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	20	10.8	0.29	10.84
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	20	10.75	3.66	10.86

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,150)	1:153:A:THR:H	1:60:A:SER:O	20	10.66	0.48	10.49
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	20	10.58	0.2	10.52
(3,128)	1:96:A:THR:H	1:60:A:SER:O	20	10.52	0.29	10.56
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	20	10.29	3.0	10.4
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	20	10.15	0.63	10.05
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	20	10.15	3.86	10.39
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	20	10.01	0.38	9.98
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	20	9.98	0.39	9.95
(3,22)	1:96:A:THR:H	1:136:A:SER:O	20	9.34	0.14	9.34
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	20	8.39	0.28	8.43
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	20	8.22	0.34	8.32
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	20	7.93	0.28	7.92
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	20	7.74	3.65	8.28
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	20	7.55	0.27	7.57
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	20	7.14	0.74	7.13
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	20	6.78	0.29	6.82
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	20	6.53	3.69	6.83
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	20	6.49	0.19	6.5
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	20	6.15	0.31	6.18
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	20	5.31	2.09	6.04
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	20	5.26	0.37	5.24
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	20	4.89	0.21	4.9
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	20	3.63	0.45	3.47
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	20	3.52	0.24	3.48
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG13	20	3.06	0.19	3.04
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	20	3.06	0.19	3.04
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	20	3.06	0.19	3.04
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB1	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB3	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG23	1:186:A:ALA:HB1	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG13	1:186:A:ALA:HB1	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG13	1:186:A:ALA:HB2	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB2	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG21	1:186:A:ALA:HB3	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG13	1:186:A:ALA:HB3	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG22	1:186:A:ALA:HB3	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG22	1:186:A:ALA:HB2	20	2.67	0.12	2.69
(1,900)	1:111:A:ILE:HG21	1:186:A:ALA:HB1	20	2.67	0.12	2.69
(1,753)	1:59:A:VAL:HG11	1:69:A:ILE:HG13	20	2.57	0.38	2.68
(1,753)	1:59:A:VAL:HG12	1:69:A:ILE:HG12	20	2.57	0.38	2.68
(1,753)	1:59:A:VAL:HG22	1:69:A:ILE:HG12	20	2.57	0.38	2.68
(1,753)	1:59:A:VAL:HG11	1:69:A:ILE:HG12	20	2.57	0.38	2.68

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,753)	1:59:A:VAL:HG21	1:69:A:ILE:HG12	20	2.57	0.38	2.68
(1,753)	1:59:A:VAL:HG22	1:69:A:ILE:HG13	20	2.57	0.38	2.68
(1,753)	1:59:A:VAL:HG12	1:69:A:ILE:HG13	20	2.57	0.38	2.68
(1,753)	1:59:A:VAL:HG21	1:69:A:ILE:HG13	20	2.57	0.38	2.68
(1,753)	1:59:A:VAL:HG13	1:69:A:ILE:HG13	20	2.57	0.38	2.68
(1,753)	1:59:A:VAL:HG23	1:69:A:ILE:HG13	20	2.57	0.38	2.68
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD13	20	2.39	0.23	2.34
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD12	20	2.39	0.23	2.34
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD11	20	2.39	0.23	2.34
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD12	20	2.39	0.23	2.34
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD11	20	2.39	0.23	2.34
(1,898)	1:111:A:ILE:HG21	1:185:A:ILE:HD11	20	2.39	0.23	2.34
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD13	20	2.39	0.23	2.34
(1,898)	1:111:A:ILE:HG23	1:185:A:ILE:HD11	20	2.39	0.23	2.34
(1,898)	1:111:A:ILE:HG21	1:185:A:ILE:HD12	20	2.39	0.23	2.34
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	20	2.24	0.52	1.97
(1,1096)	1:170:A:VAL:HG12	1:185:A:ILE:HG13	20	1.99	0.24	2.02
(1,1096)	1:170:A:VAL:HG13	1:185:A:ILE:HG13	20	1.99	0.24	2.02
(1,1096)	1:170:A:VAL:HG23	1:185:A:ILE:HG13	20	1.99	0.24	2.02
(1,1096)	1:170:A:VAL:HG11	1:185:A:ILE:HG13	20	1.99	0.24	2.02
(1,1096)	1:170:A:VAL:HG21	1:185:A:ILE:HG13	20	1.99	0.24	2.02
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	20	1.77	0.15	1.72
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG13	20	1.77	0.15	1.72
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG12	20	1.77	0.15	1.72
(1,896)	1:111:A:ILE:HD11	1:185:A:ILE:HG13	20	1.77	0.15	1.72
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG12	20	1.77	0.15	1.72
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	20	1.23	0.15	1.3
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	20	1.23	0.15	1.3
(1,1045)	1:155:A:ILE:HG21	1:183:A:PHE:HD1	20	1.07	0.27	1.05
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	20	1.07	0.27	1.05
(1,1045)	1:155:A:ILE:HG22	1:183:A:PHE:HD1	20	1.07	0.27	1.05
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD2	20	1.07	0.27	1.05
(1,1045)	1:155:A:ILE:HG22	1:183:A:PHE:HD2	20	1.07	0.27	1.05
(1,1045)	1:155:A:ILE:HG23	1:183:A:PHE:HD1	20	1.07	0.27	1.05
(1,1045)	1:155:A:ILE:HG21	1:183:A:PHE:HD2	20	1.07	0.27	1.05
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	20	1.03	0.13	1.02
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	20	1.03	0.13	1.02
(1,737)	1:155:A:ILE:HG23	1:183:A:PHE:H	20	1.03	0.13	1.02
(1,687)	1:111:A:ILE:HG13	1:183:A:PHE:H	20	0.99	0.18	1.02
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	20	0.99	0.18	1.02
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG22	20	0.96	0.05	0.96
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG13	20	0.96	0.05	0.96

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG21	20	0.96	0.05	0.96
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG23	20	0.96	0.05	0.96
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	20	0.89	0.1	0.87
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	20	0.88	0.04	0.9
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	20	0.88	0.04	0.9
(1,607)	1:155:A:ILE:HG21	1:160:A:TRP:HE3	20	0.88	0.04	0.9
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	20	0.88	0.08	0.9
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	20	0.76	0.17	0.83
(1,813)	1:76:A:ILE:HG13	1:87:A:TRP:HE3	20	0.76	0.17	0.83
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	20	0.74	0.12	0.78
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	20	0.74	0.12	0.78
(1,736)	1:155:A:ILE:HG23	1:182:A:PHE:H	20	0.74	0.12	0.78
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	20	0.74	0.16	0.75
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	20	0.65	0.21	0.62
(1,901)	1:111:A:ILE:HG23	1:155:A:ILE:HD13	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG12	1:155:A:ILE:HD11	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG22	1:155:A:ILE:HD11	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG12	1:155:A:ILE:HD12	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG22	1:155:A:ILE:HD12	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD11	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG13	1:155:A:ILE:HD13	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG23	1:155:A:ILE:HD12	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD12	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD13	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG12	1:155:A:ILE:HD13	20	0.62	0.21	0.61
(1,901)	1:111:A:ILE:HG22	1:155:A:ILE:HD13	20	0.62	0.21	0.61
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	20	0.56	0.12	0.59
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	20	0.56	0.12	0.59
(1,731)	1:155:A:ILE:HG23	1:185:A:ILE:H	20	0.56	0.12	0.59
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	20	0.36	0.12	0.36
(1,686)	1:111:A:ILE:HG12	1:182:A:PHE:H	20	0.36	0.12	0.36
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	20	0.29	0.02	0.28
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	20	0.25	0.03	0.26
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	20	0.25	0.01	0.24
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	20	0.24	0.04	0.24
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	20	0.24	0.04	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	20	0.23	0.02	0.24
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	20	0.22	0.03	0.23
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	20	0.22	0.02	0.22
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	20	0.21	0.03	0.22
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	20	0.21	0.03	0.22
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	20	0.21	0.03	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	20	0.21	0.03	0.22
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	20	0.21	0.01	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	20	0.21	0.01	0.21
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	20	0.21	0.02	0.21
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	20	0.21	0.02	0.21
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	20	0.21	0.04	0.22
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	20	0.21	0.07	0.2
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	20	0.21	0.07	0.2
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	20	0.21	0.04	0.2
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	20	0.2	0.04	0.21
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	20	0.2	0.04	0.21
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	20	0.2	0.04	0.21
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	20	0.2	0.04	0.21
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	20	0.2	0.04	0.21
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	20	0.2	0.04	0.21
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	20	0.2	0.04	0.21
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	20	0.2	0.04	0.21
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	20	0.19	0.02	0.2
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	20	0.18	0.04	0.18
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	20	0.18	0.04	0.18
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	20	0.18	0.02	0.18
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	20	0.18	0.02	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	20	0.15	0.03	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	20	0.15	0.03	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	20	0.15	0.03	0.16
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	20	0.15	0.01	0.15
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	20	0.14	0.02	0.14
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	20	0.14	0.02	0.14
(3,146)	1:145:A:MET:H	1:60:A:SER:O	19	0.99	0.25	0.95
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	19	0.79	0.17	0.72
(1,814)	1:76:A:ILE:HG13	1:87:A:TRP:HE1	19	0.79	0.17	0.72
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	19	0.21	0.07	0.21
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	19	0.21	0.07	0.21
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	19	0.21	0.07	0.21
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	19	0.2	0.05	0.22
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	19	0.17	0.04	0.16
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	19	0.17	0.02	0.17
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	19	0.17	0.02	0.17
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	19	0.16	0.04	0.15
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	19	0.16	0.03	0.15
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	19	0.14	0.02	0.15
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	19	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	19	0.14	0.01	0.14
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	19	0.12	0.01	0.12
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	19	0.12	0.01	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	19	0.12	0.01	0.11
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	19	0.11	0.01	0.11
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	18	5.01	3.75	4.76
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	18	0.19	0.06	0.18
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	18	0.19	0.06	0.18
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	18	0.19	0.06	0.18
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	18	0.19	0.06	0.18
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	18	0.19	0.06	0.18
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	18	0.19	0.06	0.18
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	18	0.19	0.06	0.18
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	18	0.19	0.06	0.18
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	18	0.19	0.06	0.18
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	18	0.18	0.05	0.18
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	18	0.18	0.05	0.18
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	18	0.17	0.05	0.16
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	18	0.17	0.05	0.16
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	18	0.17	0.04	0.17
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	18	0.17	0.04	0.17
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	18	0.17	0.04	0.17
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	18	0.17	0.02	0.17
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	18	0.17	0.05	0.15
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	18	0.14	0.02	0.14
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	18	0.13	0.03	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG21	17	1.06	0.25	1.1
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG23	17	1.06	0.25	1.1
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG22	17	1.06	0.25	1.1
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG12	17	1.06	0.25	1.1
(1,768)	1:67:A:ASP:HB3	1:94:A:ILE:HG23	17	1.06	0.25	1.1
(1,1050)	1:155:A:ILE:HG13	1:167:A:LEU:HG	17	0.7	0.35	0.85
(1,1050)	1:155:A:ILE:HG21	1:167:A:LEU:HG	17	0.7	0.35	0.85
(1,1050)	1:155:A:ILE:HG23	1:167:A:LEU:HG	17	0.7	0.35	0.85
(1,1050)	1:155:A:ILE:HG22	1:167:A:LEU:HG	17	0.7	0.35	0.85
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	17	0.23	0.06	0.21
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	17	0.23	0.06	0.21
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	17	0.21	0.03	0.21
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	17	0.21	0.03	0.21
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	17	0.19	0.06	0.2
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	17	0.19	0.06	0.2
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	17	0.18	0.08	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	17	0.18	0.08	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	17	0.18	0.08	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	17	0.18	0.08	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	17	0.18	0.08	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	17	0.18	0.08	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	17	0.18	0.08	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	17	0.18	0.08	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	17	0.18	0.08	0.16
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	17	0.18	0.03	0.18
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	17	0.17	0.04	0.17
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	17	0.13	0.02	0.13
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	17	0.13	0.02	0.13
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	17	0.13	0.02	0.13
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	17	0.13	0.02	0.13
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	16	0.22	0.06	0.2
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	16	0.22	0.06	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	16	0.18	0.04	0.18
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	16	0.14	0.03	0.14
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	16	0.12	0.02	0.12
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	16	0.12	0.01	0.12
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	16	0.11	0.01	0.11
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	16	0.11	0.01	0.11
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	15	2.84	1.03	3.27
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	15	0.19	0.04	0.18
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	15	0.17	0.02	0.17
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	15	0.15	0.03	0.15
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	15	0.13	0.04	0.12
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	15	0.13	0.01	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	15	0.13	0.01	0.13
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	15	0.13	0.01	0.13
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	14	3.48	2.53	4.11
(1,847)	1:100:A:ILE:HG12	1:143:A:ARG:HA	14	0.6	0.26	0.72
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	14	0.6	0.26	0.72
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	14	0.36	0.05	0.34
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	14	0.27	0.03	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	14	0.27	0.03	0.26
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	14	0.24	0.07	0.26
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	14	0.23	0.05	0.25
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	14	0.23	0.05	0.25
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	14	0.23	0.05	0.25
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	14	0.21	0.07	0.22
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	14	0.13	0.02	0.13
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	14	0.13	0.02	0.12
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	13	3.21	3.24	1.62
(1,671)	1:100:A:ILE:HG12	1:143:A:ARG:H	13	0.44	0.2	0.47
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	13	0.44	0.2	0.47
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	13	0.29	0.07	0.28
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	13	0.19	0.08	0.18
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	13	0.19	0.08	0.18
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	13	0.19	0.06	0.19
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	13	0.19	0.06	0.19
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	13	0.17	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	13	0.17	0.03	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	13	0.17	0.03	0.16
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	13	0.17	0.05	0.17
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	13	0.13	0.02	0.13
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	13	0.12	0.01	0.12
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	13	0.12	0.01	0.12
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	12	0.23	0.1	0.21
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	12	0.23	0.1	0.21
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	12	0.22	0.04	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	12	0.22	0.04	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	12	0.22	0.04	0.23
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	12	0.22	0.06	0.22
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	12	0.15	0.03	0.14
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	12	0.12	0.03	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	12	0.12	0.03	0.11
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	12	0.12	0.01	0.12
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	12	0.12	0.01	0.12
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	12	0.12	0.01	0.12
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	11	1.54	0.7	1.31
(1,747)	1:57:A:HIS:HB3	1:69:A:ILE:HG21	11	1.05	0.32	1.02
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG23	11	1.05	0.32	1.02
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG22	11	1.05	0.32	1.02
(1,747)	1:57:A:HIS:HB3	1:69:A:ILE:HG23	11	1.05	0.32	1.02
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG21	11	1.05	0.32	1.02
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG13	11	1.05	0.32	1.02
(1,747)	1:57:A:HIS:HB3	1:69:A:ILE:HG12	11	1.05	0.32	1.02
(1,822)	1:76:A:ILE:HG12	1:90:A:LEU:HD12	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG12	1:90:A:LEU:HD13	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG23	1:90:A:LEU:HD13	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG22	1:90:A:LEU:HD11	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG22	1:90:A:LEU:HD12	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG22	1:90:A:LEU:HD21	11	0.99	0.66	1.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,822)	1:76:A:ILE:HG12	1:90:A:LEU:HD11	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG13	1:90:A:LEU:HD12	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG21	1:90:A:LEU:HD23	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG13	1:90:A:LEU:HD11	11	0.99	0.66	1.26
(1,822)	1:76:A:ILE:HG22	1:90:A:LEU:HD13	11	0.99	0.66	1.26
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	11	0.17	0.06	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	11	0.17	0.06	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	11	0.17	0.06	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	11	0.17	0.06	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	11	0.17	0.06	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	11	0.17	0.06	0.15
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	11	0.17	0.05	0.16
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	11	0.17	0.05	0.16
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	11	0.16	0.05	0.14
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	11	0.16	0.05	0.14
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	11	0.16	0.05	0.14
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	11	0.15	0.02	0.16
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	11	0.13	0.02	0.12
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	11	0.13	0.02	0.12
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	11	0.13	0.02	0.12
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	11	0.13	0.02	0.12
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	11	0.13	0.02	0.12
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	11	0.13	0.02	0.12
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	11	0.12	0.02	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	11	0.12	0.02	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	11	0.12	0.02	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	11	0.12	0.02	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	11	0.12	0.02	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	11	0.12	0.02	0.11
(1,903)	1:111:A:ILE:HG12	1:155:A:ILE:HG13	10	0.45	0.19	0.48
(1,903)	1:111:A:ILE:HG21	1:155:A:ILE:HG13	10	0.45	0.19	0.48
(1,903)	1:111:A:ILE:HG23	1:155:A:ILE:HG13	10	0.45	0.19	0.48
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	10	0.22	0.04	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	10	0.22	0.04	0.21
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	10	0.22	0.04	0.21
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	10	0.2	0.07	0.2
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	10	0.2	0.07	0.2
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	10	0.19	0.08	0.17
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	10	0.19	0.08	0.17
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	10	0.17	0.05	0.15
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	10	0.17	0.05	0.15
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	10	0.16	0.02	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	10	0.16	0.02	0.16
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	10	0.15	0.03	0.15
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	10	0.15	0.03	0.15
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	10	0.15	0.04	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	10	0.15	0.04	0.14
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	10	0.14	0.02	0.13
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	10	0.14	0.02	0.13
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	10	0.14	0.02	0.13
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	10	0.14	0.02	0.13
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	10	0.14	0.02	0.13
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	10	0.14	0.02	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	10	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	10	0.13	0.02	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	10	0.13	0.02	0.12
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	10	0.12	0.02	0.11
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	9	2.93	0.96	2.89
(1,605)	1:155:A:ILE:HG22	1:160:A:TRP:HE1	9	0.27	0.11	0.28
(1,605)	1:155:A:ILE:HG23	1:160:A:TRP:HE1	9	0.27	0.11	0.28
(1,605)	1:155:A:ILE:HG21	1:160:A:TRP:HE1	9	0.27	0.11	0.28
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	9	0.22	0.09	0.16
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	9	0.22	0.09	0.16
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	9	0.2	0.02	0.2
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	9	0.2	0.02	0.2
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	9	0.16	0.02	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	9	0.16	0.02	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	9	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	9	0.16	0.02	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	9	0.16	0.02	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	9	0.16	0.02	0.16
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	9	0.16	0.03	0.16
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	9	0.16	0.03	0.16
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	9	0.14	0.04	0.14
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	9	0.14	0.04	0.14
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	9	0.14	0.04	0.14
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	9	0.14	0.04	0.14
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	9	0.14	0.03	0.12
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	9	0.14	0.03	0.12
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	9	0.14	0.03	0.13
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	9	0.14	0.03	0.12
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	9	0.14	0.03	0.12
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	9	0.14	0.03	0.12
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	9	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	9	0.14	0.02	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	9	0.14	0.02	0.14
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	9	0.13	0.02	0.13
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	9	0.12	0.01	0.12
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	9	0.11	0.01	0.11
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	9	0.11	0.01	0.11
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	8	1.71	0.25	1.77
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	8	0.19	0.05	0.18
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	8	0.19	0.05	0.18
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	8	0.19	0.05	0.18
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	8	0.19	0.05	0.18
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	8	0.19	0.05	0.18
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	8	0.19	0.05	0.18
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	8	0.18	0.07	0.18
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	8	0.18	0.07	0.18
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	8	0.17	0.05	0.16
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	8	0.17	0.05	0.16
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	8	0.16	0.04	0.15
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	8	0.16	0.04	0.15
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	8	0.14	0.02	0.14
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	8	0.14	0.03	0.12
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	8	0.14	0.02	0.13
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	8	0.13	0.02	0.12
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	8	0.12	0.02	0.11
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	8	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	8	0.12	0.02	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	8	0.12	0.02	0.11
(1,902)	1:111:A:ILE:HD13	1:155:A:ILE:HG21	7	0.35	0.17	0.4
(1,902)	1:111:A:ILE:HD11	1:155:A:ILE:HG13	7	0.35	0.17	0.4
(1,902)	1:111:A:ILE:HD12	1:155:A:ILE:HG13	7	0.35	0.17	0.4
(1,902)	1:111:A:ILE:HD13	1:155:A:ILE:HG13	7	0.35	0.17	0.4
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD1	7	0.25	0.07	0.29
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD2	7	0.25	0.07	0.29
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE1	7	0.24	0.03	0.24
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE2	7	0.24	0.03	0.24
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE1	7	0.24	0.03	0.24
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE2	7	0.24	0.03	0.24
(1,935)	1:117:A:PHE:HE1	1:174:A:ILE:HB	7	0.2	0.06	0.22
(1,935)	1:117:A:PHE:HE2	1:174:A:ILE:HB	7	0.2	0.06	0.22
(2,11)	1:70:A:LEU:O	1:74:A:ILE:H	7	0.2	0.04	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD11	7	0.19	0.07	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD12	7	0.19	0.07	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD13	7	0.19	0.07	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD21	7	0.19	0.07	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD22	7	0.19	0.07	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD23	7	0.19	0.07	0.18
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD1	7	0.19	0.05	0.19
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD2	7	0.19	0.05	0.19
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD1	7	0.19	0.05	0.19
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD2	7	0.19	0.05	0.19
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD1	7	0.19	0.05	0.19
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD2	7	0.19	0.05	0.19
(1,670)	1:100:A:ILE:HD11	1:143:A:ARG:H	7	0.17	0.03	0.18
(1,670)	1:100:A:ILE:HD12	1:143:A:ARG:H	7	0.17	0.03	0.18
(1,670)	1:100:A:ILE:HD13	1:143:A:ARG:H	7	0.17	0.03	0.18
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB2	7	0.15	0.03	0.14
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB3	7	0.15	0.03	0.14
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB2	7	0.15	0.03	0.14
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB3	7	0.15	0.03	0.14
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB2	7	0.15	0.03	0.14
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB3	7	0.15	0.03	0.14
(2,12)	1:70:A:LEU:O	1:74:A:ILE:N	7	0.14	0.03	0.13
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG2	7	0.14	0.01	0.14
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG3	7	0.14	0.01	0.14
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD11	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD12	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD13	7	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD21	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD22	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD23	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD11	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD12	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD13	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD21	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD22	7	0.13	0.02	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD23	7	0.13	0.02	0.13
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB2	7	0.13	0.02	0.12
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB3	7	0.13	0.02	0.12
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB2	7	0.13	0.02	0.12
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB3	7	0.13	0.02	0.12
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB2	7	0.13	0.02	0.12
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB3	7	0.13	0.02	0.12
(2,9)	1:69:A:ILE:O	1:73:A:LEU:H	7	0.12	0.02	0.12
(1,266)	1:87:A:TRP:HB2	1:88:A:GLN:H	7	0.12	0.02	0.11
(1,266)	1:87:A:TRP:HB3	1:88:A:GLN:H	7	0.12	0.02	0.11
(1,193)	1:160:A:TRP:HA	1:161:A:GLU:H	7	0.12	0.0	0.12
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB2	7	0.12	0.01	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB3	7	0.12	0.01	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB2	7	0.12	0.01	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB3	7	0.12	0.01	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB2	7	0.12	0.01	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB3	7	0.12	0.01	0.11
(3,74)	1:124:A:LEU:H	1:198:A:CYS:O	6	3.25	2.95	3.2
(3,104)	1:189:A:MET:H	1:198:A:CYS:O	6	2.17	1.14	2.64
(1,815)	1:76:A:ILE:HG13	1:87:A:TRP:HD1	6	0.35	0.12	0.3
(1,815)	1:76:A:ILE:HG22	1:87:A:TRP:HD1	6	0.35	0.12	0.3
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE1	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE2	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE1	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE2	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE1	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE2	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE1	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE2	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE1	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE2	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE1	6	0.24	0.1	0.24
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE2	6	0.24	0.1	0.24
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB2	6	0.2	0.05	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB3	6	0.2	0.05	0.22
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD11	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD12	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD13	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD11	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD12	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD13	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD11	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD12	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD13	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD11	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD12	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD13	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD11	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD12	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD13	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD11	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD12	6	0.2	0.06	0.16
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD13	6	0.2	0.06	0.16
(1,261)	1:83:A:ASP:HB3	1:84:A:SER:H	6	0.19	0.02	0.19
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD1	6	0.18	0.06	0.19
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD2	6	0.18	0.06	0.19
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD1	6	0.18	0.06	0.19
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD2	6	0.18	0.06	0.19
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD1	6	0.18	0.06	0.19
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD2	6	0.18	0.06	0.19
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD11	6	0.16	0.05	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD12	6	0.16	0.05	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD13	6	0.16	0.05	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD21	6	0.16	0.05	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD22	6	0.16	0.05	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD23	6	0.16	0.05	0.15
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB2	6	0.15	0.03	0.15
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB3	6	0.15	0.03	0.15
(1,226)	1:205:A:LYS:HA	1:206:A:LEU:H	6	0.15	0.01	0.15
(1,708)	1:125:A:LEU:H	1:146:A:LEU:HA	6	0.14	0.06	0.11
(2,45)	1:96:A:THR:O	1:100:A:ILE:H	6	0.14	0.03	0.14
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB2	6	0.14	0.02	0.14
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB3	6	0.14	0.02	0.14
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB2	6	0.14	0.02	0.14
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB3	6	0.14	0.02	0.14
(1,406)	1:118:A:GLN:HA	1:121:A:ALA:H	6	0.12	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,330)	1:145:A:MET:HB2	1:146:A:LEU:H	6	0.12	0.02	0.12
(1,330)	1:145:A:MET:HB3	1:146:A:LEU:H	6	0.12	0.02	0.12
(1,1056)	1:156:A:PHE:HA	1:185:A:ILE:HB	6	0.12	0.01	0.11
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB2	6	0.11	0.01	0.11
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB3	6	0.11	0.01	0.11
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB2	6	0.11	0.01	0.11
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB3	6	0.11	0.01	0.11
(1,904)	1:111:A:ILE:HG12	1:182:A:PHE:HD2	5	0.27	0.08	0.29
(1,904)	1:111:A:ILE:HG21	1:182:A:PHE:HD2	5	0.27	0.08	0.29
(1,904)	1:111:A:ILE:HG13	1:182:A:PHE:HD2	5	0.27	0.08	0.29
(1,904)	1:111:A:ILE:HG13	1:182:A:PHE:HD1	5	0.27	0.08	0.29
(1,891)	1:108:A:TRP:HD1	1:170:A:VAL:HB	5	0.25	0.11	0.33
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB2	5	0.19	0.03	0.19
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB3	5	0.19	0.03	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD11	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD12	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD13	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD21	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD22	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD23	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD11	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD12	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD13	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD21	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD22	5	0.18	0.04	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD23	5	0.18	0.04	0.19
(1,540)	1:115:A:LEU:HD11	1:118:A:GLN:H	5	0.18	0.03	0.18
(1,540)	1:115:A:LEU:HD12	1:118:A:GLN:H	5	0.18	0.03	0.18
(1,540)	1:115:A:LEU:HD13	1:118:A:GLN:H	5	0.18	0.03	0.18
(1,540)	1:115:A:LEU:HD21	1:118:A:GLN:H	5	0.18	0.03	0.18
(1,540)	1:115:A:LEU:HD22	1:118:A:GLN:H	5	0.18	0.03	0.18
(1,540)	1:115:A:LEU:HD23	1:118:A:GLN:H	5	0.18	0.03	0.18
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD11	5	0.17	0.04	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD12	5	0.17	0.04	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD13	5	0.17	0.04	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD21	5	0.17	0.04	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD22	5	0.17	0.04	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD23	5	0.17	0.04	0.17
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD11	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD12	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD13	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD21	5	0.17	0.05	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD22	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD23	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD11	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD12	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD13	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD21	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD22	5	0.17	0.05	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD23	5	0.17	0.05	0.16
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD1	5	0.17	0.04	0.18
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD2	5	0.17	0.04	0.18
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD1	5	0.17	0.04	0.18
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD2	5	0.17	0.04	0.18
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD1	5	0.17	0.04	0.18
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD2	5	0.17	0.04	0.18
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB2	5	0.16	0.05	0.14
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB3	5	0.16	0.05	0.14
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB2	5	0.16	0.05	0.14
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB3	5	0.16	0.05	0.14
(1,1009)	1:149:A:LEU:HD11	1:160:A:TRP:HE1	5	0.15	0.02	0.15
(1,1009)	1:149:A:LEU:HD12	1:160:A:TRP:HE1	5	0.15	0.02	0.15
(1,1009)	1:149:A:LEU:HD13	1:160:A:TRP:HE1	5	0.15	0.02	0.15
(1,1009)	1:149:A:LEU:HD21	1:160:A:TRP:HE1	5	0.15	0.02	0.15
(1,1009)	1:149:A:LEU:HD22	1:160:A:TRP:HE1	5	0.15	0.02	0.15
(1,1009)	1:149:A:LEU:HD23	1:160:A:TRP:HE1	5	0.15	0.02	0.15
(1,293)	1:110:A:ARG:HB2	1:111:A:ILE:H	5	0.15	0.01	0.14
(1,293)	1:110:A:ARG:HB3	1:111:A:ILE:H	5	0.15	0.01	0.14
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB2	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB3	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB2	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB3	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB2	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB3	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB2	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB3	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB2	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB3	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB2	5	0.15	0.01	0.15
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB3	5	0.15	0.01	0.15
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG21	5	0.14	0.01	0.13
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG22	5	0.14	0.01	0.13
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG23	5	0.14	0.01	0.13
(1,660)	1:95:A:TYR:HB2	1:139:A:THR:H	5	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,660)	1:95:A:TYR:HB3	1:139:A:THR:H	5	0.14	0.02	0.14
(1,534)	1:80:A:GLN:HG2	1:82:A:LYS:H	5	0.13	0.01	0.12
(1,534)	1:80:A:GLN:HG3	1:82:A:LYS:H	5	0.13	0.01	0.12
(1,658)	1:77:A:ARG:HB2	1:87:A:TRP:H	5	0.12	0.04	0.1
(1,658)	1:77:A:ARG:HB3	1:87:A:TRP:H	5	0.12	0.04	0.1
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB2	5	0.12	0.01	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB3	5	0.12	0.01	0.11
(1,756)	1:61:A:HIS:HB3	1:69:A:ILE:HG13	4	0.45	0.24	0.42
(1,781)	1:70:A:LEU:HG	1:94:A:ILE:HG13	4	0.38	0.11	0.44
(1,781)	1:70:A:LEU:HG	1:94:A:ILE:HG12	4	0.38	0.11	0.44
(1,749)	1:58:A:ASP:HB3	1:69:A:ILE:HG12	4	0.32	0.16	0.26
(1,749)	1:58:A:ASP:HB3	1:69:A:ILE:HG13	4	0.32	0.16	0.26
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE1	4	0.32	0.05	0.36
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE2	4	0.32	0.05	0.36
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE1	4	0.32	0.05	0.36
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE2	4	0.32	0.05	0.36
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE1	4	0.32	0.05	0.36
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE2	4	0.32	0.05	0.36
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE1	4	0.27	0.07	0.27
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE2	4	0.27	0.07	0.27
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE1	4	0.27	0.07	0.27
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE2	4	0.27	0.07	0.27
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD11	4	0.24	0.07	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD12	4	0.24	0.07	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD13	4	0.24	0.07	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD21	4	0.24	0.07	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD22	4	0.24	0.07	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD23	4	0.24	0.07	0.28
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG2	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG3	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG2	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG3	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG2	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG3	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG2	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG3	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG2	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG3	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG2	4	0.2	0.06	0.19
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG3	4	0.2	0.06	0.19
(1,316)	1:124:A:LEU:HG	1:125:A:LEU:H	4	0.2	0.04	0.18
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD1	4	0.2	0.05	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD2	4	0.2	0.05	0.22
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD1	4	0.2	0.05	0.22
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD2	4	0.2	0.05	0.22
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD1	4	0.2	0.05	0.22
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD2	4	0.2	0.05	0.22
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB1	4	0.18	0.04	0.2
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB2	4	0.18	0.04	0.2
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB3	4	0.18	0.04	0.2
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB1	4	0.18	0.04	0.2
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB2	4	0.18	0.04	0.2
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB3	4	0.18	0.04	0.2
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB2	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB3	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB2	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB3	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB2	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB3	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB2	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB3	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB2	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB3	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB2	4	0.18	0.04	0.18
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB3	4	0.18	0.04	0.18
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB2	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB3	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB2	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB3	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB2	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB3	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB2	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB3	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB2	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB3	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB2	4	0.17	0.02	0.18
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB3	4	0.17	0.02	0.18
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE1	4	0.16	0.02	0.16
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE2	4	0.16	0.02	0.16
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE1	4	0.16	0.02	0.16
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE2	4	0.16	0.02	0.16
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE1	4	0.16	0.02	0.16
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE2	4	0.16	0.02	0.16
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG2	4	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG3	4	0.16	0.01	0.16
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG2	4	0.16	0.01	0.16
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG3	4	0.16	0.01	0.16
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG2	4	0.16	0.01	0.16
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG3	4	0.16	0.01	0.16
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD11	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD12	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD13	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD21	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD22	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD23	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD11	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD12	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD13	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD21	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD22	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD23	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD11	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD12	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD13	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD21	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD22	4	0.15	0.03	0.14
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD23	4	0.15	0.03	0.14
(1,740)	1:156:A:PHE:H	1:167:A:LEU:HG	4	0.14	0.05	0.12
(1,894)	1:109:A:ARG:HG2	1:127:A:VAL:HB	4	0.14	0.03	0.14
(1,894)	1:109:A:ARG:HG3	1:127:A:VAL:HB	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE1	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE2	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE1	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE2	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE1	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE2	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE1	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE2	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE1	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE2	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE1	4	0.14	0.03	0.14
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE2	4	0.14	0.03	0.14
(1,315)	1:123:A:SER:HB2	1:124:A:LEU:H	4	0.12	0.01	0.12
(1,315)	1:123:A:SER:HB3	1:124:A:LEU:H	4	0.12	0.01	0.12
(1,1012)	1:150:A:ALA:HB1	1:159:A:SER:HA	4	0.12	0.01	0.12
(1,1012)	1:150:A:ALA:HB2	1:159:A:SER:HA	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1012)	1:150:A:ALA:HB3	1:159:A:SER:HA	4	0.12	0.01	0.12
(1,742)	1:157:A:PRO:HG2	1:186:A:ALA:H	4	0.11	0.01	0.11
(1,742)	1:157:A:PRO:HG3	1:186:A:ALA:H	4	0.11	0.01	0.11
(2,59)	1:103:A:GLU:O	1:107:A:ARG:H	4	0.11	0.01	0.11
(1,838)	1:98:A:ARG:HB2	1:142:A:ALA:HA	4	0.11	0.0	0.11
(1,838)	1:98:A:ARG:HB3	1:142:A:ALA:HA	4	0.11	0.0	0.11
(3,81)	1:148:A:LYS:H	1:198:A:CYS:O	3	1.33	0.08	1.31
(1,778)	1:70:A:LEU:HD11	1:94:A:ILE:HG13	3	0.59	0.39	0.46
(1,778)	1:70:A:LEU:HD12	1:94:A:ILE:HG13	3	0.59	0.39	0.46
(1,778)	1:70:A:LEU:HD13	1:94:A:ILE:HG13	3	0.59	0.39	0.46
(1,552)	1:151:A:GLU:HG2	1:153:A:THR:H	3	0.23	0.03	0.23
(1,552)	1:151:A:GLU:HG3	1:153:A:THR:H	3	0.23	0.03	0.23
(1,882)	1:108:A:TRP:HD1	1:155:A:ILE:HG13	3	0.2	0.11	0.14
(1,941)	1:120:A:GLU:HG2	1:183:A:PHE:HB2	3	0.18	0.05	0.18
(1,941)	1:120:A:GLU:HG2	1:183:A:PHE:HB3	3	0.18	0.05	0.18
(1,941)	1:120:A:GLU:HG3	1:183:A:PHE:HB2	3	0.18	0.05	0.18
(1,941)	1:120:A:GLU:HG3	1:183:A:PHE:HB3	3	0.18	0.05	0.18
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG11	3	0.18	0.08	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG12	3	0.18	0.08	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG13	3	0.18	0.08	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG21	3	0.18	0.08	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG22	3	0.18	0.08	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG23	3	0.18	0.08	0.14
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG11	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG12	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG13	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG21	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG22	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG23	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG11	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG12	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG13	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG21	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG22	3	0.18	0.06	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG23	3	0.18	0.06	0.16
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD11	3	0.18	0.02	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD12	3	0.18	0.02	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD13	3	0.18	0.02	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD21	3	0.18	0.02	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD22	3	0.18	0.02	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD23	3	0.18	0.02	0.18
(1,793)	1:73:A:LEU:HD11	1:90:A:LEU:HG	3	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,793)	1:73:A:LEU:HD12	1:90:A:LEU:HG	3	0.17	0.04	0.16
(1,793)	1:73:A:LEU:HD13	1:90:A:LEU:HG	3	0.17	0.04	0.16
(1,793)	1:73:A:LEU:HD21	1:90:A:LEU:HG	3	0.17	0.04	0.16
(1,793)	1:73:A:LEU:HD22	1:90:A:LEU:HG	3	0.17	0.04	0.16
(1,793)	1:73:A:LEU:HD23	1:90:A:LEU:HG	3	0.17	0.04	0.16
(2,113)	1:171:A:ASP:O	1:175:A:ALA:H	3	0.17	0.06	0.14
(1,272)	1:90:A:LEU:HB2	1:91:A:ASN:H	3	0.16	0.0	0.16
(1,272)	1:90:A:LEU:HB3	1:91:A:ASN:H	3	0.16	0.0	0.16
(1,256)	1:80:A:GLN:HG2	1:81:A:THR:H	3	0.16	0.03	0.14
(1,256)	1:80:A:GLN:HG3	1:81:A:THR:H	3	0.16	0.03	0.14
(1,934)	1:117:A:PHE:HE1	1:182:A:PHE:HE1	3	0.16	0.04	0.17
(1,934)	1:117:A:PHE:HE1	1:182:A:PHE:HE2	3	0.16	0.04	0.17
(1,934)	1:117:A:PHE:HE2	1:182:A:PHE:HE1	3	0.16	0.04	0.17
(1,934)	1:117:A:PHE:HE2	1:182:A:PHE:HE2	3	0.16	0.04	0.17
(1,816)	1:76:A:ILE:HD11	1:87:A:TRP:HD1	3	0.15	0.02	0.13
(1,816)	1:76:A:ILE:HD12	1:87:A:TRP:HD1	3	0.15	0.02	0.13
(1,816)	1:76:A:ILE:HD13	1:87:A:TRP:HD1	3	0.15	0.02	0.13
(1,783)	1:70:A:LEU:HG	1:93:A:ASP:HA	3	0.13	0.0	0.13
(1,405)	1:117:A:PHE:HA	1:120:A:GLU:H	3	0.13	0.01	0.13
(1,574)	1:162:A:LEU:HD11	1:167:A:LEU:H	3	0.13	0.02	0.12
(1,574)	1:162:A:LEU:HD12	1:167:A:LEU:H	3	0.13	0.02	0.12
(1,574)	1:162:A:LEU:HD13	1:167:A:LEU:H	3	0.13	0.02	0.12
(1,574)	1:162:A:LEU:HD21	1:167:A:LEU:H	3	0.13	0.02	0.12
(1,574)	1:162:A:LEU:HD22	1:167:A:LEU:H	3	0.13	0.02	0.12
(1,574)	1:162:A:LEU:HD23	1:167:A:LEU:H	3	0.13	0.02	0.12
(1,976)	1:124:A:LEU:HG	1:152:A:GLU:HG2	3	0.13	0.02	0.12
(1,976)	1:124:A:LEU:HG	1:152:A:GLU:HG3	3	0.13	0.02	0.12
(2,117)	1:180:A:GLU:O	1:184:A:LYS:H	3	0.13	0.0	0.13
(2,47)	1:97:A:LEU:O	1:101:A:ARG:H	3	0.12	0.01	0.12
(1,1098)	1:173:A:LEU:HD11	1:182:A:PHE:HE1	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD11	1:182:A:PHE:HE2	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD12	1:182:A:PHE:HE1	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD12	1:182:A:PHE:HE2	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD13	1:182:A:PHE:HE1	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD13	1:182:A:PHE:HE2	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD21	1:182:A:PHE:HE1	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD21	1:182:A:PHE:HE2	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD22	1:182:A:PHE:HE1	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD22	1:182:A:PHE:HE2	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD23	1:182:A:PHE:HE1	3	0.12	0.02	0.11
(1,1098)	1:173:A:LEU:HD23	1:182:A:PHE:HE2	3	0.12	0.02	0.11
(1,557)	1:153:A:THR:HA	1:155:A:ILE:H	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,826)	1:77:A:ARG:HB2	1:87:A:TRP:HB2	3	0.12	0.01	0.12
(1,826)	1:77:A:ARG:HB2	1:87:A:TRP:HB3	3	0.12	0.01	0.12
(1,826)	1:77:A:ARG:HB3	1:87:A:TRP:HB2	3	0.12	0.01	0.12
(1,826)	1:77:A:ARG:HB3	1:87:A:TRP:HB3	3	0.12	0.01	0.12
(1,637)	1:58:A:ASP:HB2	1:69:A:ILE:H	3	0.11	0.01	0.11
(1,637)	1:58:A:ASP:HB3	1:69:A:ILE:H	3	0.11	0.01	0.11
(1,1057)	1:156:A:PHE:HE1	1:166:A:TYR:HB2	3	0.11	0.0	0.11
(1,1057)	1:156:A:PHE:HE1	1:166:A:TYR:HB3	3	0.11	0.0	0.11
(1,1057)	1:156:A:PHE:HE2	1:166:A:TYR:HB2	3	0.11	0.0	0.11
(1,1057)	1:156:A:PHE:HE2	1:166:A:TYR:HB3	3	0.11	0.0	0.11
(1,536)	1:82:A:LYS:HG2	1:84:A:SER:H	3	0.11	0.01	0.11
(1,536)	1:82:A:LYS:HG3	1:84:A:SER:H	3	0.11	0.01	0.11
(1,1020)	1:152:A:GLU:HG2	1:190:A:TYR:HD1	3	0.11	0.01	0.11
(1,1020)	1:152:A:GLU:HG2	1:190:A:TYR:HD2	3	0.11	0.01	0.11
(1,1020)	1:152:A:GLU:HG3	1:190:A:TYR:HD1	3	0.11	0.01	0.11
(1,1020)	1:152:A:GLU:HG3	1:190:A:TYR:HD2	3	0.11	0.01	0.11
(1,801)	1:73:A:LEU:HD11	1:91:A:ASN:HB2	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD11	1:91:A:ASN:HB3	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD12	1:91:A:ASN:HB2	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD12	1:91:A:ASN:HB3	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD13	1:91:A:ASN:HB2	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD13	1:91:A:ASN:HB3	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD21	1:91:A:ASN:HB2	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD21	1:91:A:ASN:HB3	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD22	1:91:A:ASN:HB2	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD22	1:91:A:ASN:HB3	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD23	1:91:A:ASN:HB2	3	0.11	0.0	0.11
(1,801)	1:73:A:LEU:HD23	1:91:A:ASN:HB3	3	0.11	0.0	0.11
(1,1074)	1:158:A:ALA:HB1	1:189:A:MET:HG2	3	0.11	0.0	0.11
(1,1074)	1:158:A:ALA:HB1	1:189:A:MET:HG3	3	0.11	0.0	0.11
(1,1074)	1:158:A:ALA:HB2	1:189:A:MET:HG2	3	0.11	0.0	0.11
(1,1074)	1:158:A:ALA:HB2	1:189:A:MET:HG3	3	0.11	0.0	0.11
(1,1074)	1:158:A:ALA:HB3	1:189:A:MET:HG2	3	0.11	0.0	0.11
(1,1074)	1:158:A:ALA:HB3	1:189:A:MET:HG3	3	0.11	0.0	0.11
(1,791)	1:71:A:TYR:HE1	1:94:A:ILE:HG23	2	0.98	0.25	0.98
(1,791)	1:71:A:TYR:HE1	1:94:A:ILE:HG22	2	0.98	0.25	0.98
(1,1044)	1:155:A:ILE:HG22	1:182:A:PHE:HD2	2	0.54	0.3	0.54
(1,940)	1:117:A:PHE:HD1	1:183:A:PHE:HE1	2	0.2	0.02	0.2
(1,940)	1:117:A:PHE:HD1	1:183:A:PHE:HE2	2	0.2	0.02	0.2
(1,940)	1:117:A:PHE:HD2	1:183:A:PHE:HE1	2	0.2	0.02	0.2
(1,940)	1:117:A:PHE:HD2	1:183:A:PHE:HE2	2	0.2	0.02	0.2
(2,101)	1:165:A:ARG:O	1:169:A:VAL:H	2	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB1	2	0.16	0.06	0.16
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB2	2	0.16	0.06	0.16
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB3	2	0.16	0.06	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB1	2	0.16	0.0	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB2	2	0.16	0.0	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB3	2	0.16	0.0	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB1	2	0.16	0.0	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB2	2	0.16	0.0	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB3	2	0.16	0.0	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB1	2	0.16	0.0	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB2	2	0.16	0.0	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB3	2	0.16	0.0	0.16
(1,1034)	1:155:A:ILE:HG21	1:170:A:VAL:HB	2	0.16	0.04	0.16
(1,779)	1:70:A:LEU:HD11	1:94:A:ILE:HB	2	0.15	0.02	0.15
(1,779)	1:70:A:LEU:HD12	1:94:A:ILE:HB	2	0.15	0.02	0.15
(1,779)	1:70:A:LEU:HD13	1:94:A:ILE:HB	2	0.15	0.02	0.15
(1,779)	1:70:A:LEU:HD21	1:94:A:ILE:HB	2	0.15	0.02	0.15
(1,779)	1:70:A:LEU:HD22	1:94:A:ILE:HB	2	0.15	0.02	0.15
(1,779)	1:70:A:LEU:HD23	1:94:A:ILE:HB	2	0.15	0.02	0.15
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB1	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB2	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB3	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB1	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB2	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB3	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB1	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB2	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB3	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB1	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB2	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB3	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB1	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB2	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB3	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB1	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB2	2	0.14	0.02	0.14
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB3	2	0.14	0.02	0.14
(1,537)	1:84:A:SER:H	1:87:A:TRP:HB2	2	0.14	0.01	0.14
(1,537)	1:84:A:SER:H	1:87:A:TRP:HB3	2	0.14	0.01	0.14
(1,675)	1:101:A:ARG:H	1:164:A:GLU:HG2	2	0.14	0.02	0.14
(1,675)	1:101:A:ARG:H	1:164:A:GLU:HG3	2	0.14	0.02	0.14
(2,13)	1:71:A:TYR:O	1:75:A:VAL:H	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB1	2	0.12	0.01	0.12
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB2	2	0.12	0.01	0.12
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB3	2	0.12	0.01	0.12
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB1	2	0.12	0.01	0.12
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB2	2	0.12	0.01	0.12
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB3	2	0.12	0.01	0.12
(1,1086)	1:160:A:TRP:HZ2	1:167:A:LEU:HB2	2	0.12	0.02	0.12
(1,1086)	1:160:A:TRP:HZ2	1:167:A:LEU:HB3	2	0.12	0.02	0.12
(2,3)	1:66:A:ASP:O	1:70:A:LEU:H	2	0.12	0.01	0.12
(2,108)	1:168:A:LEU:O	1:172:A:ARG:N	2	0.12	0.01	0.12
(1,1000)	1:146:A:LEU:HG	1:164:A:GLU:HB2	2	0.12	0.01	0.12
(1,1000)	1:146:A:LEU:HG	1:164:A:GLU:HB3	2	0.12	0.01	0.12
(1,846)	1:100:A:ILE:HD11	1:143:A:ARG:HB2	2	0.12	0.0	0.12
(1,846)	1:100:A:ILE:HD11	1:143:A:ARG:HB3	2	0.12	0.0	0.12
(1,846)	1:100:A:ILE:HD12	1:143:A:ARG:HB2	2	0.12	0.0	0.12
(1,846)	1:100:A:ILE:HD12	1:143:A:ARG:HB3	2	0.12	0.0	0.12
(1,846)	1:100:A:ILE:HD13	1:143:A:ARG:HB2	2	0.12	0.0	0.12
(1,846)	1:100:A:ILE:HD13	1:143:A:ARG:HB3	2	0.12	0.0	0.12
(1,280)	1:98:A:ARG:HB2	1:99:A:GLN:H	2	0.11	0.01	0.11
(1,280)	1:98:A:ARG:HB3	1:99:A:GLN:H	2	0.11	0.01	0.11
(1,526)	1:61:A:HIS:HB2	1:63:A:GLU:H	2	0.11	0.01	0.11
(1,526)	1:61:A:HIS:HB3	1:63:A:GLU:H	2	0.11	0.01	0.11
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE1	2	0.11	0.01	0.11
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE2	2	0.11	0.01	0.11
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE3	2	0.11	0.01	0.11
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE1	2	0.11	0.01	0.11
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE2	2	0.11	0.01	0.11
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE3	2	0.11	0.01	0.11
(2,51)	1:99:A:GLN:O	1:103:A:GLU:H	2	0.11	0.0	0.11
(2,105)	1:167:A:LEU:O	1:171:A:ASP:H	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB1	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB2	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB3	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB1	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB2	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB3	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB1	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB2	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB3	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB1	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB2	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB3	2	0.11	0.0	0.11

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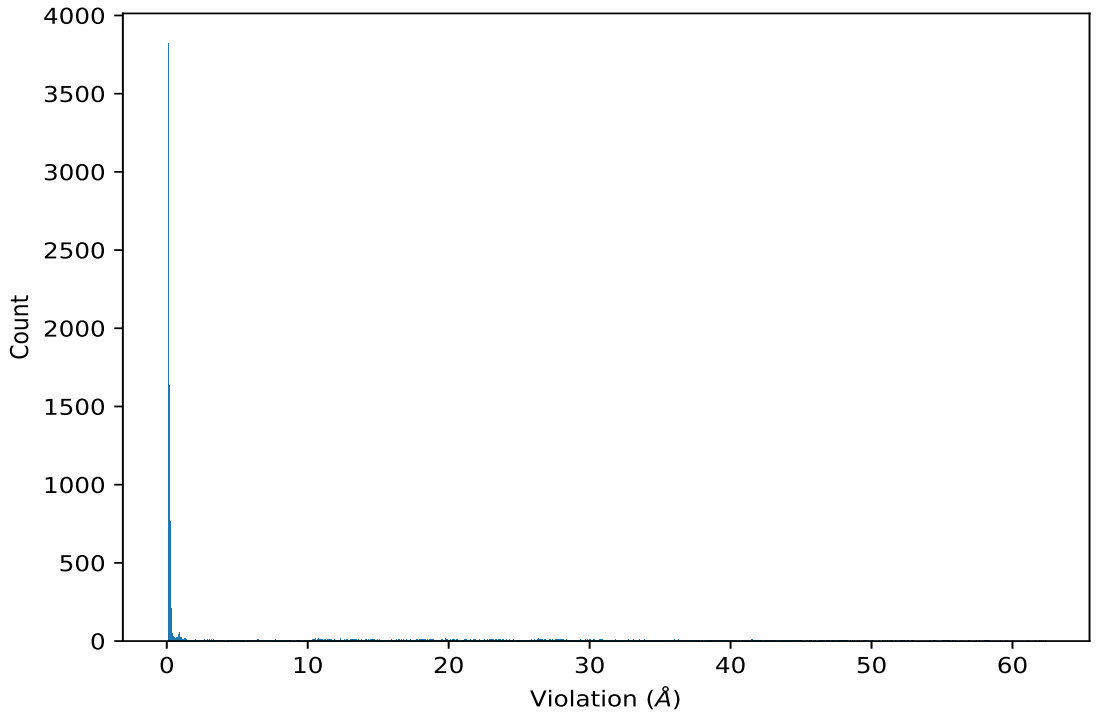
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB1	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB2	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB3	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB1	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB2	2	0.11	0.0	0.11
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB3	2	0.11	0.0	0.11
(2,20)	1:74:A:ILE:O	1:78:A:ASN:N	2	0.11	0.0	0.11
(2,57)	1:102:A:ARG:O	1:106:A:ASN:H	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	8	62.31
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	9	62.05
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	16	61.94
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	4	61.61
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	18	61.12
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	13	59.97
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	5	59.68
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	15	59.62
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	7	59.52
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	20	59.49
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	12	59.14
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	11	58.37
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	14	58.31
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	6	58.27
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	19	58.24
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	1	58.19
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	5	58.18
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	2	58.15
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	17	58.13
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	3	58.07
(3,105)	1:192:A:LYS:H	1:198:A:CYS:O	10	58.04
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	12	57.69
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	7	57.43
(2,130)	1:43:A:THR:H	1:136:A:SER:O	18	56.92
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	4	56.89
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	18	56.38
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	12	55.94
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	12	55.84
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	19	55.78
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	13	55.64
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	7	55.63
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	10	55.61
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	20	55.58
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	3	55.57
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	14	55.57
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	4	55.54
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	7	55.53
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	1	55.48
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	6	55.38
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	17	55.38
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	9	55.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	5	55.31
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	4	55.28
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	13	55.27
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	18	55.24
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	11	55.2
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	8	55.17
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	15	55.15
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	17	55.15
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	2	55.08
(3,106)	1:202:A:GLY:H	1:198:A:CYS:O	16	55.02
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	14	54.55
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	5	54.52
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	11	54.47
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	8	54.39
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	17	54.16
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	15	52.99
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	4	52.88
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	14	52.88
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	20	52.85
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	7	52.81
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	2	52.81
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	10	52.62
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	8	52.58
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	13	52.55
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	12	52.41
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	15	52.38
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	10	52.38
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	16	52.35
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	13	52.34
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	18	52.34
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	3	52.33
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	19	52.26
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	8	52.2
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	3	52.11
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	5	52.0
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	9	51.87
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	6	51.85
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	17	51.83
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	1	51.74
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	11	51.74
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	1	51.7
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	3	51.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	14	51.45
(3,107)	1:203:A:GLN:H	1:198:A:CYS:O	2	51.42
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	14	51.3
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	12	51.29
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	14	51.13
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	10	50.95
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	10	50.9
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	3	50.83
(2,130)	1:43:A:THR:H	1:136:A:SER:O	14	50.79
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	15	50.77
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	3	50.56
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	11	50.09
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	14	50.04
(2,130)	1:43:A:THR:H	1:136:A:SER:O	3	49.99
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	3	49.8
(2,130)	1:43:A:THR:H	1:136:A:SER:O	12	49.67
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	18	49.6
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	10	49.56
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	3	49.51
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	1	49.46
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	3	49.44
(2,130)	1:43:A:THR:H	1:136:A:SER:O	4	49.41
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	3	49.15
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	2	49.02
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	20	48.79
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	14	48.64
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	4	48.6
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	14	48.53
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	11	48.32
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	6	48.27
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	2	48.27
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	12	48.26
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	15	48.24
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	20	48.23
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	14	48.21
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	8	48.16
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	2	48.14
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	11	48.11
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	1	48.09
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	14	48.09
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	19	48.08
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	11	48.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	13	48.03
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	7	48.02
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	5	48.0
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	17	47.99
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	17	47.98
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	4	47.97
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	20	47.91
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	3	47.9
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	2	47.9
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	19	47.85
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	10	47.85
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	2	47.85
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	14	47.83
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	5	47.8
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	6	47.8
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	14	47.79
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	16	47.75
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	17	47.73
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	19	47.72
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	1	47.72
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	6	47.72
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	16	47.72
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	10	47.69
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	10	47.68
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	9	47.66
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	17	47.63
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	11	47.62
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	10	47.6
(3,111)	1:65:A:ASP:H	1:60:A:SER:O	18	47.6
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	6	47.57
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	12	47.56
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	5	47.49
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	3	47.46
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	10	47.45
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	1	47.41
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	14	47.38
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	12	47.34
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	1	47.34
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	3	47.32
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	5	47.26
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	2	47.21
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	6	47.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	19	47.13
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	12	47.05
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	11	47.03
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	6	47.02
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	19	46.93
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	17	46.88
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	18	46.81
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	5	46.76
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	1	46.68
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	6	46.61
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	14	46.54
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	3	46.42
(2,130)	1:43:A:THR:H	1:136:A:SER:O	19	46.37
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	3	46.31
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	12	46.29
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	10	46.26
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	13	46.04
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	14	46.01
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	10	45.9
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	14	45.8
(2,130)	1:43:A:THR:H	1:136:A:SER:O	2	45.75
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	8	45.74
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	7	45.67
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	10	45.62
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	20	45.47
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	14	45.43
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	2	45.34
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	10	45.14
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	10	45.12
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	11	45.11
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	19	45.11
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	3	45.1
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	19	45.09
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	16	45.04
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	17	44.96
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	14	44.91
(2,130)	1:43:A:THR:H	1:136:A:SER:O	20	44.85
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	5	44.84
(2,130)	1:43:A:THR:H	1:136:A:SER:O	1	44.83
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	1	44.81
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	5	44.78
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	16	44.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	10	44.71
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	6	44.67
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	14	44.6
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	3	44.55
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	3	44.51
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	14	44.51
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	11	44.5
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	8	44.49
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	10	44.47
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	12	44.46
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	4	44.43
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	12	44.43
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	14	44.41
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	17	44.41
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	14	44.38
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	9	44.37
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	3	44.34
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	2	44.32
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	6	44.3
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	10	44.3
(2,130)	1:43:A:THR:H	1:136:A:SER:O	7	44.28
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	1	44.26
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	15	44.23
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	19	44.23
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	16	44.18
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	2	44.16
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	18	44.09
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	10	44.07
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	16	44.07
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	5	44.06
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	19	44.06
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	13	44.05
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	11	44.05
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	7	44.05
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	3	44.03
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	10	44.03
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	8	44.01
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	7	43.99
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	17	43.98
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	7	43.89
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	3	43.85
(3,114)	1:70:A:LEU:H	1:60:A:SER:O	20	43.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	16	43.83
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	9	43.8
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	1	43.79
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	5	43.77
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	3	43.7
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	8	43.68
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	19	43.67
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	7	43.62
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	6	43.57
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	15	43.57
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	2	43.56
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	14	43.54
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	14	43.54
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	11	43.52
(2,130)	1:43:A:THR:H	1:136:A:SER:O	8	43.46
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	9	43.45
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	8	43.44
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	11	43.43
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	10	43.35
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	10	43.35
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	10	43.28
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	12	43.28
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	12	43.26
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	14	43.23
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	2	43.17
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	15	43.13
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	3	43.13
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	20	43.11
(2,130)	1:43:A:THR:H	1:136:A:SER:O	6	43.04
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	20	43.03
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	13	43.03
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	9	43.01
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	7	42.96
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	6	42.95
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	3	42.94
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	13	42.92
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	20	42.92
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	17	42.88
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	5	42.82
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	1	42.77
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	15	42.76
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	18	42.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	1	42.65
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	18	42.64
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	13	42.59
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	18	42.5
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	19	42.45
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	16	42.4
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	1	42.3
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	11	42.3
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	2	42.23
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	9	42.17
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	15	42.13
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	19	42.09
(2,150)	1:81:A:THR:H	1:198:A:CYS:O	4	42.07
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	16	42.03
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	6	42.03
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	19	42.01
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	20	42.01
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	8	41.99
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	12	41.99
(2,151)	1:82:A:LYS:H	1:198:A:CYS:O	4	41.98
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	11	41.97
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	12	41.96
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	11	41.95
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	10	41.94
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	18	41.91
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	14	41.9
(2,130)	1:43:A:THR:H	1:136:A:SER:O	13	41.9
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	17	41.88
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	6	41.87
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	4	41.86
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	13	41.86
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	6	41.85
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	17	41.84
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	5	41.83
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	5	41.81
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	8	41.8
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	1	41.76
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	2	41.75
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	12	41.75
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	2	41.72
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	6	41.63
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	11	41.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	2	41.61
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	7	41.61
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	12	41.6
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	17	41.6
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	1	41.59
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	3	41.59
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	15	41.59
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	15	41.58
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	9	41.58
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	1	41.57
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	2	41.57
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	11	41.56
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	13	41.55
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	14	41.55
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	8	41.54
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	10	41.54
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	20	41.53
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	5	41.51
(3,115)	1:71:A:TYR:H	1:60:A:SER:O	13	41.5
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	7	41.5
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	17	41.5
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	5	41.49
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	6	41.49
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	4	41.48
(3,64)	1:85:A:GLU:H	1:198:A:CYS:O	4	41.46
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	17	41.46
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	3	41.45
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	20	41.45
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	18	41.45
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	19	41.4
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	17	41.4
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	19	41.37
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	5	41.37
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	16	41.32
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	1	41.31
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	5	41.3
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	19	41.27
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	18	41.24
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	6	41.24
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	9	41.19
(3,110)	1:64:A:ALA:H	1:60:A:SER:O	10	41.18
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	1	41.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	3	41.08
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	7	41.06
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	10	41.03
(2,130)	1:43:A:THR:H	1:136:A:SER:O	10	41.03
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	14	41.02
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	11	40.97
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	14	40.94
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	6	40.87
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	17	40.82
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	12	40.77
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	3	40.61
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	16	40.61
(2,152)	1:86:A:GLU:H	1:198:A:CYS:O	4	40.41
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	3	40.35
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	14	40.35
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	15	40.33
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	3	40.27
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	16	40.19
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	8	40.19
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	20	40.19
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	10	40.11
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	3	40.09
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	14	40.02
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	13	39.99
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	7	39.85
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	19	39.83
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	8	39.8
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	9	39.72
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	3	39.7
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	14	39.7
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	2	39.67
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	7	39.67
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	18	39.63
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	10	39.61
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	10	39.6
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	17	39.57
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	11	39.48
(2,130)	1:43:A:THR:H	1:136:A:SER:O	5	39.43
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	16	39.39
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	5	39.37
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	15	39.31
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	19	39.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	2	39.25
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	9	39.23
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	1	39.18
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	15	39.17
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	6	39.1
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	2	39.09
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	17	39.04
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	20	39.04
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	8	38.98
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	13	38.94
(2,130)	1:43:A:THR:H	1:136:A:SER:O	15	38.9
(2,130)	1:43:A:THR:H	1:136:A:SER:O	17	38.88
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	5	38.87
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	10	38.86
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	11	38.82
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	9	38.8
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	1	38.73
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	20	38.72
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	19	38.71
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	14	38.7
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	16	38.65
(2,153)	1:87:A:TRP:H	1:198:A:CYS:O	4	38.64
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	3	38.6
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	6	38.56
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	12	38.56
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	13	38.56
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	18	38.49
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	7	38.47
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	12	38.42
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	14	38.39
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	10	38.38
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	3	38.36
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	8	38.25
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	18	38.25
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	2	38.19
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	7	38.18
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	9	38.11
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	10	38.1
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	14	37.97
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	3	37.93
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	15	37.9
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	12	37.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,149)	1:79:A:GLN:H	1:198:A:CYS:O	4	37.73
(2,130)	1:43:A:THR:H	1:136:A:SER:O	11	37.66
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	10	37.64
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	16	37.63
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	15	37.62
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	20	37.62
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	10	37.61
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	20	37.6
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	3	37.58
(2,154)	1:88:A:GLN:H	1:198:A:CYS:O	4	37.57
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	3	37.56
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	3	37.51
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	14	37.47
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	13	37.46
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	16	37.42
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	1	37.41
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	7	37.4
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	14	37.4
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	16	37.39
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	7	37.38
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	2	37.37
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	10	37.34
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	20	37.25
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	3	37.24
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	2	37.21
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	8	37.2
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	3	37.19
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	14	37.18
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	2	37.16
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	14	37.16
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	2	37.12
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	13	37.11
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	8	37.07
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	1	37.06
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	10	37.05
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	5	37.04
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	17	37.04
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	8	37.03
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	9	37.02
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	15	37.01
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	17	37.01
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	17	36.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	18	36.97
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	6	36.97
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	5	36.92
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	5	36.87
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	2	36.85
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	6	36.84
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	9	36.84
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	11	36.82
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	10	36.76
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	18	36.75
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	14	36.74
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	20	36.74
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	1	36.72
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	5	36.68
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	2	36.68
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	19	36.65
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	1	36.62
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	11	36.59
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	19	36.58
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	1	36.58
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	16	36.57
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	14	36.53
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	6	36.53
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	11	36.53
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	6	36.51
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	6	36.48
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	15	36.48
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	17	36.47
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	5	36.46
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	12	36.46
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	1	36.44
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	2	36.44
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	17	36.44
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	1	36.41
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	19	36.4
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	9	36.4
(2,147)	1:77:A:ARG:H	1:198:A:CYS:O	4	36.37
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	17	36.36
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	17	36.36
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	12	36.33
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	5	36.29
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	5	36.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	17	36.28
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	11	36.26
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	6	36.26
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	19	36.26
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	19	36.26
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	1	36.26
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	19	36.25
(2,148)	1:78:A:ASN:H	1:198:A:CYS:O	4	36.24
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	6	36.21
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	11	36.21
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	3	36.2
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	17	36.19
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	2	36.19
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	11	36.17
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	10	36.16
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	15	36.14
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	5	36.12
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	13	36.11
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	4	36.09
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	10	36.08
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	3	36.06
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	19	36.06
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	5	36.05
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	13	36.05
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	11	36.05
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	5	36.04
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	1	36.03
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	11	36.01
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	1	36.01
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	11	36.0
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	19	35.99
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	9	35.99
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	6	35.98
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	3	35.96
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	5	35.95
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	11	35.94
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	8	35.94
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	1	35.92
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	6	35.92
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	16	35.9
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	14	35.89
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	6	35.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	6	35.87
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	17	35.86
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	17	35.81
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	11	35.81
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	18	35.8
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	10	35.78
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	14	35.78
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	2	35.78
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	14	35.75
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	16	35.75
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	18	35.74
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	19	35.71
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	8	35.71
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	3	35.69
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	10	35.64
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	17	35.53
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	1	35.51
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	19	35.48
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	8	35.47
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	1	35.45
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	12	35.45
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	2	35.44
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	9	35.43
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	8	35.42
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	12	35.41
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	11	35.4
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	16	35.37
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	5	35.31
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	17	35.31
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	19	35.3
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	9	35.26
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	2	35.22
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	7	35.21
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	19	35.18
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	8	35.14
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	3	35.13
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	10	35.11
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	4	35.07
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	5	35.07
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	3	35.02
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	2	35.01
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	14	35.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:90:A:LEU:H	1:198:A:CYS:O	4	34.98
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	17	34.98
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	6	34.97
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	5	34.97
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	17	34.97
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	19	34.97
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	6	34.97
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	5	34.87
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	10	34.86
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	3	34.86
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	12	34.86
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	2	34.84
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	5	34.84
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	17	34.82
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	2	34.81
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	2	34.81
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	1	34.81
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	6	34.81
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	7	34.79
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	9	34.79
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	10	34.77
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	19	34.76
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	9	34.76
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	11	34.75
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	14	34.74
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	1	34.72
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	2	34.71
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	2	34.67
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	2	34.65
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	12	34.65
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	12	34.65
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	1	34.65
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	11	34.65
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	1	34.65
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	6	34.64
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	13	34.63
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	7	34.6
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	3	34.54
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	17	34.54
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	20	34.53
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	15	34.51
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	11	34.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	15	34.46
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	14	34.46
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	6	34.46
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	11	34.46
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	19	34.45
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	17	34.45
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	5	34.44
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	2	34.43
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	1	34.43
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	9	34.41
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	5	34.41
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	19	34.4
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	18	34.38
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	2	34.37
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	1	34.36
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	2	34.36
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	1	34.34
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	7	34.27
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	12	34.25
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	10	34.22
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	19	34.19
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	13	34.19
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	20	34.17
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	5	34.15
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	6	34.15
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	12	34.11
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	11	34.1
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	6	34.08
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	16	34.07
(4,2)	1:196:A:VAL:H	1:136:A:SER:O	2	34.06
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	11	34.04
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	14	34.03
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	3	34.0
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	5	33.98
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	10	33.96
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	4	33.94
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	4	33.94
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	20	33.93
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	19	33.93
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	19	33.92
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	15	33.92
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	9	33.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	12	33.91
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	3	33.89
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	10	33.88
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	2	33.87
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	17	33.87
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	19	33.85
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	10	33.85
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	8	33.81
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	17	33.78
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	6	33.77
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	2	33.77
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	16	33.77
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	10	33.75
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	16	33.75
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	6	33.7
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	18	33.68
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	6	33.68
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	13	33.67
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	11	33.67
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	10	33.66
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	19	33.66
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	1	33.65
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	20	33.62
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	3	33.61
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	14	33.61
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	1	33.61
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	16	33.58
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	1	33.57
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	1	33.57
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	5	33.57
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	3	33.56
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	6	33.56
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	11	33.56
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	14	33.55
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	16	33.54
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	19	33.54
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	11	33.53
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	9	33.53
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	14	33.52
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	3	33.5
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	14	33.5
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	5	33.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	17	33.49
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	10	33.47
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	6	33.47
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	19	33.46
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	4	33.46
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	5	33.45
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	12	33.45
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	17	33.44
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	3	33.43
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	20	33.43
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	6	33.42
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	17	33.37
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	11	33.36
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	7	33.35
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	5	33.34
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	12	33.34
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	17	33.33
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	1	33.33
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	8	33.33
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	7	33.31
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	10	33.3
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	15	33.29
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	11	33.26
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	5	33.25
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	1	33.23
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	19	33.23
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	16	33.23
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	5	33.23
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	6	33.21
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	11	33.21
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	17	33.21
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	14	33.17
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	4	33.14
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	11	33.14
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	10	33.12
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	18	33.11
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	19	33.11
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	3	33.11
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	1	33.1
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	6	33.1
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	19	33.09
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	3	33.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	11	33.07
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	6	33.06
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	12	33.06
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	9	33.06
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	14	33.04
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	2	33.03
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	11	33.02
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	17	33.01
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	7	32.99
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	20	32.97
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	10	32.96
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	3	32.93
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	7	32.92
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	7	32.91
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	13	32.88
(2,156)	1:91:A:ASN:H	1:198:A:CYS:O	4	32.88
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	13	32.87
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	17	32.86
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	16	32.86
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	13	32.82
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	17	32.81
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	14	32.79
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	15	32.79
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	18	32.79
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	20	32.77
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	6	32.77
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	12	32.77
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	8	32.77
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	1	32.74
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	2	32.73
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	15	32.73
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	5	32.72
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	15	32.72
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	20	32.71
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	8	32.71
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	12	32.7
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	18	32.68
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	15	32.66
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	12	32.65
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	18	32.65
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	3	32.64
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	15	32.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	19	32.64
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	16	32.62
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	2	32.61
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	7	32.61
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	12	32.59
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	20	32.59
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	19	32.58
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	19	32.56
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	3	32.56
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	2	32.51
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	8	32.51
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	7	32.51
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	8	32.5
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	16	32.49
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	20	32.45
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	5	32.42
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	12	32.42
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	8	32.41
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	15	32.4
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	14	32.38
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	15	32.38
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	9	32.37
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	20	32.37
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	12	32.36
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	2	32.34
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	13	32.34
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	3	32.32
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	9	32.32
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	7	32.31
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	16	32.3
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	17	32.29
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	20	32.29
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	10	32.26
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	1	32.25
(3,48)	1:195:A:GLY:H	1:136:A:SER:O	2	32.23
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	19	32.22
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	14	32.22
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	17	32.21
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	2	32.21
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	12	32.2
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	5	32.2
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	17	32.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	14	32.18
(1,1102)	1:131:A:SER:H	1:60:A:SER:O	10	32.16
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	12	32.13
(3,65)	1:92:A:TYR:H	1:198:A:CYS:O	4	32.13
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	2	32.12
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	19	32.12
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	9	32.11
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	1	32.1
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	6	32.09
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	16	32.08
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	12	32.07
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	5	32.06
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	12	32.06
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	1	32.05
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	6	32.05
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	5	32.05
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	8	32.02
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	11	32.01
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	16	31.99
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	8	31.98
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	6	31.97
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	12	31.97
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	5	31.96
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	11	31.96
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	17	31.95
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	6	31.94
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	13	31.94
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	2	31.93
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	5	31.92
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	1	31.92
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	13	31.92
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	20	31.89
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	19	31.88
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	8	31.87
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	9	31.87
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	15	31.87
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	7	31.87
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	9	31.85
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	19	31.83
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	1	31.83
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	6	31.83
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	6	31.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	11	31.82
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	9	31.81
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	19	31.81
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	16	31.8
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	1	31.8
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	13	31.8
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	17	31.79
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	7	31.77
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	10	31.75
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	14	31.75
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	11	31.74
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	12	31.74
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	7	31.74
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	2	31.73
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	19	31.72
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	1	31.72
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	5	31.72
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	11	31.7
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	3	31.7
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	10	31.69
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	15	31.66
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	19	31.65
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	11	31.65
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	9	31.64
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	5	31.63
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	6	31.6
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	10	31.59
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	1	31.58
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	19	31.55
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	19	31.53
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	16	31.53
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	11	31.53
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	7	31.51
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	14	31.5
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	16	31.5
(2,177)	1:176:A:LEU:H	1:60:A:SER:O	13	31.49
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	2	31.48
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	11	31.48
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	16	31.48
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	17	31.47
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	17	31.46
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	10	31.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	18	31.43
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	13	31.41
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	6	31.39
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	7	31.38
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	3	31.38
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	11	31.36
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	12	31.33
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	10	31.31
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	3	31.3
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	4	31.3
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	3	31.29
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	20	31.27
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	20	31.26
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	8	31.25
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	14	31.24
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	12	31.22
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	16	31.19
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	1	31.18
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	20	31.18
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	9	31.18
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	8	31.17
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	12	31.13
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	15	31.13
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	20	31.12
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	18	31.12
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	15	31.11
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	10	31.1
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	7	31.1
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	11	31.08
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	15	31.07
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	6	31.05
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	20	31.05
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	5	31.05
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	4	31.04
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	10	31.03
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	15	31.02
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	15	30.99
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	18	30.98
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	8	30.98
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	4	30.95
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	20	30.94
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	7	30.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	14	30.94
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	7	30.94
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	18	30.93
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	6	30.93
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	16	30.91
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	9	30.9
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	9	30.89
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	6	30.88
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	16	30.86
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	9	30.86
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	20	30.86
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	14	30.85
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	13	30.85
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	3	30.84
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	5	30.83
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	14	30.82
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	17	30.82
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	7	30.81
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	3	30.8
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	19	30.8
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	17	30.8
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	8	30.8
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	4	30.79
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	13	30.79
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	18	30.78
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	13	30.78
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	10	30.78
(3,49)	1:41:A:GLY:H	1:198:A:CYS:O	9	30.76
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	20	30.76
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	9	30.75
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	13	30.75
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	12	30.75
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	7	30.73
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	13	30.73
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	15	30.72
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	12	30.72
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	8	30.7
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	18	30.69
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	15	30.69
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	17	30.68
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	14	30.68
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	3	30.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	20	30.67
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	17	30.67
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	2	30.65
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	18	30.65
(2,171)	1:175:A:ALA:H	1:198:A:CYS:O	4	30.64
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	7	30.63
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	7	30.59
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	7	30.58
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	13	30.58
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	2	30.58
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	2	30.57
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	12	30.56
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	12	30.55
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	16	30.54
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	2	30.54
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	9	30.54
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	10	30.54
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	19	30.54
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	8	30.52
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	15	30.48
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	2	30.47
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	12	30.47
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	13	30.47
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	4	30.46
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	18	30.46
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	17	30.44
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	15	30.44
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	18	30.44
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	19	30.42
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	16	30.41
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	18	30.4
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	9	30.4
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	12	30.39
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	12	30.39
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	8	30.38
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	13	30.37
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	15	30.36
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	20	30.36
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	18	30.34
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	5	30.32
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	10	30.31
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	11	30.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	12	30.29
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	10	30.28
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	7	30.28
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	3	30.28
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	19	30.26
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	15	30.25
(2,130)	1:43:A:THR:H	1:136:A:SER:O	9	30.25
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	18	30.22
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	17	30.22
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	5	30.21
(3,47)	1:192:A:LYS:H	1:136:A:SER:O	2	30.18
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	1	30.16
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	12	30.16
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	11	30.15
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	13	30.12
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	6	30.1
(2,166)	1:137:A:LYS:H	1:198:A:CYS:O	4	30.08
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	16	30.08
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	7	30.08
(2,130)	1:43:A:THR:H	1:136:A:SER:O	16	30.08
(2,169)	1:173:A:LEU:H	1:198:A:CYS:O	4	30.07
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	5	30.07
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	5	30.06
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	12	30.06
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	14	30.02
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	20	30.01
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	14	30.01
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	11	30.01
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	5	30.01
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	1	30.01
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	1	30.0
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	3	30.0
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	3	29.99
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	19	29.99
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	11	29.98
(3,163)	1:180:A:GLU:H	1:60:A:SER:O	13	29.96
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	14	29.96
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	10	29.96
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	14	29.96
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	11	29.96
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	8	29.94
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	1	29.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	20	29.93
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	1	29.91
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	8	29.91
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	18	29.9
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	6	29.9
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	10	29.89
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	11	29.88
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	9	29.87
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	15	29.86
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	19	29.85
(2,158)	1:96:A:THR:H	1:198:A:CYS:O	4	29.85
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	17	29.84
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	11	29.84
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	17	29.84
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	3	29.84
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	8	29.83
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	15	29.83
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	8	29.83
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	6	29.82
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	13	29.8
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	4	29.8
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	2	29.8
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	10	29.77
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	1	29.76
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	19	29.76
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	20	29.73
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	1	29.73
(2,168)	1:172:A:ARG:H	1:198:A:CYS:O	4	29.73
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	6	29.72
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	16	29.72
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	9	29.72
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	1	29.71
(2,146)	1:206:A:LEU:H	1:136:A:SER:O	12	29.71
(2,129)	1:41:A:GLY:H	1:136:A:SER:O	16	29.71
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	2	29.7
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	16	29.69
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	20	29.69
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	13	29.69
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	9	29.69
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	12	29.67
(3,162)	1:179:A:ALA:H	1:60:A:SER:O	13	29.66
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	12	29.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	14	29.66
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	6	29.65
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	6	29.63
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	5	29.63
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	13	29.59
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	9	29.55
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	8	29.54
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	14	29.52
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	3	29.51
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	6	29.51
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	5	29.49
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	18	29.48
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	4	29.48
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	5	29.48
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	2	29.48
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	7	29.46
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	13	29.45
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	12	29.44
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	7	29.44
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	7	29.43
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	17	29.42
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	7	29.41
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	14	29.41
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	18	29.4
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	17	29.39
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	16	29.38
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	15	29.37
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	4	29.37
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	17	29.36
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	5	29.36
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	20	29.35
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	7	29.33
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	18	29.33
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	16	29.32
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	19	29.32
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	2	29.32
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	3	29.31
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	20	29.31
(2,157)	1:95:A:TYR:H	1:198:A:CYS:O	4	29.31
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	9	29.3
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	11	29.3
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	10	29.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	2	29.29
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	10	29.27
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	11	29.27
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	8	29.26
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	18	29.23
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	17	29.22
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	19	29.22
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	1	29.21
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	9	29.21
(3,113)	1:67:A:ASP:H	1:60:A:SER:O	18	29.16
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	19	29.14
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	6	29.1
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	3	29.07
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	18	29.05
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	19	29.05
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	4	29.04
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	15	29.03
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	15	29.01
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	17	29.01
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	20	28.99
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	18	28.98
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	5	28.96
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	15	28.96
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	10	28.95
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	12	28.94
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	6	28.91
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	2	28.9
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	13	28.9
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	18	28.9
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	2	28.89
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	14	28.88
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	2	28.85
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	18	28.83
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	9	28.82
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	12	28.8
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	3	28.8
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	18	28.8
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	17	28.79
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	18	28.78
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	2	28.78
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	1	28.77
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	20	28.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	20	28.71
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	5	28.71
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	1	28.7
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	1	28.69
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	9	28.68
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	16	28.67
(2,140)	1:184:A:LYS:H	1:136:A:SER:O	8	28.67
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	5	28.66
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	16	28.66
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	15	28.64
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	8	28.64
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	17	28.64
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	12	28.64
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	6	28.62
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	14	28.61
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	19	28.6
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	11	28.59
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	15	28.57
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	6	28.56
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	12	28.55
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	17	28.54
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	11	28.54
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	10	28.52
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	7	28.51
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	7	28.51
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	16	28.49
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	17	28.49
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	19	28.48
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	4	28.48
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	15	28.47
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	13	28.47
(2,170)	1:174:A:ILE:H	1:198:A:CYS:O	4	28.47
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	17	28.44
(2,172)	1:177:A:ASP:H	1:198:A:CYS:O	4	28.44
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	9	28.41
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	7	28.4
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	11	28.4
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	10	28.36
(3,161)	1:178:A:ALA:H	1:60:A:SER:O	13	28.36
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	7	28.35
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	17	28.34
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	18	28.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	15	28.34
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	11	28.34
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	5	28.33
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	10	28.33
(2,167)	1:171:A:ASP:H	1:198:A:CYS:O	4	28.33
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	3	28.32
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	8	28.32
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	6	28.31
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	11	28.31
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	15	28.27
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	12	28.27
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	5	28.26
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	19	28.26
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	6	28.25
(3,97)	1:176:A:LEU:H	1:198:A:CYS:O	4	28.24
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	17	28.24
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	2	28.24
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	3	28.2
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	13	28.19
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	11	28.19
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	5	28.18
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	11	28.18
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	1	28.17
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	8	28.16
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	1	28.15
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	5	28.15
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	4	28.15
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	16	28.14
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	11	28.14
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	1	28.14
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	5	28.14
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	13	28.14
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	10	28.13
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	11	28.12
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	20	28.1
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	1	28.1
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	9	28.08
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	2	28.07
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	12	28.06
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	15	28.06
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	12	28.05
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	6	28.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	6	28.05
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	6	28.05
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	18	28.05
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	6	28.05
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	13	28.05
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	4	28.04
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	5	28.04
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	2	28.04
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	9	28.04
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	2	28.03
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	16	28.02
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	19	28.01
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	19	28.01
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	12	28.01
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	7	27.99
(2,159)	1:99:A:GLN:H	1:198:A:CYS:O	4	27.99
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	18	27.98
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	19	27.97
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	2	27.95
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	5	27.95
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	1	27.95
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	19	27.93
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	20	27.93
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	7	27.93
(2,145)	1:205:A:LYS:H	1:136:A:SER:O	20	27.93
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	17	27.92
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	14	27.91
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	20	27.91
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	7	27.91
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	1	27.9
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	14	27.9
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	4	27.89
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	8	27.89
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	1	27.89
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	11	27.87
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	12	27.87
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	1	27.86
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	2	27.86
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	7	27.85
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	13	27.85
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	11	27.85
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	17	27.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	8	27.83
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	16	27.83
(2,176)	1:112:A:LEU:H	1:60:A:SER:O	14	27.82
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	8	27.81
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	19	27.81
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	1	27.8
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	20	27.79
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	17	27.79
(2,173)	1:178:A:ALA:H	1:198:A:CYS:O	4	27.78
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	9	27.78
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	16	27.78
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	5	27.76
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	19	27.75
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	16	27.75
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	6	27.75
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	16	27.75
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	19	27.75
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	3	27.74
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	1	27.74
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	19	27.73
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	20	27.73
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	3	27.73
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	9	27.73
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	12	27.73
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	2	27.72
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	16	27.71
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	11	27.69
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	15	27.69
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	11	27.69
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	3	27.67
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	7	27.67
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	5	27.67
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	20	27.67
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	16	27.66
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	19	27.66
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	1	27.66
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	9	27.65
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	20	27.65
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	13	27.65
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	13	27.64
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	2	27.63
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	6	27.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	11	27.62
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	8	27.62
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	16	27.61
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	13	27.61
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	15	27.61
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	8	27.6
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	6	27.59
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	16	27.59
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	3	27.59
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	14	27.58
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	10	27.58
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	13	27.58
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	5	27.57
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	19	27.56
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	3	27.55
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	7	27.55
(3,112)	1:66:A:ASP:H	1:60:A:SER:O	18	27.53
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	13	27.53
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	9	27.53
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	8	27.52
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	17	27.5
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	14	27.49
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	15	27.48
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	16	27.48
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	1	27.46
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	15	27.44
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	6	27.44
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	8	27.44
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	13	27.43
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	11	27.42
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	5	27.42
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	7	27.41
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	18	27.4
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	12	27.4
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	9	27.39
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	5	27.39
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	2	27.38
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	19	27.37
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	7	27.37
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	14	27.37
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	16	27.36
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	2	27.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	10	27.36
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	7	27.35
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	13	27.34
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	3	27.33
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	20	27.32
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	10	27.31
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	9	27.3
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	8	27.3
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	16	27.28
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	14	27.26
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	15	27.25
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	14	27.25
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	16	27.24
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	14	27.24
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	4	27.24
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	15	27.24
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	11	27.23
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	16	27.23
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	20	27.23
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	9	27.21
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	8	27.21
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	4	27.2
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	20	27.2
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	17	27.2
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	20	27.19
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	10	27.19
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	3	27.19
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	19	27.19
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	20	27.19
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	18	27.18
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	10	27.17
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	18	27.16
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	8	27.16
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	8	27.15
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	6	27.14
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	8	27.12
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	13	27.12
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	12	27.12
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	16	27.12
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	15	27.12
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	10	27.11
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	4	27.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,50)	1:43:A:THR:H	1:198:A:CYS:O	9	27.11
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	20	27.09
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	16	27.09
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	4	27.07
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	18	27.06
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	6	27.06
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	15	27.05
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	1	27.02
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	3	27.01
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	7	27.01
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	1	27.01
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	5	27.01
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	7	27.01
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	15	27.01
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	16	26.99
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	8	26.99
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	13	26.97
(3,61)	1:70:A:LEU:H	1:198:A:CYS:O	9	26.96
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	17	26.96
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	4	26.94
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	6	26.94
(2,139)	1:160:A:TRP:H	1:136:A:SER:O	2	26.93
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	17	26.91
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	19	26.91
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	6	26.89
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	10	26.89
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	16	26.89
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	8	26.88
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	19	26.88
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	4	26.87
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	12	26.86
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	11	26.86
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	8	26.85
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	12	26.85
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	7	26.85
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	2	26.84
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	12	26.84
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	18	26.82
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	6	26.81
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	19	26.8
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	7	26.79
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	10	26.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	15	26.79
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	18	26.77
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	16	26.77
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	17	26.77
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	17	26.77
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	9	26.76
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	2	26.75
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	18	26.74
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	2	26.74
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	5	26.72
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	4	26.71
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	5	26.71
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	3	26.7
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	3	26.7
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	6	26.69
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	9	26.68
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	9	26.67
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	3	26.66
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	1	26.66
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	16	26.66
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	18	26.65
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	7	26.65
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	9	26.65
(3,51)	1:57:A:HIS:H	1:198:A:CYS:O	9	26.64
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	17	26.64
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	16	26.63
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	20	26.62
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	10	26.61
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	11	26.6
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	5	26.59
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	20	26.59
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	15	26.58
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	18	26.58
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	15	26.57
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	6	26.56
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	18	26.56
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	12	26.55
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	1	26.55
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	7	26.55
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	9	26.54
(3,66)	1:97:A:LEU:H	1:198:A:CYS:O	4	26.54
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	14	26.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	2	26.54
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	7	26.53
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	8	26.53
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	11	26.51
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	9	26.51
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	9	26.51
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	9	26.51
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	15	26.5
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	14	26.49
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	8	26.49
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	8	26.48
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	17	26.46
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	4	26.45
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	18	26.45
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	5	26.44
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	3	26.44
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	13	26.42
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	9	26.42
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	12	26.41
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	19	26.41
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	16	26.41
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	11	26.4
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	19	26.4
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	12	26.4
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	6	26.4
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	4	26.4
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	17	26.39
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	20	26.39
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	10	26.39
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	5	26.39
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	4	26.38
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	10	26.38
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	15	26.37
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	3	26.37
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	2	26.35
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	8	26.34
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	4	26.34
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	7	26.33
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	18	26.32
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	13	26.32
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	5	26.32
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	9	26.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	20	26.3
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	19	26.3
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	1	26.29
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	8	26.28
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	1	26.28
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	1	26.26
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	17	26.26
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	7	26.26
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	12	26.24
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	8	26.23
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	7	26.23
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	18	26.22
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	18	26.21
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	13	26.21
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	7	26.2
(3,52)	1:58:A:ASP:H	1:198:A:CYS:O	9	26.2
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	15	26.18
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	12	26.17
(3,166)	1:184:A:LYS:H	1:60:A:SER:O	14	26.16
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	2	26.16
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	12	26.16
(3,45)	1:180:A:GLU:H	1:136:A:SER:O	13	26.15
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	19	26.15
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	7	26.15
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	20	26.15
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	12	26.13
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	8	26.13
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	17	26.09
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	3	26.09
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	14	26.08
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	11	26.08
(3,137)	1:119:A:ARG:H	1:60:A:SER:O	13	26.07
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	7	26.07
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	7	26.07
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	6	26.05
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	20	26.05
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	16	26.04
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	15	26.03
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	12	26.01
(3,44)	1:176:A:LEU:H	1:136:A:SER:O	13	26.01
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	19	26.01
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	8	25.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	20	25.99
(3,46)	1:188:A:GLN:H	1:136:A:SER:O	2	25.95
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	15	25.92
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	15	25.91
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	2	25.91
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	18	25.9
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	14	25.89
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	10	25.88
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	12	25.88
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	11	25.87
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	18	25.87
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	20	25.87
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	9	25.86
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	2	25.84
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	3	25.84
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	15	25.83
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	11	25.83
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	5	25.82
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	9	25.82
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	8	25.79
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	16	25.78
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	14	25.75
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	3	25.75
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	5	25.75
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	18	25.74
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	13	25.74
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	5	25.72
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	11	25.72
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	20	25.72
(3,62)	1:71:A:TYR:H	1:198:A:CYS:O	4	25.71
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	7	25.7
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	20	25.69
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	1	25.67
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	10	25.67
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	11	25.67
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	14	25.66
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	13	25.64
(3,164)	1:182:A:PHE:H	1:60:A:SER:O	14	25.64
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	13	25.64
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	18	25.63
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	1	25.61
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	8	25.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	10	25.59
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	13	25.59
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	17	25.59
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	19	25.58
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	20	25.58
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	14	25.55
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	2	25.54
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	10	25.53
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	16	25.53
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	6	25.52
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	13	25.51
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	17	25.48
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	15	25.48
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	20	25.48
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	1	25.48
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	9	25.47
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	15	25.45
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	13	25.44
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	13	25.44
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	1	25.42
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	6	25.4
(3,96)	1:170:A:VAL:H	1:198:A:CYS:O	4	25.37
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	16	25.35
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	8	25.35
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	18	25.34
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	15	25.32
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	8	25.29
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	9	25.29
(3,95)	1:169:A:VAL:H	1:198:A:CYS:O	4	25.28
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	20	25.28
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	12	25.26
(2,160)	1:103:A:GLU:H	1:198:A:CYS:O	4	25.26
(2,138)	1:154:A:SER:H	1:136:A:SER:O	11	25.23
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	3	25.22
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	6	25.21
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	15	25.19
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	10	25.18
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	16	25.15
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	13	25.14
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	4	25.12
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	20	25.12
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	7	25.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	16	25.12
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	13	25.11
(3,58)	1:66:A:ASP:H	1:198:A:CYS:O	9	25.09
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	11	25.08
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	10	25.05
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	18	25.04
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	17	25.03
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	15	25.02
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	3	25.01
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	4	25.0
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	9	25.0
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	15	24.99
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	6	24.99
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	10	24.99
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	9	24.98
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	16	24.96
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	14	24.95
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	8	24.95
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	11	24.95
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	9	24.94
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	7	24.92
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	1	24.92
(2,138)	1:154:A:SER:H	1:136:A:SER:O	4	24.92
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	5	24.9
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	19	24.89
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	18	24.89
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	7	24.88
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	8	24.87
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	2	24.85
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	18	24.84
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	12	24.82
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	14	24.78
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	12	24.77
(3,160)	1:174:A:ILE:H	1:60:A:SER:O	13	24.76
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	4	24.76
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	5	24.76
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	4	24.74
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	10	24.73
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	16	24.73
(2,138)	1:154:A:SER:H	1:136:A:SER:O	7	24.73
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	15	24.72
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	20	24.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:154:A:SER:H	1:136:A:SER:O	1	24.65
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	5	24.63
(2,178)	1:192:A:LYS:H	1:60:A:SER:O	14	24.61
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	20	24.61
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	15	24.6
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	7	24.59
(3,93)	1:165:A:ARG:H	1:198:A:CYS:O	4	24.58
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	1	24.58
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	12	24.57
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	19	24.56
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	19	24.56
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	3	24.55
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	9	24.55
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	18	24.55
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	17	24.55
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	14	24.54
(2,138)	1:154:A:SER:H	1:136:A:SER:O	5	24.54
(2,138)	1:154:A:SER:H	1:136:A:SER:O	6	24.52
(2,138)	1:154:A:SER:H	1:136:A:SER:O	16	24.52
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	16	24.51
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	14	24.5
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	20	24.46
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	13	24.45
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	11	24.44
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	13	24.44
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	2	24.43
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	10	24.43
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	6	24.41
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	16	24.41
(2,138)	1:154:A:SER:H	1:136:A:SER:O	17	24.4
(2,138)	1:154:A:SER:H	1:136:A:SER:O	9	24.38
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	19	24.38
(2,138)	1:154:A:SER:H	1:136:A:SER:O	15	24.36
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	3	24.34
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	6	24.34
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	11	24.34
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	12	24.33
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	10	24.32
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	9	24.32
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	1	24.32
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	20	24.31
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	19	24.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	7	24.3
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	8	24.3
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	4	24.28
(2,138)	1:154:A:SER:H	1:136:A:SER:O	18	24.28
(2,138)	1:154:A:SER:H	1:136:A:SER:O	20	24.28
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	13	24.27
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	3	24.27
(2,138)	1:154:A:SER:H	1:136:A:SER:O	3	24.26
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	9	24.25
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	3	24.24
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	18	24.24
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	7	24.23
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	18	24.23
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	18	24.22
(2,138)	1:154:A:SER:H	1:136:A:SER:O	19	24.21
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	9	24.2
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	4	24.19
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	4	24.18
(2,138)	1:154:A:SER:H	1:136:A:SER:O	8	24.18
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	18	24.17
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	3	24.14
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	17	24.13
(2,138)	1:154:A:SER:H	1:136:A:SER:O	14	24.13
(2,138)	1:154:A:SER:H	1:136:A:SER:O	13	24.12
(2,144)	1:204:A:ARG:H	1:136:A:SER:O	13	24.11
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	10	24.1
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	16	24.1
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	19	24.09
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	14	24.08
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	4	24.08
(2,138)	1:154:A:SER:H	1:136:A:SER:O	12	24.08
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	3	24.07
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	10	24.07
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	1	24.05
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	18	24.05
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	7	24.04
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	20	24.03
(2,138)	1:154:A:SER:H	1:136:A:SER:O	10	24.03
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	6	23.95
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	10	23.95
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	20	23.94
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	10	23.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	17	23.92
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	2	23.91
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	15	23.91
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	13	23.89
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	3	23.87
(2,134)	1:117:A:PHE:H	1:136:A:SER:O	2	23.87
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	18	23.86
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	8	23.86
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	4	23.86
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	5	23.85
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	8	23.85
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	4	23.85
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	20	23.84
(2,143)	1:203:A:GLN:H	1:136:A:SER:O	4	23.84
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	18	23.82
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	9	23.81
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	7	23.81
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	20	23.81
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	16	23.8
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	8	23.8
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	15	23.8
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	17	23.79
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	7	23.79
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	4	23.77
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	11	23.76
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	16	23.76
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	12	23.75
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	17	23.75
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	7	23.73
(2,142)	1:202:A:GLY:H	1:136:A:SER:O	4	23.73
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	3	23.72
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	7	23.68
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	8	23.68
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	15	23.67
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	6	23.67
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	7	23.67
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	14	23.66
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	20	23.66
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	8	23.66
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	13	23.66
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	20	23.66
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	5	23.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	19	23.65
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	18	23.64
(2,138)	1:154:A:SER:H	1:136:A:SER:O	2	23.64
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	10	23.63
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	18	23.63
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	1	23.61
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	9	23.61
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	7	23.6
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	6	23.6
(3,63)	1:72:A:ASN:H	1:198:A:CYS:O	9	23.59
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	7	23.58
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	14	23.57
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	4	23.56
(2,161)	1:107:A:ARG:H	1:198:A:CYS:O	4	23.55
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	13	23.54
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	20	23.53
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	7	23.53
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	13	23.53
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	13	23.52
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	12	23.51
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	15	23.51
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	8	23.5
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	5	23.5
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	9	23.5
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	15	23.49
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	11	23.48
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	3	23.46
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	13	23.46
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	3	23.44
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	1	23.44
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	12	23.44
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	15	23.42
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	8	23.42
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	11	23.41
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	15	23.4
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	9	23.4
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	15	23.4
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	7	23.39
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	1	23.37
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	13	23.36
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	12	23.36
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	6	23.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	5	23.34
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	11	23.34
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	19	23.33
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	17	23.32
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	10	23.32
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	12	23.32
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	15	23.32
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	5	23.31
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	6	23.3
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	9	23.3
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	15	23.3
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	16	23.3
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	16	23.28
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	10	23.26
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	1	23.25
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	16	23.25
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	19	23.25
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	16	23.22
(2,174)	1:180:A:GLU:H	1:198:A:CYS:O	4	23.22
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	5	23.21
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	7	23.2
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	16	23.18
(3,165)	1:183:A:PHE:H	1:60:A:SER:O	14	23.18
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	16	23.18
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	13	23.18
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	7	23.18
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	3	23.17
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	11	23.16
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	4	23.16
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	20	23.14
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	20	23.14
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	5	23.13
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	14	23.12
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	14	23.11
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	8	23.11
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	16	23.11
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	14	23.11
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	20	23.11
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	16	23.09
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	10	23.09
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	2	23.09
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	17	23.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	9	23.06
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	2	23.05
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	17	23.04
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	7	23.04
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	8	23.03
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	18	23.02
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	11	23.02
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	18	23.01
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	14	23.01
(2,163)	1:111:A:ILE:H	1:198:A:CYS:O	4	23.01
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	2	23.0
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	15	23.0
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	4	22.99
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	19	22.98
(4,1)	1:156:A:PHE:H	1:136:A:SER:O	2	22.98
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	12	22.98
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	13	22.98
(3,57)	1:65:A:ASP:H	1:198:A:CYS:O	9	22.97
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	9	22.97
(2,133)	1:116:A:GLY:H	1:136:A:SER:O	18	22.97
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	12	22.96
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	9	22.96
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	19	22.95
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	4	22.95
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	15	22.95
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	20	22.94
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	15	22.94
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	2	22.92
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	12	22.92
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	14	22.92
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	20	22.92
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	16	22.9
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	3	22.88
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	15	22.88
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	19	22.88
(3,136)	1:107:A:ARG:H	1:60:A:SER:O	2	22.87
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	6	22.87
(3,138)	1:120:A:GLU:H	1:60:A:SER:O	13	22.85
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	8	22.85
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	15	22.85
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	8	22.83
(3,53)	1:60:A:SER:H	1:198:A:CYS:O	8	22.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	1	22.82
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	16	22.81
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	9	22.8
(2,141)	1:201:A:ASP:H	1:136:A:SER:O	4	22.8
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	3	22.79
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	20	22.78
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	6	22.77
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	2	22.77
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	3	22.77
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	5	22.77
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	15	22.76
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	7	22.76
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	1	22.75
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	6	22.74
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	10	22.74
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	13	22.74
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	15	22.72
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	20	22.71
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	17	22.69
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	18	22.67
(3,59)	1:67:A:ASP:H	1:198:A:CYS:O	9	22.63
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	4	22.62
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	1	22.6
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	20	22.58
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	7	22.54
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	12	22.53
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	13	22.53
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	14	22.52
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	6	22.51
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	8	22.51
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	19	22.5
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	11	22.5
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	7	22.48
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	6	22.48
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	19	22.46
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	18	22.44
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	10	22.43
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	13	22.39
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	9	22.37
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	4	22.37
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	8	22.36
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	13	22.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	10	22.35
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	18	22.32
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	12	22.32
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	15	22.32
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	11	22.29
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	9	22.29
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	7	22.28
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	9	22.25
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	1	22.25
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	10	22.25
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	4	22.25
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	20	22.24
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	15	22.24
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	16	22.24
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	3	22.23
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	18	22.23
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	7	22.23
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	4	22.21
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	17	22.19
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	5	22.19
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	6	22.17
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	18	22.17
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	18	22.17
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	7	22.16
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	8	22.16
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	14	22.16
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	13	22.16
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	6	22.15
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	20	22.14
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	7	22.14
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	18	22.14
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	17	22.13
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	14	22.11
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	18	22.1
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	15	22.09
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	8	22.06
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	11	22.06
(3,169)	1:187:A:SER:H	1:60:A:SER:O	9	22.04
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	20	22.02
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	20	22.01
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	3	22.0
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	17	21.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:109:A:ARG:H	1:198:A:CYS:O	4	21.98
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	7	21.97
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	17	21.97
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	5	21.96
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	18	21.96
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	15	21.95
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	20	21.94
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	13	21.93
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	18	21.93
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	5	21.93
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	10	21.9
(3,159)	1:171:A:ASP:H	1:60:A:SER:O	13	21.89
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	17	21.89
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	15	21.89
(5,1)	1:174:A:ILE:H	1:136:A:SER:O	13	21.88
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	20	21.88
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	3	21.88
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	11	21.87
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	2	21.87
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	13	21.86
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	18	21.86
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	15	21.86
(3,172)	1:195:A:GLY:H	1:60:A:SER:O	4	21.84
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	8	21.84
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	10	21.84
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	7	21.83
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	13	21.83
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	11	21.83
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	20	21.83
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	17	21.82
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	1	21.82
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	18	21.82
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	13	21.81
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	1	21.8
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	12	21.8
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	9	21.79
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	4	21.79
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	11	21.79
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	1	21.78
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	4	21.78
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	18	21.77
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	17	21.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	12	21.76
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	13	21.74
(3,77)	1:138:A:ASN:H	1:198:A:CYS:O	4	21.71
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	20	21.71
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	12	21.69
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	5	21.67
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	16	21.66
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	16	21.66
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	18	21.65
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	2	21.64
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	8	21.63
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	1	21.62
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	19	21.61
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	3	21.58
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	1	21.58
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	5	21.57
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	4	21.56
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	17	21.55
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	12	21.54
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	2	21.53
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	8	21.53
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	5	21.53
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	14	21.52
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	12	21.51
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	19	21.51
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	2	21.5
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	20	21.49
(3,169)	1:187:A:SER:H	1:60:A:SER:O	16	21.48
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	19	21.48
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	3	21.47
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	18	21.45
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	15	21.44
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	6	21.44
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	9	21.43
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	14	21.43
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	11	21.42
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	5	21.41
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	16	21.39
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	11	21.39
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	7	21.39
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	11	21.35
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	19	21.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	9	21.35
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	2	21.32
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	6	21.32
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	13	21.32
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	6	21.31
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	7	21.31
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	11	21.3
(3,169)	1:187:A:SER:H	1:60:A:SER:O	19	21.29
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	5	21.29
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	13	21.29
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	6	21.29
(5,2)	1:109:A:ARG:H	1:60:A:SER:O	14	21.28
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	19	21.27
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	15	21.26
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	20	21.26
(3,140)	1:123:A:SER:H	1:60:A:SER:O	16	21.24
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	16	21.24
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	3	21.21
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	10	21.2
(3,94)	1:167:A:LEU:H	1:198:A:CYS:O	4	21.2
(3,140)	1:123:A:SER:H	1:60:A:SER:O	19	21.19
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	17	21.17
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	16	21.17
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	18	21.17
(3,171)	1:189:A:MET:H	1:60:A:SER:O	9	21.16
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	4	21.16
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	8	21.15
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	12	21.15
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	1	21.14
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	15	21.14
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	15	21.11
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	12	21.11
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	3	21.1
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	11	21.1
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	18	21.09
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	8	21.07
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	14	21.06
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	4	21.06
(3,167)	1:185:A:ILE:H	1:60:A:SER:O	1	21.05
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	4	21.04
(3,157)	1:169:A:VAL:H	1:60:A:SER:O	13	21.03
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	14	21.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	19	21.02
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	8	21.02
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	3	21.0
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	13	21.0
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	19	20.98
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	18	20.97
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	9	20.97
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	17	20.97
(2,135)	1:120:A:GLU:H	1:136:A:SER:O	2	20.96
(3,140)	1:123:A:SER:H	1:60:A:SER:O	2	20.95
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	16	20.95
(3,140)	1:123:A:SER:H	1:60:A:SER:O	9	20.94
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	3	20.93
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	2	20.93
(3,60)	1:68:A:ARG:H	1:198:A:CYS:O	9	20.93
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	10	20.92
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	17	20.89
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	15	20.87
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	3	20.86
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	8	20.86
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	17	20.86
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	8	20.85
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	1	20.85
(3,67)	1:102:A:ARG:H	1:198:A:CYS:O	4	20.84
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	18	20.84
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	10	20.81
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	2	20.81
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	16	20.8
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	10	20.8
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	6	20.74
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	12	20.74
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	18	20.73
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	5	20.72
(3,171)	1:189:A:MET:H	1:60:A:SER:O	16	20.71
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	5	20.71
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	18	20.71
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	20	20.7
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	12	20.7
(2,164)	1:116:A:GLY:H	1:198:A:CYS:O	4	20.7
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	7	20.66
(3,92)	1:164:A:GLU:H	1:198:A:CYS:O	4	20.66
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	14	20.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	20	20.66
(3,169)	1:187:A:SER:H	1:60:A:SER:O	10	20.64
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	7	20.63
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	8	20.63
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	17	20.63
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	19	20.63
(3,54)	1:61:A:HIS:H	1:198:A:CYS:O	9	20.63
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	20	20.62
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	6	20.62
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	14	20.6
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	1	20.6
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	7	20.6
(3,171)	1:189:A:MET:H	1:60:A:SER:O	19	20.59
(3,169)	1:187:A:SER:H	1:60:A:SER:O	6	20.59
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	2	20.59
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	3	20.59
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	6	20.59
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	9	20.58
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	6	20.56
(3,169)	1:187:A:SER:H	1:60:A:SER:O	18	20.54
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	6	20.54
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	15	20.54
(3,140)	1:123:A:SER:H	1:60:A:SER:O	10	20.53
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	13	20.53
(2,175)	1:182:A:PHE:H	1:198:A:CYS:O	4	20.53
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	4	20.53
(3,169)	1:187:A:SER:H	1:60:A:SER:O	20	20.52
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	1	20.51
(3,43)	1:172:A:ARG:H	1:136:A:SER:O	13	20.51
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	16	20.51
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	10	20.5
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	15	20.49
(3,169)	1:187:A:SER:H	1:60:A:SER:O	4	20.48
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	4	20.48
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	16	20.48
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	4	20.48
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	9	20.47
(3,140)	1:123:A:SER:H	1:60:A:SER:O	6	20.45
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	7	20.45
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	7	20.44
(3,140)	1:123:A:SER:H	1:60:A:SER:O	18	20.43
(3,38)	1:153:A:THR:H	1:136:A:SER:O	11	20.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	13	20.43
(3,140)	1:123:A:SER:H	1:60:A:SER:O	4	20.42
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	5	20.42
(3,140)	1:123:A:SER:H	1:60:A:SER:O	8	20.41
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	12	20.41
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	11	20.4
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	16	20.4
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	9	20.39
(3,169)	1:187:A:SER:H	1:60:A:SER:O	2	20.38
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	18	20.38
(2,137)	1:151:A:GLU:H	1:136:A:SER:O	2	20.37
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	6	20.36
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	11	20.36
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	14	20.34
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	9	20.32
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	19	20.32
(3,169)	1:187:A:SER:H	1:60:A:SER:O	17	20.31
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	18	20.31
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	1	20.31
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	5	20.31
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	1	20.31
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	11	20.31
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	14	20.3
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	14	20.29
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	8	20.28
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	20	20.28
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	17	20.28
(3,169)	1:187:A:SER:H	1:60:A:SER:O	3	20.27
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	17	20.27
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	4	20.27
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	20	20.27
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	18	20.26
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	14	20.26
(3,169)	1:187:A:SER:H	1:60:A:SER:O	8	20.25
(3,140)	1:123:A:SER:H	1:60:A:SER:O	15	20.25
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	10	20.25
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	5	20.24
(3,140)	1:123:A:SER:H	1:60:A:SER:O	3	20.23
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	13	20.23
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	16	20.22
(3,38)	1:153:A:THR:H	1:136:A:SER:O	4	20.22
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	17	20.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	20	20.21
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	17	20.2
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	6	20.19
(3,140)	1:123:A:SER:H	1:60:A:SER:O	5	20.18
(3,140)	1:123:A:SER:H	1:60:A:SER:O	7	20.18
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	7	20.18
(3,169)	1:187:A:SER:H	1:60:A:SER:O	7	20.15
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	5	20.14
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	2	20.14
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	19	20.13
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	1	20.12
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	9	20.11
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	4	20.1
(3,140)	1:123:A:SER:H	1:60:A:SER:O	20	20.1
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	10	20.1
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	20	20.1
(3,68)	1:106:A:ASN:H	1:198:A:CYS:O	4	20.09
(3,55)	1:62:A:THR:H	1:198:A:CYS:O	9	20.09
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	11	20.08
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	3	20.08
(3,10)	1:79:A:GLN:H	1:136:A:SER:O	10	20.07
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	15	20.05
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	20	20.05
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	3	20.04
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	15	20.04
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	3	20.03
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	15	20.03
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	5	20.01
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	18	20.01
(3,140)	1:123:A:SER:H	1:60:A:SER:O	1	20.0
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	16	19.98
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	2	19.97
(3,169)	1:187:A:SER:H	1:60:A:SER:O	15	19.96
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	9	19.96
(3,135)	1:106:A:ASN:H	1:60:A:SER:O	14	19.94
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	12	19.94
(3,169)	1:187:A:SER:H	1:60:A:SER:O	12	19.93
(3,169)	1:187:A:SER:H	1:60:A:SER:O	13	19.93
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	1	19.93
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	5	19.93
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	6	19.92
(3,38)	1:153:A:THR:H	1:136:A:SER:O	7	19.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	12	19.92
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	18	19.92
(3,38)	1:153:A:THR:H	1:136:A:SER:O	1	19.91
(3,169)	1:187:A:SER:H	1:60:A:SER:O	11	19.9
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	7	19.9
(3,140)	1:123:A:SER:H	1:60:A:SER:O	12	19.89
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	19	19.89
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	13	19.89
(3,140)	1:123:A:SER:H	1:60:A:SER:O	13	19.88
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	13	19.88
(3,171)	1:189:A:MET:H	1:60:A:SER:O	18	19.87
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	2	19.86
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	1	19.85
(3,33)	1:132:A:THR:H	1:136:A:SER:O	1	19.85
(3,171)	1:189:A:MET:H	1:60:A:SER:O	10	19.83
(3,169)	1:187:A:SER:H	1:60:A:SER:O	5	19.83
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	2	19.83
(3,33)	1:132:A:THR:H	1:136:A:SER:O	4	19.83
(3,140)	1:123:A:SER:H	1:60:A:SER:O	17	19.82
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	10	19.82
(3,38)	1:153:A:THR:H	1:136:A:SER:O	5	19.81
(3,171)	1:189:A:MET:H	1:60:A:SER:O	4	19.79
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	12	19.79
(3,140)	1:123:A:SER:H	1:60:A:SER:O	11	19.79
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	8	19.79
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	11	19.79
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	8	19.79
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	17	19.78
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	15	19.78
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	5	19.78
(3,171)	1:189:A:MET:H	1:60:A:SER:O	6	19.77
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	8	19.77
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	13	19.77
(3,33)	1:132:A:THR:H	1:136:A:SER:O	17	19.77
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	19	19.77
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	9	19.76
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	19	19.76
(3,38)	1:153:A:THR:H	1:136:A:SER:O	16	19.76
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	16	19.76
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	8	19.75
(3,38)	1:153:A:THR:H	1:136:A:SER:O	17	19.74
(3,33)	1:132:A:THR:H	1:136:A:SER:O	13	19.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	16	19.73
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	11	19.73
(3,38)	1:153:A:THR:H	1:136:A:SER:O	6	19.73
(3,169)	1:187:A:SER:H	1:60:A:SER:O	1	19.71
(3,33)	1:132:A:THR:H	1:136:A:SER:O	18	19.71
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	12	19.68
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	19	19.68
(3,33)	1:132:A:THR:H	1:136:A:SER:O	3	19.67
(3,171)	1:189:A:MET:H	1:60:A:SER:O	20	19.66
(3,69)	1:112:A:LEU:H	1:198:A:CYS:O	4	19.66
(3,33)	1:132:A:THR:H	1:136:A:SER:O	11	19.65
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	12	19.64
(3,33)	1:132:A:THR:H	1:136:A:SER:O	8	19.64
(3,33)	1:132:A:THR:H	1:136:A:SER:O	15	19.62
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	18	19.62
(3,38)	1:153:A:THR:H	1:136:A:SER:O	9	19.61
(3,38)	1:153:A:THR:H	1:136:A:SER:O	15	19.61
(3,171)	1:189:A:MET:H	1:60:A:SER:O	2	19.59
(3,140)	1:123:A:SER:H	1:60:A:SER:O	14	19.59
(3,38)	1:153:A:THR:H	1:136:A:SER:O	18	19.58
(3,33)	1:132:A:THR:H	1:136:A:SER:O	5	19.58
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	8	19.57
(3,33)	1:132:A:THR:H	1:136:A:SER:O	20	19.57
(3,38)	1:153:A:THR:H	1:136:A:SER:O	20	19.56
(3,33)	1:132:A:THR:H	1:136:A:SER:O	19	19.56
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	12	19.56
(3,33)	1:132:A:THR:H	1:136:A:SER:O	9	19.55
(3,38)	1:153:A:THR:H	1:136:A:SER:O	3	19.54
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	11	19.54
(3,33)	1:132:A:THR:H	1:136:A:SER:O	6	19.53
(3,171)	1:189:A:MET:H	1:60:A:SER:O	8	19.52
(3,33)	1:132:A:THR:H	1:136:A:SER:O	16	19.52
(3,169)	1:187:A:SER:H	1:60:A:SER:O	14	19.51
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	10	19.51
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	11	19.5
(3,33)	1:132:A:THR:H	1:136:A:SER:O	12	19.5
(3,33)	1:132:A:THR:H	1:136:A:SER:O	7	19.49
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	19	19.48
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	4	19.46
(3,33)	1:132:A:THR:H	1:136:A:SER:O	10	19.46
(3,171)	1:189:A:MET:H	1:60:A:SER:O	3	19.45
(3,38)	1:153:A:THR:H	1:136:A:SER:O	8	19.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:132:A:THR:H	1:136:A:SER:O	2	19.45
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	3	19.42
(3,171)	1:189:A:MET:H	1:60:A:SER:O	17	19.41
(3,38)	1:153:A:THR:H	1:136:A:SER:O	19	19.41
(3,33)	1:132:A:THR:H	1:136:A:SER:O	14	19.41
(3,38)	1:153:A:THR:H	1:136:A:SER:O	13	19.38
(3,171)	1:189:A:MET:H	1:60:A:SER:O	7	19.35
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	14	19.35
(3,38)	1:153:A:THR:H	1:136:A:SER:O	14	19.34
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	20	19.33
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	2	19.31
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	1	19.29
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	10	19.28
(3,38)	1:153:A:THR:H	1:136:A:SER:O	12	19.24
(3,171)	1:189:A:MET:H	1:60:A:SER:O	12	19.23
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	4	19.23
(3,171)	1:189:A:MET:H	1:60:A:SER:O	13	19.22
(3,171)	1:189:A:MET:H	1:60:A:SER:O	15	19.22
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	4	19.21
(3,171)	1:189:A:MET:H	1:60:A:SER:O	11	19.18
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	6	19.18
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	7	19.15
(3,38)	1:153:A:THR:H	1:136:A:SER:O	10	19.15
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	17	19.14
(3,28)	1:119:A:ARG:H	1:136:A:SER:O	2	19.14
(3,158)	1:170:A:VAL:H	1:60:A:SER:O	13	19.11
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	8	19.09
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	5	19.08
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	7	19.07
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	18	19.06
(3,171)	1:189:A:MET:H	1:60:A:SER:O	5	19.04
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	19	19.04
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	13	19.01
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	16	18.97
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	13	18.97
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	17	18.96
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	6	18.95
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	6	18.95
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	15	18.94
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	9	18.94
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	16	18.94
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	18	18.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	16	18.93
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	4	18.93
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	13	18.92
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	3	18.91
(3,171)	1:189:A:MET:H	1:60:A:SER:O	1	18.9
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	10	18.9
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	17	18.9
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	3	18.89
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	15	18.89
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	20	18.89
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	18	18.87
(3,38)	1:153:A:THR:H	1:136:A:SER:O	2	18.86
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	20	18.85
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	7	18.84
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	5	18.83
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	1	18.83
(2,136)	1:122:A:ASP:H	1:136:A:SER:O	2	18.82
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	20	18.81
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	15	18.81
(2,165)	1:117:A:PHE:H	1:198:A:CYS:O	4	18.81
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	1	18.81
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	13	18.8
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	7	18.8
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	6	18.79
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	1	18.79
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	3	18.79
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	4	18.77
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	2	18.77
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	14	18.77
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	15	18.77
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	19	18.77
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	18	18.76
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	20	18.76
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	6	18.75
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	15	18.75
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	9	18.74
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	14	18.73
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	7	18.72
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	7	18.71
(3,171)	1:189:A:MET:H	1:60:A:SER:O	14	18.7
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	12	18.7
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	11	18.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:65:A:ASP:H	1:136:A:SER:O	14	18.7
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	19	18.69
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	8	18.68
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	9	18.67
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	10	18.67
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	17	18.67
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	18	18.67
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	3	18.66
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	5	18.65
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	3	18.64
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	2	18.64
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	11	18.64
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	14	18.63
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	19	18.63
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	9	18.62
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	5	18.61
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	17	18.6
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	12	18.6
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	8	18.6
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	17	18.59
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	11	18.59
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	12	18.59
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	9	18.58
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	16	18.57
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	20	18.57
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	7	18.55
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	13	18.54
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	5	18.54
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	20	18.54
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	2	18.54
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	11	18.53
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	8	18.52
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	12	18.51
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	4	18.51
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	17	18.49
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	9	18.49
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	12	18.49
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	16	18.49
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	16	18.48
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	6	18.47
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	8	18.45
(3,56)	1:64:A:ALA:H	1:198:A:CYS:O	9	18.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	5	18.45
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	19	18.45
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	12	18.44
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	9	18.42
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	10	18.42
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	1	18.41
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	3	18.41
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	2	18.4
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	7	18.39
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	16	18.39
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	6	18.39
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	18	18.39
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	10	18.38
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	1	18.37
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	19	18.37
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	11	18.36
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	19	18.36
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	18	18.36
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	19	18.35
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	10	18.35
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	5	18.34
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	19	18.33
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	12	18.33
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	17	18.32
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	8	18.31
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	20	18.3
(3,139)	1:122:A:ASP:H	1:60:A:SER:O	14	18.29
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	11	18.29
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	10	18.29
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	8	18.29
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	13	18.29
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	4	18.28
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	2	18.26
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	6	18.26
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	18	18.26
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	17	18.25
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	3	18.24
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	7	18.24
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	13	18.24
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	15	18.24
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	4	18.23
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	9	18.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	3	18.23
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	6	18.22
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	8	18.21
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	17	18.21
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	13	18.21
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	6	18.21
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	3	18.2
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	20	18.19
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	12	18.18
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	12	18.18
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	16	18.17
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	18	18.17
(2,131)	1:67:A:ASP:H	1:136:A:SER:O	14	18.17
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	2	18.16
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	2	18.14
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	4	18.14
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	9	18.14
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	20	18.13
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	12	18.12
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	17	18.12
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	18	18.12
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	10	18.11
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	16	18.11
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	1	18.1
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	7	18.09
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	9	18.08
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	15	18.07
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	19	18.07
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	14	18.07
(3,37)	1:152:A:GLU:H	1:136:A:SER:O	2	18.07
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	11	18.06
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	8	18.06
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	2	18.05
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	6	18.05
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	6	18.05
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	3	18.05
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	14	18.05
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	8	18.04
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	1	18.04
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	5	18.03
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	13	18.03
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	8	18.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	1:81:A:THR:H	1:136:A:SER:O	19	18.02
(2,132)	1:68:A:ARG:H	1:136:A:SER:O	10	18.02
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	13	18.01
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	13	18.01
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	17	18.0
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	5	17.99
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	14	17.99
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	4	17.98
(3,21)	1:95:A:TYR:H	1:136:A:SER:O	2	17.98
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	1	17.98
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	5	17.97
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	18	17.96
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	10	17.96
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	1	17.96
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	15	17.96
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	15	17.94
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	20	17.94
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	16	17.93
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	15	17.93
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	16	17.92
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	18	17.92
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	6	17.91
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	10	17.91
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	15	17.91
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	7	17.89
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	11	17.89
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	2	17.89
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	15	17.87
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	4	17.86
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	11	17.85
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	7	17.83
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	5	17.83
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	2	17.81
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	8	17.81
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	1	17.8
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	11	17.8
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	3	17.79
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	19	17.78
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	17	17.78
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	5	17.78
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	16	17.78
(3,34)	1:142:A:ALA:H	1:136:A:SER:O	4	17.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	12	17.76
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	12	17.76
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	3	17.75
(3,11)	1:81:A:THR:H	1:136:A:SER:O	8	17.75
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	1	17.74
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	11	17.74
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	20	17.74
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	14	17.74
(3,168)	1:186:A:ALA:H	1:60:A:SER:O	14	17.73
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	9	17.73
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	5	17.72
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	14	17.72
(3,11)	1:81:A:THR:H	1:136:A:SER:O	18	17.71
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	20	17.71
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	10	17.7
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	6	17.68
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	19	17.67
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	17	17.66
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	3	17.65
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	10	17.62
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	15	17.62
(3,11)	1:81:A:THR:H	1:136:A:SER:O	3	17.6
(3,11)	1:81:A:THR:H	1:136:A:SER:O	13	17.6
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	18	17.59
(3,11)	1:81:A:THR:H	1:136:A:SER:O	2	17.59
(3,121)	1:85:A:GLU:H	1:60:A:SER:O	19	17.58
(3,11)	1:81:A:THR:H	1:136:A:SER:O	15	17.58
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	4	17.58
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	13	17.57
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	4	17.56
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	16	17.54
(3,29)	1:123:A:SER:H	1:136:A:SER:O	11	17.53
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	7	17.53
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	8	17.5
(3,11)	1:81:A:THR:H	1:136:A:SER:O	4	17.5
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	12	17.49
(3,11)	1:81:A:THR:H	1:136:A:SER:O	17	17.49
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	9	17.47
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	20	17.43
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	13	17.43
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	3	17.42
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	7	17.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,29)	1:123:A:SER:H	1:136:A:SER:O	1	17.4
(3,11)	1:81:A:THR:H	1:136:A:SER:O	12	17.4
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	16	17.38
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	11	17.37
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	7	17.35
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	1	17.35
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	18	17.33
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	18	17.32
(3,3)	1:66:A:ASP:H	1:136:A:SER:O	14	17.29
(3,11)	1:81:A:THR:H	1:136:A:SER:O	20	17.28
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	8	17.27
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	9	17.27
(3,11)	1:81:A:THR:H	1:136:A:SER:O	14	17.26
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	19	17.26
(3,11)	1:81:A:THR:H	1:136:A:SER:O	5	17.25
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	17	17.25
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	12	17.24
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	7	17.23
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	1	17.19
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	20	17.19
(3,141)	1:125:A:LEU:H	1:60:A:SER:O	14	17.18
(3,11)	1:81:A:THR:H	1:136:A:SER:O	9	17.18
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	13	17.17
(3,11)	1:81:A:THR:H	1:136:A:SER:O	6	17.13
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	15	17.12
(3,11)	1:81:A:THR:H	1:136:A:SER:O	16	17.11
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	12	17.08
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	4	17.08
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	18	17.07
(3,9)	1:78:A:ASN:H	1:136:A:SER:O	10	17.07
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	6	17.05
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	1	17.04
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	3	17.04
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	9	17.03
(3,98)	1:183:A:PHE:H	1:198:A:CYS:O	4	17.03
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	10	17.02
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	4	17.01
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	20	17.01
(3,11)	1:81:A:THR:H	1:136:A:SER:O	7	17.0
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	6	16.97
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	13	16.97
(3,11)	1:81:A:THR:H	1:136:A:SER:O	10	16.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	5	16.94
(3,29)	1:123:A:SER:H	1:136:A:SER:O	4	16.94
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	15	16.91
(3,29)	1:123:A:SER:H	1:136:A:SER:O	6	16.91
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	20	16.9
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	11	16.9
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	11	16.9
(3,11)	1:81:A:THR:H	1:136:A:SER:O	11	16.9
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	10	16.9
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	12	16.84
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	19	16.83
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	14	16.8
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	1	16.8
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	12	16.8
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	17	16.79
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	19	16.79
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	15	16.79
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	16	16.79
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	10	16.77
(3,29)	1:123:A:SER:H	1:136:A:SER:O	7	16.77
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	7	16.77
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	2	16.76
(3,29)	1:123:A:SER:H	1:136:A:SER:O	9	16.74
(3,11)	1:81:A:THR:H	1:136:A:SER:O	1	16.74
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	8	16.73
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	13	16.71
(3,29)	1:123:A:SER:H	1:136:A:SER:O	16	16.7
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	2	16.69
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	20	16.69
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	3	16.67
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	7	16.66
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	16	16.66
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	17	16.64
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	6	16.64
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	16	16.63
(3,29)	1:123:A:SER:H	1:136:A:SER:O	14	16.63
(3,29)	1:123:A:SER:H	1:136:A:SER:O	17	16.62
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	11	16.61
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	13	16.61
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	5	16.6
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	6	16.6
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	7	16.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	2	16.58
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	5	16.58
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	9	16.55
(3,151)	1:154:A:SER:H	1:60:A:SER:O	9	16.54
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	1	16.54
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	9	16.52
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	2	16.51
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	8	16.5
(3,29)	1:123:A:SER:H	1:136:A:SER:O	5	16.5
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	5	16.49
(3,29)	1:123:A:SER:H	1:136:A:SER:O	20	16.49
(3,134)	1:104:A:VAL:H	1:60:A:SER:O	2	16.48
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	18	16.48
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	4	16.48
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	17	16.47
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	16	16.47
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	15	16.45
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	12	16.44
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	17	16.44
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	8	16.43
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	14	16.43
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	8	16.43
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	18	16.42
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	11	16.41
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	13	16.41
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	6	16.41
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	3	16.4
(3,29)	1:123:A:SER:H	1:136:A:SER:O	10	16.4
(3,29)	1:123:A:SER:H	1:136:A:SER:O	3	16.38
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	3	16.37
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	19	16.36
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	2	16.35
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	6	16.35
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	4	16.34
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	16	16.34
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	15	16.34
(3,29)	1:123:A:SER:H	1:136:A:SER:O	18	16.34
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	11	16.33
(3,29)	1:123:A:SER:H	1:136:A:SER:O	15	16.32
(3,99)	1:184:A:LYS:H	1:198:A:CYS:O	4	16.3
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	16	16.3
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	5	16.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	3	16.28
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	5	16.24
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	4	16.22
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	9	16.21
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	20	16.21
(3,29)	1:123:A:SER:H	1:136:A:SER:O	13	16.2
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	8	16.2
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	17	16.2
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	18	16.19
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	18	16.18
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	19	16.17
(3,29)	1:123:A:SER:H	1:136:A:SER:O	8	16.15
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	7	16.13
(3,42)	1:169:A:VAL:H	1:136:A:SER:O	13	16.12
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	8	16.11
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	2	16.11
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	10	16.1
(3,29)	1:123:A:SER:H	1:136:A:SER:O	12	16.1
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	1	16.09
(3,151)	1:154:A:SER:H	1:60:A:SER:O	16	16.09
(3,29)	1:123:A:SER:H	1:136:A:SER:O	19	16.09
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	12	16.06
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	15	16.06
(3,151)	1:154:A:SER:H	1:60:A:SER:O	19	16.05
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	12	16.05
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	3	16.04
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	19	16.03
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	16	16.0
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	7	15.97
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	1	15.95
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	18	15.94
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	17	15.94
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	20	15.92
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	11	15.92
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	1	15.91
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	16	15.91
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	8	15.9
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	6	15.9
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	12	15.9
(3,170)	1:188:A:GLN:H	1:60:A:SER:O	14	15.88
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	5	15.88
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	13	15.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	8	15.86
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	9	15.85
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	8	15.83
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	18	15.83
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	20	15.82
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	9	15.81
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	20	15.77
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	12	15.77
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	15	15.76
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	13	15.75
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	16	15.73
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	15	15.72
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	7	15.71
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	16	15.7
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	10	15.69
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	3	15.68
(3,29)	1:123:A:SER:H	1:136:A:SER:O	2	15.67
(3,4)	1:70:A:LEU:H	1:136:A:SER:O	14	15.66
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	8	15.65
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	15	15.64
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	11	15.63
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	19	15.62
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	12	15.62
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	9	15.62
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	5	15.61
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	16	15.58
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	9	15.55
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	16	15.5
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	11	15.5
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	13	15.5
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	17	15.5
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	14	15.49
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	13	15.49
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	2	15.48
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	14	15.47
(3,151)	1:154:A:SER:H	1:60:A:SER:O	10	15.45
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	18	15.45
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	11	15.44
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	3	15.43
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	4	15.41
(3,151)	1:154:A:SER:H	1:60:A:SER:O	6	15.4
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	5	15.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	10	15.39
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	7	15.38
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	1	15.38
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	19	15.36
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	17	15.34
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	4	15.34
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	7	15.33
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	12	15.33
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	4	15.32
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	9	15.32
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	19	15.3
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	14	15.29
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	9	15.27
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	11	15.27
(3,151)	1:154:A:SER:H	1:60:A:SER:O	18	15.26
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	8	15.26
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	1	15.24
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	18	15.23
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	9	15.22
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	13	15.22
(3,151)	1:154:A:SER:H	1:60:A:SER:O	4	15.21
(3,133)	1:103:A:GLU:H	1:60:A:SER:O	2	15.19
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	10	15.17
(3,151)	1:154:A:SER:H	1:60:A:SER:O	20	15.15
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	10	15.15
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	6	15.15
(3,151)	1:154:A:SER:H	1:60:A:SER:O	2	15.14
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	6	15.14
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	9	15.13
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	4	15.12
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	8	15.12
(3,1)	1:64:A:ALA:H	1:136:A:SER:O	14	15.12
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	7	15.11
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	6	15.1
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	9	15.1
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	18	15.09
(3,6)	1:72:A:ASN:H	1:136:A:SER:O	10	15.09
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	19	15.07
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	1	15.07
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	20	15.07
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	5	15.06
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	5	15.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	7	15.05
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	12	15.05
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	3	15.05
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	1	15.04
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	14	15.03
(3,151)	1:154:A:SER:H	1:60:A:SER:O	3	15.0
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	15	15.0
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	19	15.0
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	3	14.98
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	14	14.98
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	3	14.97
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	14	14.96
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	18	14.95
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	20	14.94
(3,151)	1:154:A:SER:H	1:60:A:SER:O	8	14.94
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	18	14.93
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	10	14.92
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	20	14.92
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	2	14.92
(3,151)	1:154:A:SER:H	1:60:A:SER:O	17	14.91
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	20	14.91
(3,100)	1:185:A:ILE:H	1:198:A:CYS:O	4	14.9
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	9	14.87
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	6	14.87
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	16	14.86
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	11	14.86
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	5	14.86
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	18	14.84
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	20	14.82
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	6	14.8
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	13	14.79
(3,151)	1:154:A:SER:H	1:60:A:SER:O	7	14.78
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	20	14.78
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	8	14.78
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	17	14.78
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	20	14.77
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	11	14.74
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	16	14.74
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	10	14.73
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	15	14.73
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	16	14.73
(3,151)	1:154:A:SER:H	1:60:A:SER:O	15	14.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	3	14.72
(3,40)	1:165:A:ARG:H	1:136:A:SER:O	15	14.72
(2,179)	1:205:A:LYS:H	1:60:A:SER:O	8	14.72
(3,151)	1:154:A:SER:H	1:60:A:SER:O	13	14.71
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	3	14.71
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	7	14.7
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	14	14.7
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	7	14.7
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	5	14.69
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	7	14.69
(3,151)	1:154:A:SER:H	1:60:A:SER:O	12	14.67
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	8	14.66
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	2	14.66
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	4	14.66
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	17	14.64
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	13	14.63
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	7	14.62
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	1	14.61
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	6	14.6
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	5	14.6
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	3	14.59
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	10	14.59
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	8	14.58
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	9	14.58
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	18	14.58
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	17	14.57
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	15	14.56
(3,151)	1:154:A:SER:H	1:60:A:SER:O	11	14.55
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	8	14.55
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	19	14.55
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	2	14.55
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	12	14.54
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	8	14.53
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	17	14.53
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	11	14.53
(3,151)	1:154:A:SER:H	1:60:A:SER:O	5	14.51
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	17	14.51
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	8	14.51
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	14	14.5
(3,151)	1:154:A:SER:H	1:60:A:SER:O	1	14.5
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	11	14.49
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	17	14.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	1	14.46
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	12	14.45
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	12	14.45
(3,151)	1:154:A:SER:H	1:60:A:SER:O	14	14.44
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	4	14.44
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	6	14.44
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	11	14.43
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	12	14.43
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	13	14.43
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	4	14.42
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	18	14.4
(3,41)	1:167:A:LEU:H	1:136:A:SER:O	2	14.4
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	3	14.4
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	2	14.39
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	13	14.39
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	17	14.39
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	14	14.38
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	18	14.38
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	3	14.38
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	15	14.35
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	15	14.34
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	10	14.34
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	16	14.33
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	20	14.33
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	7	14.32
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	8	14.32
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	3	14.31
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	19	14.31
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	1	14.3
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	20	14.28
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	1	14.27
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	3	14.25
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	14	14.25
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	5	14.24
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	10	14.24
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	12	14.21
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	7	14.21
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	10	14.2
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	13	14.2
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	9	14.2
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	9	14.19
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	5	14.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	9	14.18
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	6	14.18
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	9	14.17
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	5	14.16
(3,101)	1:186:A:ALA:H	1:198:A:CYS:O	4	14.16
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	4	14.16
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	20	14.15
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	15	14.14
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	16	14.13
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	1	14.13
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	3	14.13
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	7	14.13
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	1	14.12
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	15	14.11
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	15	14.11
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	20	14.11
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	14	14.1
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	19	14.09
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	6	14.08
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	12	14.06
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	7	14.06
(3,122)	1:86:A:GLU:H	1:60:A:SER:O	19	14.06
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	2	14.06
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	17	14.05
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	13	14.04
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	2	14.03
(3,131)	1:100:A:ILE:H	1:60:A:SER:O	11	14.02
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	16	14.0
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	2	14.0
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	5	13.97
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	12	13.97
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	17	13.94
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	2	13.91
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	5	13.91
(3,39)	1:164:A:GLU:H	1:136:A:SER:O	16	13.9
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	14	13.87
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	10	13.87
(3,79)	1:143:A:ARG:H	1:198:A:CYS:O	4	13.85
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	15	13.85
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	19	13.84
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	10	13.84
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	4	13.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	8	13.82
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	13	13.82
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	10	13.81
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	16	13.76
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	18	13.76
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	6	13.75
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	18	13.75
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	14	13.72
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	4	13.71
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	13	13.71
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	6	13.71
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	10	13.7
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	16	13.7
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	11	13.69
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	10	13.69
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	17	13.66
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	7	13.65
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	14	13.64
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	16	13.64
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	1	13.63
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	2	13.63
(3,142)	1:126:A:SER:H	1:60:A:SER:O	16	13.61
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	3	13.61
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	6	13.61
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	10	13.61
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	12	13.6
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	9	13.6
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	4	13.6
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	9	13.59
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	15	13.59
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	14	13.59
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	20	13.58
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	19	13.58
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	16	13.57
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	10	13.55
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	3	13.54
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	4	13.53
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	13	13.52
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	11	13.49
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	20	13.49
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	3	13.49
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	14	13.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,125)	1:92:A:TYR:H	1:60:A:SER:O	19	13.48
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	15	13.47
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	6	13.46
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	1	13.46
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	18	13.46
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	3	13.44
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	8	13.42
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	9	13.4
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	17	13.4
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	19	13.4
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	15	13.39
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	17	13.39
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	4	13.38
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	19	13.38
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	9	13.37
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	14	13.37
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	13	13.37
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	3	13.36
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	13	13.36
(3,12)	1:82:A:LYS:H	1:136:A:SER:O	11	13.34
(3,156)	1:167:A:LEU:H	1:60:A:SER:O	13	13.33
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	1	13.33
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	17	13.33
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	18	13.32
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	19	13.32
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	6	13.31
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	2	13.3
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	20	13.29
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	5	13.29
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	8	13.26
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	18	13.26
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	5	13.25
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	6	13.25
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	17	13.25
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	2	13.25
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	2	13.24
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	10	13.23
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	15	13.23
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	8	13.23
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	18	13.22
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	20	13.21
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	11	13.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	1	13.19
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	13	13.18
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	14	13.18
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	7	13.17
(3,120)	1:82:A:LYS:H	1:60:A:SER:O	19	13.17
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	5	13.16
(3,173)	1:200:A:VAL:H	1:60:A:SER:O	8	13.15
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	12	13.15
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	9	13.14
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	10	13.14
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	16	13.14
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	9	13.13
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	20	13.13
(3,142)	1:126:A:SER:H	1:60:A:SER:O	19	13.12
(3,142)	1:126:A:SER:H	1:60:A:SER:O	9	13.11
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	15	13.11
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	7	13.11
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	12	13.11
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	2	13.1
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	14	13.1
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	15	13.09
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	6	13.09
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	15	13.08
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	7	13.07
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	17	13.07
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	14	13.06
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	6	13.06
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	19	13.06
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	3	13.05
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	15	13.05
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	11	13.04
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	4	13.03
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	13	13.01
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	1	13.01
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	16	13.01
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	19	13.01
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	5	13.0
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	5	13.0
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	5	13.0
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	8	12.99
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	20	12.98
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	9	12.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	20	12.97
(3,142)	1:126:A:SER:H	1:60:A:SER:O	6	12.96
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	2	12.96
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	7	12.94
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	19	12.93
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	16	12.93
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	12	12.91
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	4	12.9
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	5	12.89
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	11	12.89
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	6	12.89
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	9	12.89
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	11	12.87
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	13	12.86
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	1	12.86
(3,142)	1:126:A:SER:H	1:60:A:SER:O	4	12.85
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	17	12.84
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	3	12.82
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	18	12.82
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	14	12.82
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	19	12.81
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	11	12.81
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	20	12.8
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	8	12.79
(3,142)	1:126:A:SER:H	1:60:A:SER:O	2	12.79
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	16	12.77
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	1	12.77
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	12	12.76
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	1	12.76
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	7	12.76
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	8	12.76
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	12	12.75
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	14	12.73
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	12	12.72
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	1	12.71
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	9	12.69
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	3	12.68
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	16	12.67
(3,142)	1:126:A:SER:H	1:60:A:SER:O	11	12.66
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	4	12.66
(3,132)	1:102:A:ARG:H	1:60:A:SER:O	2	12.65
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	10	12.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	18	12.63
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	13	12.63
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	15	12.63
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	8	12.62
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	5	12.62
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	20	12.61
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	18	12.6
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	6	12.6
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	1	12.59
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	18	12.58
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	11	12.58
(3,24)	1:102:A:ARG:H	1:136:A:SER:O	11	12.58
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	2	12.58
(3,142)	1:126:A:SER:H	1:60:A:SER:O	8	12.56
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	12	12.55
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	7	12.54
(3,142)	1:126:A:SER:H	1:60:A:SER:O	1	12.52
(3,8)	1:77:A:ARG:H	1:136:A:SER:O	10	12.52
(3,142)	1:126:A:SER:H	1:60:A:SER:O	15	12.51
(3,5)	1:71:A:TYR:H	1:136:A:SER:O	10	12.51
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	17	12.5
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	16	12.49
(3,142)	1:126:A:SER:H	1:60:A:SER:O	10	12.47
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	12	12.46
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	14	12.45
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	19	12.44
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	16	12.43
(3,142)	1:126:A:SER:H	1:60:A:SER:O	18	12.42
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	7	12.41
(3,142)	1:126:A:SER:H	1:60:A:SER:O	7	12.4
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	3	12.4
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	2	12.39
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	3	12.36
(3,142)	1:126:A:SER:H	1:60:A:SER:O	13	12.35
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	20	12.35
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	4	12.34
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	6	12.33
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	11	12.32
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	9	12.32
(3,142)	1:126:A:SER:H	1:60:A:SER:O	5	12.31
(3,142)	1:126:A:SER:H	1:60:A:SER:O	17	12.31
(3,142)	1:126:A:SER:H	1:60:A:SER:O	20	12.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	16	12.3
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	9	12.3
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	14	12.3
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	1	12.3
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	11	12.3
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	2	12.29
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	5	12.27
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	7	12.22
(3,142)	1:126:A:SER:H	1:60:A:SER:O	3	12.19
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	14	12.18
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	7	12.16
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	17	12.11
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	5	12.1
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	18	12.1
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	17	12.09
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	9	12.08
(3,142)	1:126:A:SER:H	1:60:A:SER:O	12	12.07
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	10	12.06
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	17	12.06
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	2	12.03
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	12	12.03
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	4	12.03
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	13	12.0
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	3	12.0
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	8	11.99
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	7	11.99
(3,7)	1:74:A:ILE:H	1:136:A:SER:O	10	11.99
(3,155)	1:165:A:ARG:H	1:60:A:SER:O	13	11.97
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	4	11.97
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	20	11.96
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	16	11.95
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	10	11.94
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	5	11.91
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	1	11.89
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	15	11.88
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	9	11.87
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	17	11.87
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	18	11.87
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	6	11.86
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	13	11.86
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	11	11.86
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	16	11.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	18	11.82
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	16	11.81
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	6	11.81
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	12	11.81
(3,31)	1:126:A:SER:H	1:136:A:SER:O	1	11.8
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	10	11.79
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	11	11.79
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	19	11.78
(3,31)	1:126:A:SER:H	1:136:A:SER:O	11	11.78
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	2	11.77
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	18	11.76
(3,78)	1:142:A:ALA:H	1:198:A:CYS:O	4	11.75
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	15	11.74
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	4	11.72
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	6	11.72
(3,150)	1:153:A:THR:H	1:60:A:SER:O	9	11.72
(3,142)	1:126:A:SER:H	1:60:A:SER:O	14	11.7
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	5	11.7
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	3	11.69
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	13	11.68
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	17	11.67
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	1	11.66
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	12	11.66
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	15	11.66
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	12	11.66
(3,174)	1:201:A:ASP:H	1:60:A:SER:O	8	11.65
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	8	11.64
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	18	11.64
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	16	11.63
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	6	11.62
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	3	11.61
(3,150)	1:153:A:THR:H	1:60:A:SER:O	16	11.61
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	14	11.61
(3,119)	1:81:A:THR:H	1:60:A:SER:O	15	11.61
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	9	11.61
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	13	11.61
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	2	11.6
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	20	11.59
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	5	11.58
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	8	11.58
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	15	11.57
(3,30)	1:125:A:LEU:H	1:136:A:SER:O	19	11.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	20	11.56
(3,119)	1:81:A:THR:H	1:60:A:SER:O	7	11.54
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	14	11.54
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	9	11.53
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	15	11.53
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	6	11.52
(3,119)	1:81:A:THR:H	1:60:A:SER:O	11	11.51
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	12	11.51
(3,126)	1:93:A:ASP:H	1:60:A:SER:O	11	11.5
(3,150)	1:153:A:THR:H	1:60:A:SER:O	19	11.49
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	13	11.49
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	18	11.49
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	4	11.48
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	1	11.48
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	7	11.48
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	18	11.48
(3,119)	1:81:A:THR:H	1:60:A:SER:O	14	11.46
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	8	11.46
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	14	11.45
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	16	11.45
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	20	11.45
(3,86)	1:155:A:ILE:H	1:198:A:CYS:O	4	11.43
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	12	11.43
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	3	11.42
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	17	11.41
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	7	11.41
(3,119)	1:81:A:THR:H	1:60:A:SER:O	20	11.41
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	6	11.41
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	8	11.4
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	7	11.4
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	1	11.39
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	3	11.38
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	17	11.38
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	19	11.37
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	8	11.36
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	8	11.36
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	19	11.36
(3,31)	1:126:A:SER:H	1:136:A:SER:O	4	11.36
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	20	11.33
(3,119)	1:81:A:THR:H	1:60:A:SER:O	3	11.32
(3,119)	1:81:A:THR:H	1:60:A:SER:O	12	11.3
(3,31)	1:126:A:SER:H	1:136:A:SER:O	6	11.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	9	11.29
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	8	11.28
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	20	11.28
(3,31)	1:126:A:SER:H	1:136:A:SER:O	14	11.28
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	12	11.28
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	16	11.26
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	3	11.26
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	10	11.26
(3,119)	1:81:A:THR:H	1:60:A:SER:O	5	11.25
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	7	11.24
(3,119)	1:81:A:THR:H	1:60:A:SER:O	6	11.24
(3,119)	1:81:A:THR:H	1:60:A:SER:O	8	11.23
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	19	11.23
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	4	11.22
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	18	11.21
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	7	11.19
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	9	11.19
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	16	11.18
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	19	11.18
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	13	11.17
(3,31)	1:126:A:SER:H	1:136:A:SER:O	7	11.16
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	3	11.15
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	16	11.15
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	10	11.14
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	9	11.12
(3,31)	1:126:A:SER:H	1:136:A:SER:O	17	11.12
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	2	11.12
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	11	11.12
(3,119)	1:81:A:THR:H	1:60:A:SER:O	1	11.11
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	15	11.11
(3,150)	1:153:A:THR:H	1:60:A:SER:O	2	11.1
(3,119)	1:81:A:THR:H	1:60:A:SER:O	13	11.1
(3,119)	1:81:A:THR:H	1:60:A:SER:O	4	11.09
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	5	11.09
(3,31)	1:126:A:SER:H	1:136:A:SER:O	9	11.08
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	10	11.06
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	5	11.05
(3,108)	1:204:A:ARG:H	1:198:A:CYS:O	2	11.05
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	5	11.04
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	2	11.03
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	8	11.01
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	17	11.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,31)	1:126:A:SER:H	1:136:A:SER:O	16	11.0
(3,23)	1:99:A:GLN:H	1:136:A:SER:O	1	11.0
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	12	10.99
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	14	10.99
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	11	10.99
(3,119)	1:81:A:THR:H	1:60:A:SER:O	2	10.98
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	4	10.97
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	1	10.97
(3,150)	1:153:A:THR:H	1:60:A:SER:O	6	10.96
(3,150)	1:153:A:THR:H	1:60:A:SER:O	10	10.96
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	17	10.94
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	13	10.94
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	10	10.94
(3,128)	1:96:A:THR:H	1:60:A:SER:O	18	10.93
(3,31)	1:126:A:SER:H	1:136:A:SER:O	5	10.93
(3,128)	1:96:A:THR:H	1:60:A:SER:O	3	10.91
(3,31)	1:126:A:SER:H	1:136:A:SER:O	10	10.91
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	7	10.91
(3,119)	1:81:A:THR:H	1:60:A:SER:O	17	10.9
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	12	10.89
(3,31)	1:126:A:SER:H	1:136:A:SER:O	3	10.89
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	11	10.89
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	5	10.88
(3,128)	1:96:A:THR:H	1:60:A:SER:O	10	10.87
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	6	10.87
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	8	10.86
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	15	10.85
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	12	10.85
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	11	10.85
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	2	10.84
(3,128)	1:96:A:THR:H	1:60:A:SER:O	20	10.83
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	11	10.82
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	16	10.82
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	19	10.82
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	14	10.81
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	16	10.81
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	4	10.8
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	11	10.8
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	9	10.79
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	11	10.79
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	1	10.78
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	5	10.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,128)	1:96:A:THR:H	1:60:A:SER:O	7	10.78
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	11	10.78
(3,31)	1:126:A:SER:H	1:136:A:SER:O	20	10.78
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	19	10.77
(3,128)	1:96:A:THR:H	1:60:A:SER:O	4	10.77
(3,175)	1:203:A:GLN:H	1:60:A:SER:O	9	10.76
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	4	10.76
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	19	10.76
(3,31)	1:126:A:SER:H	1:136:A:SER:O	18	10.76
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	16	10.76
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	7	10.75
(3,36)	1:148:A:LYS:H	1:136:A:SER:O	2	10.75
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	13	10.74
(3,150)	1:153:A:THR:H	1:60:A:SER:O	18	10.73
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	5	10.73
(3,128)	1:96:A:THR:H	1:60:A:SER:O	9	10.72
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	6	10.72
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	1	10.72
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	5	10.71
(3,150)	1:153:A:THR:H	1:60:A:SER:O	4	10.71
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	17	10.71
(3,31)	1:126:A:SER:H	1:136:A:SER:O	2	10.7
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	20	10.7
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	6	10.69
(3,128)	1:96:A:THR:H	1:60:A:SER:O	17	10.68
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	13	10.67
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	15	10.66
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	20	10.62
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	10	10.61
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	1	10.61
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	1	10.61
(3,128)	1:96:A:THR:H	1:60:A:SER:O	5	10.6
(3,31)	1:126:A:SER:H	1:136:A:SER:O	13	10.6
(3,31)	1:126:A:SER:H	1:136:A:SER:O	15	10.6
(3,128)	1:96:A:THR:H	1:60:A:SER:O	8	10.59
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	9	10.59
(3,119)	1:81:A:THR:H	1:60:A:SER:O	16	10.59
(3,119)	1:81:A:THR:H	1:60:A:SER:O	19	10.58
(3,31)	1:126:A:SER:H	1:136:A:SER:O	12	10.58
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	6	10.56
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	14	10.56
(3,150)	1:153:A:THR:H	1:60:A:SER:O	20	10.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	11	10.56
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	18	10.56
(3,31)	1:126:A:SER:H	1:136:A:SER:O	8	10.56
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	2	10.55
(3,150)	1:153:A:THR:H	1:60:A:SER:O	8	10.54
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	20	10.54
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	12	10.54
(3,128)	1:96:A:THR:H	1:60:A:SER:O	16	10.53
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	10	10.53
(3,152)	1:156:A:PHE:H	1:60:A:SER:O	1	10.52
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	6	10.52
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	1	10.51
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	3	10.51
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	18	10.5
(3,31)	1:126:A:SER:H	1:136:A:SER:O	19	10.49
(3,130)	1:99:A:GLN:H	1:60:A:SER:O	2	10.48
(3,119)	1:81:A:THR:H	1:60:A:SER:O	9	10.48
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	17	10.48
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	14	10.48
(3,128)	1:96:A:THR:H	1:60:A:SER:O	6	10.46
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	15	10.46
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	1	10.46
(3,128)	1:96:A:THR:H	1:60:A:SER:O	19	10.45
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	8	10.45
(3,150)	1:153:A:THR:H	1:60:A:SER:O	15	10.44
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	15	10.44
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	17	10.44
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	7	10.43
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	4	10.43
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	8	10.43
(3,150)	1:153:A:THR:H	1:60:A:SER:O	3	10.41
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	13	10.4
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	7	10.4
(3,128)	1:96:A:THR:H	1:60:A:SER:O	13	10.39
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	20	10.36
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	7	10.36
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	19	10.36
(3,150)	1:153:A:THR:H	1:60:A:SER:O	17	10.33
(3,119)	1:81:A:THR:H	1:60:A:SER:O	18	10.33
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	6	10.33
(3,128)	1:96:A:THR:H	1:60:A:SER:O	2	10.32
(3,124)	1:90:A:LEU:H	1:60:A:SER:O	19	10.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	13	10.31
(3,150)	1:153:A:THR:H	1:60:A:SER:O	7	10.3
(3,150)	1:153:A:THR:H	1:60:A:SER:O	13	10.3
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	4	10.29
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	16	10.29
(3,150)	1:153:A:THR:H	1:60:A:SER:O	1	10.27
(3,119)	1:81:A:THR:H	1:60:A:SER:O	10	10.27
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	15	10.27
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	9	10.27
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	9	10.25
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	15	10.23
(3,150)	1:153:A:THR:H	1:60:A:SER:O	5	10.23
(3,150)	1:153:A:THR:H	1:60:A:SER:O	11	10.22
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	10	10.22
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	6	10.19
(3,150)	1:153:A:THR:H	1:60:A:SER:O	12	10.18
(3,128)	1:96:A:THR:H	1:60:A:SER:O	1	10.18
(3,128)	1:96:A:THR:H	1:60:A:SER:O	12	10.17
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	4	10.16
(3,19)	1:92:A:TYR:H	1:136:A:SER:O	2	10.16
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	16	10.15
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	20	10.14
(3,128)	1:96:A:THR:H	1:60:A:SER:O	11	10.13
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	5	10.13
(3,150)	1:153:A:THR:H	1:60:A:SER:O	14	10.09
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	10	10.09
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	7	10.08
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	5	10.08
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	6	10.08
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	11	10.07
(3,128)	1:96:A:THR:H	1:60:A:SER:O	15	10.05
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	9	10.03
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	14	10.02
(3,128)	1:96:A:THR:H	1:60:A:SER:O	14	10.01
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	15	9.98
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	18	9.98
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	14	9.98
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	15	9.97
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	20	9.97
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	12	9.96
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	17	9.96
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	5	9.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	14	9.93
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	15	9.91
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	17	9.9
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	12	9.88
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	20	9.88
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	1	9.87
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	3	9.87
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	7	9.85
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	8	9.82
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	10	9.8
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	12	9.76
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	19	9.75
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	3	9.67
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	3	9.66
(3,22)	1:96:A:THR:H	1:136:A:SER:O	7	9.6
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	19	9.59
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	18	9.57
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	14	9.56
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	20	9.56
(3,22)	1:96:A:THR:H	1:136:A:SER:O	14	9.54
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	18	9.53
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	8	9.53
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	13	9.51
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	13	9.51
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	13	9.5
(3,22)	1:96:A:THR:H	1:136:A:SER:O	10	9.5
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	2	9.49
(3,22)	1:96:A:THR:H	1:136:A:SER:O	9	9.48
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	8	9.46
(3,22)	1:96:A:THR:H	1:136:A:SER:O	11	9.45
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	17	9.44
(3,22)	1:96:A:THR:H	1:136:A:SER:O	20	9.44
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	18	9.43
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	15	9.43
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	11	9.41
(3,22)	1:96:A:THR:H	1:136:A:SER:O	13	9.4
(3,22)	1:96:A:THR:H	1:136:A:SER:O	12	9.38
(3,27)	1:109:A:ARG:H	1:136:A:SER:O	2	9.37
(3,22)	1:96:A:THR:H	1:136:A:SER:O	3	9.35
(3,22)	1:96:A:THR:H	1:136:A:SER:O	5	9.35
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	17	9.34
(3,22)	1:96:A:THR:H	1:136:A:SER:O	16	9.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,22)	1:96:A:THR:H	1:136:A:SER:O	17	9.34
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	2	9.33
(3,22)	1:96:A:THR:H	1:136:A:SER:O	18	9.33
(3,26)	1:107:A:ARG:H	1:136:A:SER:O	2	9.32
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	10	9.3
(3,22)	1:96:A:THR:H	1:136:A:SER:O	6	9.29
(3,22)	1:96:A:THR:H	1:136:A:SER:O	1	9.28
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	9	9.27
(3,70)	1:119:A:ARG:H	1:198:A:CYS:O	4	9.24
(3,22)	1:96:A:THR:H	1:136:A:SER:O	8	9.22
(3,22)	1:96:A:THR:H	1:136:A:SER:O	4	9.2
(3,22)	1:96:A:THR:H	1:136:A:SER:O	15	9.2
(3,22)	1:96:A:THR:H	1:136:A:SER:O	19	9.2
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	14	9.04
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	13	9.03
(3,154)	1:164:A:GLU:H	1:60:A:SER:O	13	9.02
(3,22)	1:96:A:THR:H	1:136:A:SER:O	2	9.01
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	5	8.99
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	14	8.96
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	6	8.89
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	7	8.87
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	1	8.86
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	9	8.85
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	3	8.85
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	19	8.81
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	16	8.79
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	20	8.7
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	6	8.67
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	11	8.67
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	3	8.62
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	18	8.62
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	17	8.6
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	8	8.59
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	12	8.57
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	5	8.55
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	11	8.55
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	4	8.54
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	16	8.53
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	9	8.5
(3,90)	1:160:A:TRP:H	1:198:A:CYS:O	9	8.5
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	3	8.48
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	12	8.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	2	8.48
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	6	8.47
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	18	8.47
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	8	8.46
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	12	8.45
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	7	8.44
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	19	8.44
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	17	8.43
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	19	8.42
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	16	8.42
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	1	8.42
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	9	8.38
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	2	8.36
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	4	8.35
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	13	8.34
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	1	8.32
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	20	8.32
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	15	8.32
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	8	8.31
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	16	8.3
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	18	8.29
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	13	8.29
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	19	8.27
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	13	8.23
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	8	8.21
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	18	8.19
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	17	8.17
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	18	8.16
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	16	8.15
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	5	8.13
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	12	8.08
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	3	8.06
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	15	8.05
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	10	8.04
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	2	8.03
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	15	8.03
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	3	8.02
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	14	8.01
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	4	8.0
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	19	7.95
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	10	7.94
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	7	7.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	13	7.93
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	2	7.91
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	9	7.91
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	3	7.9
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	12	7.9
(3,123)	1:87:A:TRP:H	1:60:A:SER:O	19	7.88
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	11	7.86
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	12	7.86
(3,83)	1:152:A:GLU:H	1:198:A:CYS:O	10	7.85
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	5	7.83
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	17	7.82
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	8	7.81
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	18	7.81
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	17	7.78
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	20	7.78
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	4	7.76
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	8	7.76
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	14	7.75
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	10	7.73
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	6	7.73
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	14	7.73
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	18	7.72
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	5	7.71
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	15	7.7
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	9	7.7
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	16	7.7
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	4	7.69
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	18	7.68
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	3	7.68
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	12	7.64
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	7	7.58
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	15	7.57
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	1	7.57
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	11	7.57
(3,13)	1:85:A:GLU:H	1:136:A:SER:O	10	7.54
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	1	7.52
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	14	7.51
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	4	7.48
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	5	7.46
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	10	7.43
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	19	7.43
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	20	7.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,91)	1:162:A:LEU:H	1:198:A:CYS:O	4	7.37
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	16	7.36
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	20	7.35
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	11	7.32
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	6	7.32
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	16	7.31
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	3	7.29
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	6	7.29
(3,143)	1:142:A:ALA:H	1:60:A:SER:O	14	7.27
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	8	7.27
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	1	7.27
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	9	7.24
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	2	7.23
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	6	7.22
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	19	7.22
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	17	7.21
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	2	7.21
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	11	7.21
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	7	7.19
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	13	7.18
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	7	7.17
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	20	7.17
(3,14)	1:86:A:GLU:H	1:136:A:SER:O	10	7.17
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	13	7.14
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	18	7.1
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	8	7.09
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	17	7.08
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	7	7.08
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	2	7.07
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	9	7.01
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	17	7.0
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	15	6.95
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	4	6.94
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	8	6.94
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	3	6.92
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	1	6.89
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	5	6.88
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	6	6.88
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	14	6.84
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	12	6.82
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	12	6.8
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	2	6.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	10	6.77
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	7	6.75
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	4	6.74
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	19	6.73
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	15	6.71
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	11	6.69
(3,87)	1:156:A:PHE:H	1:198:A:CYS:O	4	6.69
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	14	6.69
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	5	6.69
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	11	6.67
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	2	6.63
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	20	6.63
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	16	6.61
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	9	6.6
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	5	6.58
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	18	6.56
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	3	6.55
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	9	6.54
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	12	6.54
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	6	6.53
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	6	6.51
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	8	6.51
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	1	6.51
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	16	6.51
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	10	6.49
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	19	6.49
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	15	6.47
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	16	6.47
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	9	6.45
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	15	6.45
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	4	6.43
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	16	6.43
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	17	6.42
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	20	6.42
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	7	6.42
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	20	6.41
(3,74)	1:124:A:LEU:H	1:198:A:CYS:O	10	6.4
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	11	6.4
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	18	6.4
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	11	6.4
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	13	6.39
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	3	6.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	17	6.38
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	9	6.38
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	7	6.37
(3,15)	1:87:A:TRP:H	1:136:A:SER:O	10	6.33
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	13	6.32
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	13	6.32
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	5	6.28
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	14	6.26
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	20	6.23
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	16	6.22
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	19	6.2
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	8	6.2
(3,74)	1:124:A:LEU:H	1:198:A:CYS:O	14	6.18
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	8	6.17
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	1	6.16
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	6	6.14
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	5	6.13
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	11	6.11
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	13	6.08
(3,74)	1:124:A:LEU:H	1:198:A:CYS:O	3	6.02
(3,32)	1:130:A:LEU:H	1:136:A:SER:O	4	6.0
(3,153)	1:160:A:TRP:H	1:60:A:SER:O	1	5.99
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	8	5.98
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	8	5.94
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	1	5.87
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	2	5.86
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	12	5.86
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	18	5.81
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	12	5.79
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	16	5.79
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	1	5.78
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	11	5.7
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	15	5.66
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	7	5.63
(3,129)	1:97:A:LEU:H	1:60:A:SER:O	14	5.62
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	18	5.62
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	16	5.54
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	4	5.52
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	9	5.52
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	12	5.41
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	5	5.37
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	9	5.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	6	5.34
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	10	5.34
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	17	5.27
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	12	5.26
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	16	5.25
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	20	5.24
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	14	5.23
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	17	5.23
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	17	5.22
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	20	5.22
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	3	5.21
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	15	5.18
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	7	5.14
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	5	5.14
(3,71)	1:120:A:GLU:H	1:198:A:CYS:O	4	5.13
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	18	5.08
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	4	5.05
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	19	4.99
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	7	4.97
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	5	4.95
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	6	4.94
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	10	4.94
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	19	4.93
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	9	4.93
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	3	4.93
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	8	4.92
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	18	4.91
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	19	4.88
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	9	4.87
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	13	4.87
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	16	4.84
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	18	4.84
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	4	4.82
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	6	4.82
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	14	4.8
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	13	4.8
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	1	4.77
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	8	4.75
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	11	4.74
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	13	4.72
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	12	4.69
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	1	4.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	2	4.64
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	11	4.6
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	2	4.59
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	16	4.58
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	8	4.58
(3,25)	1:106:A:ASN:H	1:136:A:SER:O	2	4.58
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	9	4.57
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	8	4.51
(3,127)	1:95:A:TYR:H	1:60:A:SER:O	15	4.49
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	9	4.44
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	19	4.41
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	7	4.41
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	20	4.41
(3,89)	1:159:A:SER:H	1:198:A:CYS:O	16	4.39
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	2	4.28
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	15	4.23
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	15	4.09
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	15	4.08
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	20	4.03
(3,72)	1:122:A:ASP:H	1:198:A:CYS:O	4	4.02
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	20	3.99
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	10	3.99
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	17	3.92
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	6	3.9
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	13	3.88
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	2	3.86
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	7	3.83
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	10	3.81
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	9	3.78
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	11	3.78
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	16	3.76
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	18	3.75
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	1	3.74
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	13	3.72
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	18	3.67
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	5	3.67
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	4	3.65
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	1	3.65
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	6	3.63
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	20	3.63
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	6	3.62
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	5	3.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	19	3.57
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	9	3.57
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	8	3.55
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	15	3.53
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	9	3.52
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	7	3.51
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	12	3.51
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	7	3.48
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	11	3.45
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	14	3.45
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	20	3.41
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	15	3.41
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	3	3.4
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	20	3.37
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	8	3.36
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	18	3.36
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	1	3.34
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	5	3.33
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	7	3.33
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	9	3.33
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	10	3.32
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	17	3.32
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	11	3.31
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	13	3.31
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	3	3.3
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	4	3.29
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	17	3.28
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	3	3.27
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG13	6	3.27
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	12	3.23
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	13	3.22
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	17	3.21
(3,104)	1:189:A:MET:H	1:198:A:CYS:O	8	3.2
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	15	3.2
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	13	3.2
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	18	3.19
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	19	3.19
(3,18)	1:91:A:ASN:H	1:136:A:SER:O	2	3.18
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	3	3.18
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	10	3.17
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	18	3.17
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	19	3.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,104)	1:189:A:MET:H	1:198:A:CYS:O	9	3.16
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	12	3.12
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	18	3.12
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	8	3.11
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	14	3.11
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	16	3.1
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG13	1	3.05
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	19	3.04
(3,149)	1:152:A:GLU:H	1:60:A:SER:O	14	3.03
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	11	3.02
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	5	3.01
(3,104)	1:189:A:MET:H	1:198:A:CYS:O	16	3.0
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	10	3.0
(1,753)	1:59:A:VAL:HG11	1:69:A:ILE:HG12	5	3.0
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	9	2.99
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	12	2.99
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	14	2.98
(1,753)	1:59:A:VAL:HG12	1:69:A:ILE:HG13	11	2.95
(1,753)	1:59:A:VAL:HG12	1:69:A:ILE:HG13	15	2.95
(1,753)	1:59:A:VAL:HG11	1:69:A:ILE:HG13	14	2.92
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	16	2.9
(1,753)	1:59:A:VAL:HG11	1:69:A:ILE:HG13	1	2.9
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	16	2.89
(1,900)	1:111:A:ILE:HG22	1:186:A:ALA:HB2	18	2.88
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	4	2.88
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	8	2.87
(1,897)	1:111:A:ILE:HG12	1:185:A:ILE:HG12	2	2.86
(1,753)	1:59:A:VAL:HG12	1:69:A:ILE:HG12	8	2.86
(1,753)	1:59:A:VAL:HG21	1:69:A:ILE:HG12	7	2.85
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB2	11	2.84
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	16	2.83
(1,753)	1:59:A:VAL:HG21	1:69:A:ILE:HG12	20	2.83
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	13	2.82
(1,753)	1:59:A:VAL:HG22	1:69:A:ILE:HG12	3	2.82
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	20	2.81
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB1	13	2.8
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	15	2.78
(1,900)	1:111:A:ILE:HG23	1:186:A:ALA:HB1	3	2.76
(1,900)	1:111:A:ILE:HG13	1:186:A:ALA:HB3	15	2.76
(1,898)	1:111:A:ILE:HG21	1:185:A:ILE:HD12	17	2.76
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB1	12	2.75
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD11	13	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB3	10	2.72
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB2	8	2.71
(1,900)	1:111:A:ILE:HG22	1:186:A:ALA:HB3	17	2.71
(1,898)	1:111:A:ILE:HG21	1:185:A:ILE:HD11	6	2.7
(1,753)	1:59:A:VAL:HG12	1:69:A:ILE:HG12	2	2.7
(1,900)	1:111:A:ILE:HG13	1:186:A:ALA:HB1	4	2.69
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB2	14	2.69
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB2	19	2.69
(1,898)	1:111:A:ILE:HG23	1:185:A:ILE:HD11	20	2.69
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB2	16	2.67
(1,897)	1:111:A:ILE:HG13	1:185:A:ILE:HG12	7	2.67
(1,898)	1:111:A:ILE:HG23	1:185:A:ILE:HD11	9	2.66
(1,753)	1:59:A:VAL:HG11	1:69:A:ILE:HG12	13	2.66
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	9	2.64
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB3	6	2.64
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	10	2.63
(1,900)	1:111:A:ILE:HG21	1:186:A:ALA:HB3	9	2.62
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD13	18	2.62
(1,753)	1:59:A:VAL:HG12	1:69:A:ILE:HG12	12	2.62
(1,900)	1:111:A:ILE:HG21	1:186:A:ALA:HB1	20	2.58
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	13	2.57
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	8	2.55
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB1	5	2.54
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	3	2.52
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD13	16	2.51
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	14	2.5
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD12	11	2.5
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB1	1	2.48
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD11	12	2.48
(1,900)	1:111:A:ILE:HG13	1:186:A:ALA:HB2	7	2.45
(1,900)	1:111:A:ILE:HG12	1:186:A:ALA:HB3	2	2.43
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	18	2.42
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	12	2.4
(1,753)	1:59:A:VAL:HG21	1:69:A:ILE:HG13	16	2.4
(1,753)	1:59:A:VAL:HG11	1:69:A:ILE:HG13	4	2.37
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD13	1	2.36
(1,753)	1:59:A:VAL:HG13	1:69:A:ILE:HG13	17	2.36
(1,1096)	1:170:A:VAL:HG12	1:185:A:ILE:HG13	2	2.33
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD11	5	2.32
(1,753)	1:59:A:VAL:HG21	1:69:A:ILE:HG12	10	2.32
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	2	2.3
(1,753)	1:59:A:VAL:HG11	1:69:A:ILE:HG12	6	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	17	2.27
(3,104)	1:189:A:MET:H	1:198:A:CYS:O	4	2.27
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	4	2.26
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD12	14	2.26
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD11	19	2.25
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD12	10	2.23
(1,1096)	1:170:A:VAL:HG13	1:185:A:ILE:HG13	9	2.22
(1,1096)	1:170:A:VAL:HG12	1:185:A:ILE:HG13	13	2.21
(1,1096)	1:170:A:VAL:HG11	1:185:A:ILE:HG13	17	2.21
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD12	4	2.21
(1,1096)	1:170:A:VAL:HG12	1:185:A:ILE:HG13	12	2.18
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD13	8	2.17
(1,1096)	1:170:A:VAL:HG13	1:185:A:ILE:HG13	6	2.16
(1,1096)	1:170:A:VAL:HG11	1:185:A:ILE:HG13	20	2.16
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	15	2.15
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD11	3	2.15
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD11	15	2.14
(3,80)	1:145:A:MET:H	1:198:A:CYS:O	4	2.13
(1,898)	1:111:A:ILE:HG12	1:185:A:ILE:HD12	2	2.12
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	2	2.1
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG12	17	2.07
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	16	2.04
(1,1096)	1:170:A:VAL:HG11	1:185:A:ILE:HG13	18	2.04
(1,1096)	1:170:A:VAL:HG11	1:185:A:ILE:HG13	10	2.03
(1,1096)	1:170:A:VAL:HG13	1:185:A:ILE:HG13	4	2.02
(1,1096)	1:170:A:VAL:HG11	1:185:A:ILE:HG13	11	2.02
(1,1096)	1:170:A:VAL:HG11	1:185:A:ILE:HG13	19	2.02
(1,1096)	1:170:A:VAL:HG12	1:185:A:ILE:HG13	8	2.01
(1,753)	1:59:A:VAL:HG23	1:69:A:ILE:HG13	18	2.01
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	3	2.0
(1,1096)	1:170:A:VAL:HG11	1:185:A:ILE:HG13	16	2.0
(1,898)	1:111:A:ILE:HG13	1:185:A:ILE:HD11	7	2.0
(1,896)	1:111:A:ILE:HD11	1:185:A:ILE:HG13	13	2.0
(1,1096)	1:170:A:VAL:HG23	1:185:A:ILE:HG13	5	1.98
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	1	1.97
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	13	1.97
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	20	1.97
(1,1096)	1:170:A:VAL:HG13	1:185:A:ILE:HG13	14	1.96
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG12	20	1.96
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	5	1.94
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	17	1.94
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	8	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	20	1.93
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG12	9	1.93
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	18	1.93
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	19	1.9
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	6	1.89
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	12	1.89
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	15	1.88
(1,1096)	1:170:A:VAL:HG12	1:185:A:ILE:HG13	1	1.88
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG13	16	1.87
(1,896)	1:111:A:ILE:HD11	1:185:A:ILE:HG13	6	1.86
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	14	1.84
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	11	1.84
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	12	1.81
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	2	1.8
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	6	1.79
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	7	1.78
(1,753)	1:59:A:VAL:HG22	1:69:A:ILE:HG13	9	1.78
(1,753)	1:59:A:VAL:HG23	1:69:A:ILE:HG13	19	1.78
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	5	1.76
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	5	1.75
(3,117)	1:78:A:ASN:H	1:60:A:SER:O	11	1.74
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG13	10	1.74
(1,822)	1:76:A:ILE:HG21	1:90:A:LEU:HD23	18	1.72
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	1	1.71
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	11	1.71
(1,896)	1:111:A:ILE:HD11	1:185:A:ILE:HG13	4	1.7
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	14	1.69
(1,822)	1:76:A:ILE:HG22	1:90:A:LEU:HD21	10	1.69
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	8	1.68
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	1	1.67
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG13	5	1.65
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG13	15	1.64
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	7	1.63
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG13	19	1.63
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	17	1.62
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	8	1.61
(1,896)	1:111:A:ILE:HD12	1:185:A:ILE:HG12	3	1.6
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG22	14	1.58
(3,146)	1:145:A:MET:H	1:60:A:SER:O	16	1.55
(3,84)	1:153:A:THR:H	1:198:A:CYS:O	7	1.54
(1,822)	1:76:A:ILE:HG12	1:90:A:LEU:HD11	13	1.54
(1,1096)	1:170:A:VAL:HG23	1:185:A:ILE:HG13	7	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:76:A:ILE:HG13	1:90:A:LEU:HD11	19	1.53
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	7	1.5
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	20	1.5
(1,1045)	1:155:A:ILE:HG23	1:183:A:PHE:HD1	11	1.48
(1,896)	1:111:A:ILE:HD13	1:185:A:ILE:HG13	2	1.48
(1,1096)	1:170:A:VAL:HG21	1:185:A:ILE:HG13	15	1.47
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	19	1.46
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	17	1.45
(1,822)	1:76:A:ILE:HG12	1:90:A:LEU:HD13	2	1.45
(3,81)	1:148:A:LYS:H	1:198:A:CYS:O	3	1.44
(1,1096)	1:170:A:VAL:HG13	1:185:A:ILE:HG13	3	1.43
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG21	11	1.42
(1,1045)	1:155:A:ILE:HG21	1:183:A:PHE:HD1	1	1.39
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	16	1.39
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG21	14	1.39
(3,102)	1:187:A:SER:H	1:198:A:CYS:O	4	1.38
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	2	1.38
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	12	1.38
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	12	1.37
(3,146)	1:145:A:MET:H	1:60:A:SER:O	6	1.36
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	6	1.36
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	17	1.36
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	4	1.35
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	7	1.34
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG22	5	1.34
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG21	8	1.34
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	16	1.33
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	2	1.32
(3,146)	1:145:A:MET:H	1:60:A:SER:O	19	1.31
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	19	1.31
(3,81)	1:148:A:LYS:H	1:198:A:CYS:O	10	1.31
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	14	1.31
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	20	1.31
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG22	19	1.31
(3,104)	1:189:A:MET:H	1:198:A:CYS:O	18	1.3
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD2	6	1.3
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	3	1.3
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	18	1.29
(1,1045)	1:155:A:ILE:HG22	1:183:A:PHE:HD1	5	1.29
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	13	1.29
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	19	1.29
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG21	18	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	6	1.28
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	11	1.28
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	20	1.28
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	3	1.28
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	5	1.27
(1,822)	1:76:A:ILE:HG12	1:90:A:LEU:HD12	1	1.26
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	19	1.26
(3,81)	1:148:A:LYS:H	1:198:A:CYS:O	14	1.25
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG23	17	1.25
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	6	1.24
(1,1045)	1:155:A:ILE:HG22	1:183:A:PHE:HD2	9	1.24
(1,1045)	1:155:A:ILE:HG21	1:183:A:PHE:HD2	17	1.24
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG22	11	1.24
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	14	1.24
(3,146)	1:145:A:MET:H	1:60:A:SER:O	9	1.23
(1,791)	1:71:A:TYR:HE1	1:94:A:ILE:HG23	2	1.23
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG23	4	1.23
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD2	20	1.22
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	5	1.22
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	19	1.22
(1,1050)	1:155:A:ILE:HG23	1:167:A:LEU:HG	20	1.21
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	1	1.2
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	1	1.2
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	10	1.2
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	2	1.2
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	8	1.2
(3,146)	1:145:A:MET:H	1:60:A:SER:O	4	1.19
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	11	1.19
(1,1050)	1:155:A:ILE:HG22	1:167:A:LEU:HG	17	1.19
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	15	1.18
(1,814)	1:76:A:ILE:HG13	1:87:A:TRP:HE1	9	1.18
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG21	1	1.18
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG23	15	1.18
(1,822)	1:76:A:ILE:HG13	1:90:A:LEU:HD12	15	1.13
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	4	1.13
(1,687)	1:111:A:ILE:HG13	1:183:A:PHE:H	10	1.13
(1,737)	1:155:A:ILE:HG23	1:183:A:PHE:H	14	1.12
(1,687)	1:111:A:ILE:HG13	1:183:A:PHE:H	1	1.12
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	2	1.12
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	5	1.12
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	20	1.12
(1,1050)	1:155:A:ILE:HG23	1:167:A:LEU:HG	9	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:70:A:LEU:HD11	1:94:A:ILE:HG13	16	1.11
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG23	7	1.1
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	10	1.1
(3,88)	1:158:A:ALA:H	1:198:A:CYS:O	12	1.09
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG21	20	1.09
(1,814)	1:76:A:ILE:HG13	1:87:A:TRP:HE1	13	1.08
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	9	1.08
(3,146)	1:145:A:MET:H	1:60:A:SER:O	17	1.07
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	13	1.07
(1,747)	1:57:A:HIS:HB3	1:69:A:ILE:HG21	1	1.07
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	18	1.07
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	17	1.07
(3,146)	1:145:A:MET:H	1:60:A:SER:O	1	1.06
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG22	9	1.06
(1,737)	1:155:A:ILE:HG23	1:183:A:PHE:H	15	1.06
(3,146)	1:145:A:MET:H	1:60:A:SER:O	2	1.05
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG23	14	1.05
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	7	1.05
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG13	2	1.04
(1,823)	1:76:A:ILE:HG23	1:86:A:GLU:HB2	14	1.04
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG23	3	1.04
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	7	1.04
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	11	1.04
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	14	1.04
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG13	7	1.03
(1,1050)	1:155:A:ILE:HG23	1:167:A:LEU:HG	7	1.03
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	8	1.03
(1,814)	1:76:A:ILE:HG13	1:87:A:TRP:HE1	7	1.03
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	11	1.03
(3,146)	1:145:A:MET:H	1:60:A:SER:O	13	1.02
(1,747)	1:57:A:HIS:HB3	1:69:A:ILE:HG12	20	1.02
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	9	1.02
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG22	1	1.01
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	8	1.01
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	15	1.01
(1,814)	1:76:A:ILE:HG13	1:87:A:TRP:HE1	11	1.01
(1,747)	1:57:A:HIS:HB3	1:69:A:ILE:HG21	15	1.01
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	6	1.01
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	6	1.01
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	14	1.0
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG21	6	1.0
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG22	12	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG23	15	0.99
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG13	16	0.99
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	2	0.99
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	14	0.99
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	9	0.99
(1,848)	1:100:A:ILE:HG13	1:143:A:ARG:HB2	18	0.99
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	11	0.99
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG13	3	0.98
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	6	0.98
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	6	0.98
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	16	0.98
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG22	5	0.97
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG22	18	0.97
(1,1050)	1:155:A:ILE:HG22	1:167:A:LEU:HG	15	0.97
(1,901)	1:111:A:ILE:HG22	1:155:A:ILE:HD13	18	0.97
(1,814)	1:76:A:ILE:HG13	1:87:A:TRP:HE1	6	0.97
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	3	0.97
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	4	0.96
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	10	0.96
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	7	0.96
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	9	0.96
(3,146)	1:145:A:MET:H	1:60:A:SER:O	20	0.95
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	10	0.95
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	20	0.95
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG23	9	0.94
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG23	11	0.94
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	3	0.94
(1,848)	1:100:A:ILE:HG12	1:143:A:ARG:HB2	1	0.94
(1,821)	1:76:A:ILE:HG13	1:87:A:TRP:HB3	14	0.94
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	14	0.94
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	16	0.94
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	1	0.94
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	16	0.94
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	5	0.94
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG21	19	0.93
(1,1050)	1:155:A:ILE:HG21	1:167:A:LEU:HG	4	0.93
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	15	0.93
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	17	0.93
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	18	0.93
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG21	8	0.92
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG13	17	0.92
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	12	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	4	0.92
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	5	0.92
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	5	0.92
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	3	0.92
(1,607)	1:155:A:ILE:HG21	1:160:A:TRP:HE3	11	0.92
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	19	0.92
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	11	0.91
(1,1050)	1:155:A:ILE:HG23	1:167:A:LEU:HG	10	0.91
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	20	0.91
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	19	0.91
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	5	0.91
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	8	0.91
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	9	0.91
(1,607)	1:155:A:ILE:HG21	1:160:A:TRP:HE3	12	0.91
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	13	0.91
(3,146)	1:145:A:MET:H	1:60:A:SER:O	5	0.9
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG21	4	0.9
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG23	6	0.9
(1,1050)	1:155:A:ILE:HG21	1:167:A:LEU:HG	8	0.9
(1,901)	1:111:A:ILE:HG12	1:155:A:ILE:HD12	4	0.9
(1,813)	1:76:A:ILE:HG13	1:87:A:TRP:HE3	15	0.9
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	3	0.9
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	8	0.9
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	12	0.9
(1,737)	1:155:A:ILE:HG22	1:183:A:PHE:H	9	0.9
(1,737)	1:155:A:ILE:HG23	1:183:A:PHE:H	12	0.9
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	20	0.9
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	1	0.9
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	19	0.9
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	8	0.9
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	12	0.9
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	1	0.9
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	7	0.89
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG22	10	0.89
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG23	13	0.89
(1,901)	1:111:A:ILE:HG12	1:155:A:ILE:HD11	10	0.89
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	2	0.89
(1,737)	1:155:A:ILE:HG21	1:183:A:PHE:H	13	0.89
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	18	0.89
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	16	0.89
(3,146)	1:145:A:MET:H	1:60:A:SER:O	15	0.88
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	11	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,901)	1:111:A:ILE:HG12	1:155:A:ILE:HD11	8	0.88
(1,813)	1:76:A:ILE:HG13	1:87:A:TRP:HE3	19	0.88
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	17	0.88
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	4	0.88
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	13	0.88
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	16	0.88
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	17	0.88
(3,103)	1:188:A:GLN:H	1:198:A:CYS:O	13	0.87
(1,1052)	1:156:A:PHE:HB3	1:185:A:ILE:HG22	20	0.87
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	18	0.87
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	1	0.87
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	10	0.87
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	16	0.87
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	2	0.87
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	7	0.87
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	5	0.87
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	18	0.86
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG23	3	0.86
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	3	0.86
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	4	0.86
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	6	0.86
(1,607)	1:155:A:ILE:HG21	1:160:A:TRP:HE3	14	0.86
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	17	0.86
(1,1050)	1:155:A:ILE:HG23	1:167:A:LEU:HG	13	0.85
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	5	0.85
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	10	0.85
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	18	0.85
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	7	0.84
(1,1044)	1:155:A:ILE:HG22	1:182:A:PHE:HD2	7	0.84
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	13	0.84
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	8	0.84
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	2	0.84
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	4	0.84
(3,146)	1:145:A:MET:H	1:60:A:SER:O	8	0.83
(1,901)	1:111:A:ILE:HG23	1:155:A:ILE:HD12	13	0.83
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	8	0.83
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	4	0.83
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	8	0.83
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	17	0.83
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG13	13	0.83
(1,737)	1:155:A:ILE:HG23	1:183:A:PHE:H	11	0.83
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	19	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	20	0.83
(3,146)	1:145:A:MET:H	1:60:A:SER:O	7	0.82
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	9	0.82
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	3	0.82
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	10	0.82
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	19	0.82
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	4	0.82
(1,687)	1:111:A:ILE:HG13	1:183:A:PHE:H	8	0.82
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	11	0.82
(1,607)	1:155:A:ILE:HG22	1:160:A:TRP:HE3	10	0.82
(1,607)	1:155:A:ILE:HG21	1:160:A:TRP:HE3	15	0.82
(3,146)	1:145:A:MET:H	1:60:A:SER:O	3	0.81
(3,146)	1:145:A:MET:H	1:60:A:SER:O	18	0.81
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	12	0.81
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD11	17	0.81
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	17	0.81
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	18	0.81
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	19	0.81
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	20	0.8
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	7	0.8
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	15	0.8
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	13	0.8
(1,607)	1:155:A:ILE:HG23	1:160:A:TRP:HE3	7	0.8
(3,146)	1:145:A:MET:H	1:60:A:SER:O	11	0.79
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	1	0.79
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	1	0.79
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	15	0.79
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	10	0.79
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	18	0.79
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	18	0.79
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	18	0.79
(1,756)	1:61:A:HIS:HB3	1:69:A:ILE:HG13	4	0.78
(1,736)	1:155:A:ILE:HG23	1:182:A:PHE:H	14	0.78
(1,736)	1:155:A:ILE:HG23	1:182:A:PHE:H	15	0.78
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	4	0.77
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	3	0.77
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	1	0.77
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	3	0.76
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	3	0.76
(1,687)	1:111:A:ILE:HG13	1:183:A:PHE:H	4	0.76
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	16	0.75
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG23	8	0.75
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	16	0.75
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	8	0.75
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	10	0.75
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	16	0.75
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	15	0.75
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	20	0.74
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	7	0.74
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	12	0.74
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	8	0.74
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD12	20	0.73
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	16	0.73
(1,791)	1:71:A:TYR:HE1	1:94:A:ILE:HG22	13	0.73
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG22	5	0.73
(1,768)	1:67:A:ASP:HB3	1:94:A:ILE:HG23	12	0.73
(1,687)	1:111:A:ILE:HG13	1:183:A:PHE:H	15	0.73
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	12	0.72
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	10	0.72
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	14	0.72
(1,687)	1:111:A:ILE:HG12	1:183:A:PHE:H	12	0.72
(1,652)	1:74:A:ILE:HG12	1:88:A:GLN:H	2	0.72
(1,903)	1:111:A:ILE:HG12	1:155:A:ILE:HG13	4	0.71
(1,901)	1:111:A:ILE:HG23	1:155:A:ILE:HD12	9	0.71
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	19	0.71
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	17	0.71
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	6	0.71
(1,901)	1:111:A:ILE:HG12	1:155:A:ILE:HD13	15	0.7
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	4	0.7
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	5	0.7
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	20	0.7
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	20	0.7
(1,903)	1:111:A:ILE:HG12	1:155:A:ILE:HG13	15	0.69
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	6	0.69
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	8	0.69
(1,687)	1:111:A:ILE:HG13	1:183:A:PHE:H	7	0.69
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	12	0.68
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	15	0.68
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	6	0.68
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	3	0.68
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	1	0.68
(1,736)	1:155:A:ILE:HG23	1:182:A:PHE:H	12	0.68
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	12	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD11	16	0.67
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	13	0.67
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	13	0.66
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	18	0.66
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	5	0.66
(1,686)	1:111:A:ILE:HG12	1:182:A:PHE:H	3	0.66
(1,814)	1:76:A:ILE:HG12	1:87:A:TRP:HE1	2	0.65
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	13	0.65
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	6	0.64
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	11	0.64
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	4	0.64
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	10	0.64
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	17	0.63
(1,810)	1:74:A:ILE:HG12	1:91:A:ASN:HB2	2	0.63
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	2	0.63
(3,146)	1:145:A:MET:H	1:60:A:SER:O	10	0.62
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	18	0.62
(1,731)	1:155:A:ILE:HG23	1:185:A:ILE:H	14	0.62
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	20	0.62
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	5	0.61
(1,902)	1:111:A:ILE:HD13	1:155:A:ILE:HG13	17	0.61
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	6	0.61
(1,736)	1:155:A:ILE:HG23	1:182:A:PHE:H	11	0.61
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	20	0.61
(3,75)	1:125:A:LEU:H	1:198:A:CYS:O	4	0.6
(1,903)	1:111:A:ILE:HG21	1:155:A:ILE:HG13	8	0.6
(1,749)	1:58:A:ASP:HB3	1:69:A:ILE:HG13	18	0.6
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	18	0.6
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	9	0.59
(1,747)	1:57:A:HIS:HB3	1:69:A:ILE:HG23	7	0.59
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	17	0.59
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	7	0.59
(1,731)	1:155:A:ILE:HG23	1:185:A:ILE:H	15	0.59
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	6	0.59
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	7	0.58
(1,903)	1:111:A:ILE:HG12	1:155:A:ILE:HG13	7	0.58
(1,814)	1:76:A:ILE:HG13	1:87:A:TRP:HE1	15	0.58
(1,1050)	1:155:A:ILE:HG13	1:167:A:LEU:HG	12	0.57
(1,813)	1:76:A:ILE:HG12	1:87:A:TRP:HE3	7	0.57
(1,756)	1:61:A:HIS:HB3	1:69:A:ILE:HG13	17	0.57
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	3	0.56
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	18	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:76:A:ILE:HG13	1:87:A:TRP:HE1	19	0.56
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	13	0.56
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	1	0.55
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD11	6	0.55
(1,815)	1:76:A:ILE:HG22	1:87:A:TRP:HD1	14	0.55
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	3	0.55
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	17	0.55
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	19	0.54
(1,747)	1:57:A:HIS:HB2	1:69:A:ILE:HG13	12	0.54
(1,736)	1:155:A:ILE:HG21	1:182:A:PHE:H	13	0.54
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	20	0.53
(1,902)	1:111:A:ILE:HD11	1:155:A:ILE:HG13	9	0.52
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	17	0.52
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	7	0.52
(3,146)	1:145:A:MET:H	1:60:A:SER:O	12	0.51
(1,1050)	1:155:A:ILE:HG23	1:167:A:LEU:HG	6	0.51
(1,1045)	1:155:A:ILE:HG12	1:183:A:PHE:HD1	19	0.51
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD11	14	0.51
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	16	0.5
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	19	0.5
(1,903)	1:111:A:ILE:HG23	1:155:A:ILE:HG13	9	0.49
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	18	0.49
(1,736)	1:155:A:ILE:HG22	1:182:A:PHE:H	9	0.49
(1,731)	1:155:A:ILE:HG23	1:185:A:ILE:H	12	0.49
(1,903)	1:111:A:ILE:HG21	1:155:A:ILE:HG13	17	0.48
(1,901)	1:111:A:ILE:HG13	1:155:A:ILE:HD13	7	0.48
(1,815)	1:76:A:ILE:HG13	1:87:A:TRP:HD1	9	0.48
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	13	0.47
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	13	0.47
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	13	0.47
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	13	0.47
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	13	0.47
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	13	0.47
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	13	0.47
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	13	0.47
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	13	0.47
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	13	0.47
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	13	0.47
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	13	0.47
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	5	0.47
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	9	0.47
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	13	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	4	0.46
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	8	0.46
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD12	11	0.46
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD13	12	0.46
(1,778)	1:70:A:LEU:HD12	1:94:A:ILE:HG13	2	0.46
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	1	0.46
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	17	0.46
(1,1050)	1:155:A:ILE:HG13	1:167:A:LEU:HG	1	0.45
(1,781)	1:70:A:LEU:HG	1:94:A:ILE:HG12	1	0.45
(1,781)	1:70:A:LEU:HG	1:94:A:ILE:HG13	16	0.45
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	2	0.44
(1,768)	1:67:A:ASP:HB2	1:94:A:ILE:HG12	10	0.44
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	3	0.44
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	6	0.44
(1,605)	1:155:A:ILE:HG23	1:160:A:TRP:HE1	9	0.44
(1,781)	1:70:A:LEU:HG	1:94:A:ILE:HG12	15	0.43
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	19	0.43
(1,605)	1:155:A:ILE:HG22	1:160:A:TRP:HE1	17	0.43
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	13	0.42
(1,731)	1:155:A:ILE:HG23	1:185:A:ILE:H	11	0.42
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	7	0.42
(1,583)	1:76:A:ILE:HG13	1:80:A:GLN:HG2	19	0.42
(1,902)	1:111:A:ILE:HD13	1:155:A:ILE:HG13	20	0.41
(1,901)	1:111:A:ILE:HG12	1:155:A:ILE:HD11	2	0.41
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	4	0.41
(1,902)	1:111:A:ILE:HD12	1:155:A:ILE:HG13	11	0.4
(1,901)	1:111:A:ILE:HG22	1:155:A:ILE:HD12	5	0.4
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	10	0.4
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	18	0.4
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	12	0.4
(3,74)	1:124:A:LEU:H	1:198:A:CYS:O	17	0.39
(3,73)	1:123:A:SER:H	1:198:A:CYS:O	9	0.39
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	19	0.39
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	15	0.38
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	2	0.38
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	2	0.38
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	2	0.38
(1,904)	1:111:A:ILE:HG12	1:182:A:PHE:HD2	1	0.38
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	20	0.38
(1,731)	1:155:A:ILE:HG21	1:185:A:ILE:H	17	0.38
(1,696)	1:122:A:ASP:H	1:155:A:ILE:HG12	2	0.38
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	9	0.38
(1,901)	1:111:A:ILE:HG22	1:155:A:ILE:HD11	3	0.37
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	3	0.37
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	5	0.37
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	3	0.37
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	4	0.37
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	14	0.37
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE1	17	0.37
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE2	17	0.37
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE1	17	0.37
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE2	17	0.37
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE1	17	0.37
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE2	17	0.37
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE1	17	0.37
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE2	17	0.37
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE1	17	0.37
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE2	17	0.37
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE1	17	0.37
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE2	17	0.37
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE1	9	0.36
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE2	9	0.36
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE1	9	0.36
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE2	9	0.36
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE1	9	0.36
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE2	9	0.36
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE1	17	0.36
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE2	17	0.36
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE1	17	0.36
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE2	17	0.36
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE1	17	0.36
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE2	17	0.36
(1,882)	1:108:A:TRP:HD1	1:155:A:ILE:HG13	6	0.36
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	8	0.36
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	1	0.36
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE1	1	0.36
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE2	1	0.36
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE1	1	0.36
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE2	1	0.36
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	12	0.35
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	12	0.35
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	12	0.35
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	12	0.35
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	12	0.35
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	12	0.35
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	12	0.35
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	12	0.35
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	12	0.35
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	12	0.35
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	12	0.35
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE1	20	0.35
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE2	20	0.35
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE1	20	0.35
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE2	20	0.35
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE1	20	0.35
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE2	20	0.35
(1,891)	1:108:A:TRP:HD1	1:170:A:VAL:HB	20	0.35
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	17	0.35
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	17	0.35
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	17	0.35
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	17	0.35
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	17	0.35
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	17	0.35
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	17	0.35
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	17	0.35
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	17	0.35
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	17	0.35
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	17	0.35
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	17	0.35
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	1	0.35
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	14	0.35
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	14	0.35
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	14	0.35
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	11	0.34
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	14	0.34
(1,1050)	1:155:A:ILE:HG13	1:167:A:LEU:HG	14	0.34
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	1	0.34
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	1	0.34
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	1	0.34
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	1	0.34
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	1	0.34
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	1	0.34
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	1	0.34
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	1	0.34
(1,931)	1:112:A:LEU:HG	1:118:A:GLN:HA	6	0.34
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD1	17	0.34
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD2	17	0.34
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	16	0.34
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	17	0.34
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	4	0.34
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	4	0.34
(3,74)	1:124:A:LEU:H	1:198:A:CYS:O	5	0.33
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	13	0.33
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	11	0.33
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	11	0.33
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	11	0.33
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	11	0.33
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	11	0.33
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	11	0.33
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	11	0.33
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	11	0.33
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	11	0.33
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	11	0.33
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	11	0.33
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	11	0.33
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD11	2	0.33
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD12	2	0.33
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD13	2	0.33
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD11	2	0.33
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD12	2	0.33
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD13	2	0.33
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD11	2	0.33
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD12	2	0.33
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD13	2	0.33
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD11	2	0.33
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD12	2	0.33
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD13	2	0.33
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD11	2	0.33
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD12	2	0.33
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD13	2	0.33
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD11	2	0.33
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD12	2	0.33
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD13	2	0.33
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	5	0.33
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	5	0.33
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	5	0.33
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	5	0.33
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	5	0.33
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	5	0.33
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	5	0.33
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	5	0.33
(1,891)	1:108:A:TRP:HD1	1:170:A:VAL:HB	9	0.33
(1,891)	1:108:A:TRP:HD1	1:170:A:VAL:HB	17	0.33
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	5	0.33
(1,688)	1:112:A:LEU:HD11	1:183:A:PHE:H	6	0.33
(1,688)	1:112:A:LEU:HD12	1:183:A:PHE:H	6	0.33
(1,688)	1:112:A:LEU:HD13	1:183:A:PHE:H	6	0.33
(1,688)	1:112:A:LEU:HD21	1:183:A:PHE:H	6	0.33
(1,688)	1:112:A:LEU:HD22	1:183:A:PHE:H	6	0.33
(1,688)	1:112:A:LEU:HD23	1:183:A:PHE:H	6	0.33
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	16	0.33
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	1	0.33
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	1	0.33
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE1	20	0.33
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE2	20	0.33
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE1	20	0.33
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE2	20	0.33
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE1	20	0.33
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE2	20	0.33
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE1	20	0.33
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE2	20	0.33
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE1	20	0.33
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE2	20	0.33
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE1	20	0.33
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE2	20	0.33
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	1	0.32
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	1	0.32
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	1	0.32
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	1	0.32
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	1	0.32
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	1	0.32
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	1	0.32
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	1	0.32
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	1	0.32
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	1	0.32
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	1	0.32
(1,901)	1:111:A:ILE:HG21	1:155:A:ILE:HD13	19	0.32
(1,815)	1:76:A:ILE:HG13	1:87:A:TRP:HD1	7	0.32
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	18	0.32
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	18	0.32
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	4	0.32
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	8	0.32
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	15	0.32
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	20	0.32
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	11	0.32
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	11	0.32
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	11	0.32
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	17	0.32
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	17	0.32
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE1	9	0.32
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE2	9	0.32
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE1	9	0.32
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE2	9	0.32
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE1	9	0.32
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE2	9	0.32
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE1	9	0.32
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE2	9	0.32
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE1	9	0.32
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE2	9	0.32
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE1	9	0.32
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE2	9	0.32
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	6	0.32
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	13	0.32
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	9	0.32
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	9	0.32
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	11	0.31
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	19	0.31
(1,1050)	1:155:A:ILE:HG13	1:167:A:LEU:HG	3	0.31
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	6	0.31
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	6	0.31
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	6	0.31
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	6	0.31
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	6	0.31
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	6	0.31
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	6	0.31
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	6	0.31
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	6	0.31
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	6	0.31
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	6	0.31
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	15	0.31
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	15	0.31
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	15	0.31
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	15	0.31
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	15	0.31
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	15	0.31
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	15	0.31
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	15	0.31
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	15	0.31
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	15	0.31
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	15	0.31
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	15	0.31
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	2	0.31
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	2	0.31
(1,904)	1:111:A:ILE:HG13	1:182:A:PHE:HD1	11	0.31
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	9	0.31
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	9	0.31
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	9	0.31
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	9	0.31
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	9	0.31
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	9	0.31
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	9	0.31
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	9	0.31
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	9	0.31
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	9	0.31
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	9	0.31
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	9	0.31
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	17	0.31
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	17	0.31
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	8	0.31
(1,605)	1:155:A:ILE:HG21	1:160:A:TRP:HE1	11	0.31
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	9	0.31
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	9	0.31
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	16	0.31
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	1	0.3
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	11	0.3
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	1	0.3
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	15	0.3
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	7	0.3
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	9	0.3
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	9	0.3
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	9	0.3
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	9	0.3
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	9	0.3
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	9	0.3
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	9	0.3
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	9	0.3
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	9	0.3
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	9	0.3
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	9	0.3
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	9	0.3
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	14	0.3
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	14	0.3
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	2	0.3
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	2	0.3
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD1	20	0.3
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD2	20	0.3
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	9	0.3
(1,731)	1:155:A:ILE:HG22	1:185:A:ILE:H	9	0.3
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	2	0.3
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	15	0.3
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD11	10	0.3
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD12	10	0.3
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD13	10	0.3
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD21	10	0.3
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD22	10	0.3
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD23	10	0.3
(1,605)	1:155:A:ILE:HG23	1:160:A:TRP:HE1	5	0.3
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE1	19	0.3
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE2	19	0.3
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE1	19	0.3
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE2	19	0.3
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	20	0.3
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	20	0.3
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	5	0.3
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	3	0.3
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	2	0.29
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	12	0.29
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	18	0.29
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	8	0.29
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	8	0.29
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	13	0.29
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	13	0.29
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	16	0.29
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	16	0.29
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	16	0.29
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	16	0.29
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	16	0.29
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	16	0.29
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	16	0.29
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	16	0.29
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	16	0.29
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	16	0.29
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	16	0.29
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	16	0.29
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	11	0.29
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	11	0.29
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	11	0.29
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	11	0.29
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	11	0.29
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	11	0.29
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	11	0.29
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	11	0.29
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	11	0.29
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	19	0.29
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	19	0.29
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	19	0.29
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	19	0.29
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	19	0.29
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	19	0.29
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	19	0.29
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	19	0.29
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	19	0.29
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	19	0.29
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	19	0.29
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	19	0.29
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	19	0.29
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	19	0.29
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	19	0.29
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE1	2	0.29
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE2	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE1	2	0.29
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE2	2	0.29
(1,935)	1:117:A:PHE:HE1	1:174:A:ILE:HB	5	0.29
(1,935)	1:117:A:PHE:HE2	1:174:A:ILE:HB	5	0.29
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD1	6	0.29
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD2	6	0.29
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD1	9	0.29
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD2	9	0.29
(1,904)	1:111:A:ILE:HG13	1:182:A:PHE:HD1	5	0.29
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG2	10	0.29
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG3	10	0.29
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG2	10	0.29
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG3	10	0.29
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG2	10	0.29
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG3	10	0.29
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG2	10	0.29
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG3	10	0.29
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG2	10	0.29
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG3	10	0.29
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG2	10	0.29
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG3	10	0.29
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	2	0.29
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	2	0.29
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	2	0.29
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	2	0.29
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	2	0.29
(1,811)	1:74:A:ILE:HG12	1:87:A:TRP:HB2	12	0.29
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	17	0.29
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	17	0.29
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	17	0.29
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	17	0.29
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	17	0.29
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	17	0.29
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	17	0.29
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	17	0.29
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	17	0.29
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	17	0.29
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	17	0.29
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	17	0.29
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	17	0.29
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	17	0.29
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	17	0.29
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	17	0.29
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	17	0.29
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	3	0.29
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG11	2	0.29
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG12	2	0.29
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG13	2	0.29
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG21	2	0.29
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG22	2	0.29
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG23	2	0.29
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	6	0.29
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	6	0.29
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD11	3	0.29
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD12	3	0.29
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD13	3	0.29
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD21	3	0.29
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD22	3	0.29
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD23	3	0.29
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	17	0.29
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	17	0.29
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	9	0.29
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	6	0.29
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	6	0.29
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	5	0.28
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	6	0.28
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	7	0.28
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	8	0.28
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	9	0.28
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	16	0.28
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	2	0.28
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	10	0.28
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	5	0.28
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	5	0.28
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	5	0.28
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	5	0.28
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	5	0.28
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	5	0.28
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	5	0.28
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	5	0.28
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	5	0.28
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	5	0.28
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	5	0.28
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	5	0.28
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	5	0.28
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE1	10	0.28
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE2	10	0.28
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE1	10	0.28
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE2	10	0.28
(1,935)	1:117:A:PHE:HE1	1:174:A:ILE:HB	19	0.28
(1,935)	1:117:A:PHE:HE2	1:174:A:ILE:HB	19	0.28
(1,903)	1:111:A:ILE:HG23	1:155:A:ILE:HG13	20	0.28
(1,901)	1:111:A:ILE:HG23	1:155:A:ILE:HD13	1	0.28
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	20	0.28
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	20	0.28
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	20	0.28
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	20	0.28
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	20	0.28
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	20	0.28
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	20	0.28
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	20	0.28
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	20	0.28
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	5	0.28
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	5	0.28
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	5	0.28
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	5	0.28
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	5	0.28
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	5	0.28
(1,815)	1:76:A:ILE:HG13	1:87:A:TRP:HD1	6	0.28
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	8	0.28
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	8	0.28
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	10	0.28
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	10	0.28
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	6	0.28
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	5	0.28
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	5	0.28
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	5	0.28
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	6	0.28
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	6	0.28
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	6	0.28
(1,756)	1:61:A:HIS:HB3	1:69:A:ILE:HG13	16	0.28
(1,749)	1:58:A:ASP:HB3	1:69:A:ILE:HG12	16	0.28
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	9	0.28
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	20	0.28
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	20	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD11	1	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD12	1	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD13	1	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD21	1	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD22	1	0.28
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD23	1	0.28
(1,605)	1:155:A:ILE:HG22	1:160:A:TRP:HE1	1	0.28
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	12	0.28
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	13	0.28
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	13	0.28
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	14	0.28
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	14	0.28
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	11	0.28
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	3	0.27
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	6	0.27
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	3	0.27
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	4	0.27
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	17	0.27
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	5	0.27
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	8	0.27
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	18	0.27
(2,11)	1:70:A:LEU:O	1:74:A:ILE:H	13	0.27
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	17	0.27
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	17	0.27
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	17	0.27
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	17	0.27
(1,1050)	1:155:A:ILE:HG23	1:167:A:LEU:HG	18	0.27
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	9	0.27
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	9	0.27
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	11	0.27
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	11	0.27
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	16	0.27
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	16	0.27
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	1	0.27
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	1	0.27
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	1	0.27
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	1	0.27
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	1	0.27
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	1	0.27
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	1	0.27
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	1	0.27
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	1	0.27
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	1	0.27
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	1	0.27
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	12	0.27
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	12	0.27
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	12	0.27
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	12	0.27
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	12	0.27
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	12	0.27
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	12	0.27
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	12	0.27
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	12	0.27
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	12	0.27
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	12	0.27
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	12	0.27
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	7	0.27
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	8	0.27
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	19	0.27
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD1	6	0.27
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD2	6	0.27
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD1	6	0.27
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD2	6	0.27
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD1	6	0.27
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD2	6	0.27
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	1	0.27
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	1	0.27
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	1	0.27
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	10	0.27
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	10	0.27
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	10	0.27
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	12	0.27
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	12	0.27
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	7	0.27
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	8	0.27
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	8	0.27
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	8	0.27
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	2	0.27
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	19	0.27
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	12	0.27
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	13	0.27
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	14	0.27
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	14	0.27
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD11	14	0.27
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD12	14	0.27
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD13	14	0.27
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD21	14	0.27
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD22	14	0.27
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD23	14	0.27
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD11	15	0.27
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD12	15	0.27
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD13	15	0.27
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD21	15	0.27
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD22	15	0.27
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD23	15	0.27
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	16	0.27
(1,552)	1:151:A:GLU:HG2	1:153:A:THR:H	13	0.27
(1,552)	1:151:A:GLU:HG3	1:153:A:THR:H	13	0.27
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	7	0.27
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	12	0.27
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	12	0.27
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	20	0.27
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	20	0.27
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	6	0.27
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	11	0.26
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	13	0.26
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	7	0.26
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	2	0.26
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	20	0.26
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	10	0.26
(2,21)	1:75:A:VAL:O	1:79:A:GLN:H	20	0.26
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	1	0.26
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	3	0.26
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	6	0.26
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	12	0.26
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	13	0.26
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	15	0.26
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	16	0.26
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	20	0.26
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	9	0.26
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	12	0.26
(2,11)	1:70:A:LEU:O	1:74:A:ILE:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	9	0.26
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	9	0.26
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	9	0.26
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	9	0.26
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	13	0.26
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	13	0.26
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	13	0.26
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	13	0.26
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	4	0.26
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	4	0.26
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	7	0.26
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	7	0.26
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	15	0.26
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	15	0.26
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	16	0.26
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	16	0.26
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	18	0.26
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	18	0.26
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	3	0.26
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	3	0.26
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	13	0.26
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	13	0.26
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	19	0.26
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	19	0.26
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	8	0.26
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	3	0.26
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	3	0.26
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE1	14	0.26
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE2	14	0.26
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE1	14	0.26
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE2	14	0.26
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD1	3	0.26
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD2	3	0.26
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD1	3	0.26
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD2	3	0.26
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD1	3	0.26
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD2	3	0.26
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	11	0.26
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	11	0.26
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	11	0.26
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	11	0.26
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	11	0.26
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	11	0.26
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	11	0.26
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	11	0.26
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	1	0.26
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	1	0.26
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG11	4	0.26
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG12	4	0.26
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG13	4	0.26
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG21	4	0.26
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG22	4	0.26
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG23	4	0.26
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG11	4	0.26
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG12	4	0.26
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG13	4	0.26
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG21	4	0.26
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG22	4	0.26
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG23	4	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	5	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	5	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	5	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	5	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	5	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	5	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	5	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	5	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	5	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	5	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	5	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	5	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	5	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	5	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	5	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	5	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	5	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	5	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	5	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	5	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	5	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	5	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	5	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	5	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	5	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	5	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	5	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	5	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	5	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	5	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	5	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	5	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	5	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	5	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	5	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	16	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	16	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	16	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	16	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	16	0.26
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	16	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	16	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	16	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	16	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	16	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	16	0.26
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	16	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	16	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	16	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	16	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	16	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	16	0.26
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	16	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	16	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	16	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	16	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	16	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	16	0.26
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	16	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	16	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	16	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	16	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	16	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	16	0.26
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	16	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	16	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	16	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	16	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	16	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	16	0.26
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	16	0.26
(1,824)	1:76:A:ILE:HD11	1:86:A:GLU:HG2	14	0.26
(1,824)	1:76:A:ILE:HD11	1:86:A:GLU:HG3	14	0.26
(1,824)	1:76:A:ILE:HD12	1:86:A:GLU:HG2	14	0.26
(1,824)	1:76:A:ILE:HD12	1:86:A:GLU:HG3	14	0.26
(1,824)	1:76:A:ILE:HD13	1:86:A:GLU:HG2	14	0.26
(1,824)	1:76:A:ILE:HD13	1:86:A:GLU:HG3	14	0.26
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	3	0.26
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	3	0.26
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	3	0.26
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	18	0.26
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	18	0.26
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	18	0.26
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	20	0.26
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	20	0.26
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	20	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	3	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	3	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	4	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	4	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	5	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	5	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	16	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	16	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	20	0.26
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	20	0.26
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	17	0.26
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	4	0.26
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	4	0.26
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	4	0.26
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	4	0.26
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	4	0.26
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	4	0.26
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	4	0.26
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	4	0.26
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	4	0.26
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	4	0.26
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	4	0.26
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	4	0.26
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	4	0.26
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	4	0.26
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	4	0.26
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	4	0.26
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	4	0.26
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	20	0.26
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	20	0.26
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	20	0.26
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	20	0.26
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	20	0.26
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	20	0.26
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	20	0.26
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	20	0.26
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	20	0.26
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	20	0.26
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	20	0.26
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	20	0.26
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	20	0.26
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	20	0.26
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	20	0.26
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	20	0.26
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	20	0.26
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	20	0.26
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	2	0.26
(1,708)	1:125:A:LEU:H	1:146:A:LEU:HA	14	0.26
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD11	2	0.26
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD12	2	0.26
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD13	2	0.26
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD21	2	0.26
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD22	2	0.26
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD23	2	0.26
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	4	0.26
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	5	0.26
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	6	0.26
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	3	0.26
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	3	0.26
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	10	0.26
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	10	0.26
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	18	0.26
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	13	0.26
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	13	0.26
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	13	0.26
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	13	0.26
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	13	0.26
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	13	0.26
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	16	0.26
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	16	0.26
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	16	0.26
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	16	0.26
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	16	0.26
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	16	0.26
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	18	0.26
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	18	0.26
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	18	0.26
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	18	0.26
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	18	0.26
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	18	0.26
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	19	0.26
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	15	0.26
(1,316)	1:124:A:LEU:HG	1:125:A:LEU:H	3	0.26
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	17	0.26
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	17	0.26
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	9	0.26
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	9	0.26
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	1	0.26
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	14	0.26
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	3	0.25
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	9	0.25
(2,113)	1:171:A:ASP:O	1:175:A:ALA:H	3	0.25
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	1	0.25
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	6	0.25
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	8	0.25
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	17	0.25
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	3	0.25
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	4	0.25
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	8	0.25
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	17	0.25
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	20	0.25
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	20	0.25
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	20	0.25
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	3	0.25
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	3	0.25
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	5	0.25
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	5	0.25
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	19	0.25
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	19	0.25
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD11	11	0.25
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD12	11	0.25
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD13	11	0.25
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD21	11	0.25
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD22	11	0.25
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD23	11	0.25
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD11	11	0.25
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD12	11	0.25
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD13	11	0.25
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD21	11	0.25
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD22	11	0.25
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD23	11	0.25
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	7	0.25
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	7	0.25
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD1	9	0.25
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD2	9	0.25
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD1	9	0.25
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD2	9	0.25
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD1	9	0.25
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD2	9	0.25
(1,903)	1:111:A:ILE:HG21	1:155:A:ILE:HG13	10	0.25
(1,903)	1:111:A:ILE:HG23	1:155:A:ILE:HG13	13	0.25
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	17	0.25
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	17	0.25
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	17	0.25
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	17	0.25
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	17	0.25
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	17	0.25
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	17	0.25
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	17	0.25
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	17	0.25
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	18	0.25
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	18	0.25
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	18	0.25
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	18	0.25
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	18	0.25
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	18	0.25
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	18	0.25
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	18	0.25
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	18	0.25
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	18	0.25
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	18	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	9	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	9	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	9	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	9	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	9	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	9	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	9	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	9	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	9	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	9	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	9	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	9	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	9	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	9	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	9	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	9	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	9	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	9	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	9	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	9	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	9	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	9	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	9	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	9	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	9	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	9	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	9	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	9	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	9	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	9	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	9	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	9	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	9	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	9	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	9	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	15	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	15	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	15	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	15	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	15	0.25
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	15	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	15	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	15	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	15	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	15	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	15	0.25
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	15	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	15	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	15	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	15	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	15	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	15	0.25
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	15	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	15	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	15	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	15	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	15	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	15	0.25
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	15	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	15	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	15	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	15	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	15	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	15	0.25
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	15	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	15	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	15	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	15	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	15	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	15	0.25
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	15	0.25
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	4	0.25
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	4	0.25
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	4	0.25
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	16	0.25
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	16	0.25
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	1	0.25
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	1	0.25
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	7	0.25
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	7	0.25
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	7	0.25
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	9	0.25
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	20	0.25
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	5	0.25
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	16	0.25
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	16	0.25
(1,657)	1:76:A:ILE:HD11	1:90:A:LEU:H	14	0.25
(1,657)	1:76:A:ILE:HD12	1:90:A:LEU:H	14	0.25
(1,657)	1:76:A:ILE:HD13	1:90:A:LEU:H	14	0.25
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	19	0.25
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	19	0.25
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	3	0.25
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	3	0.25
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	3	0.25
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	3	0.25
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	3	0.25
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	3	0.25
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	20	0.25
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	20	0.25
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	20	0.25
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	20	0.25
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	20	0.25
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	20	0.25
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	11	0.25
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	18	0.25
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	2	0.25
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	5	0.25
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	11	0.25
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	11	0.25
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	11	0.25
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	13	0.25
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	13	0.25
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB2	7	0.25
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB3	7	0.25
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB2	7	0.25
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB3	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	3	0.25
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	3	0.25
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	2	0.25
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	7	0.25
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	16	0.25
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	20	0.25
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	16	0.24
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	18	0.24
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	4	0.24
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	12	0.24
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	16	0.24
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	10	0.24
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	18	0.24
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	19	0.24
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	4	0.24
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	7	0.24
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	9	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	5	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	6	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	7	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	10	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	11	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	16	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	19	0.24
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	20	0.24
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	1	0.24
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	1	0.24
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	1	0.24
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	1	0.24
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	1	0.24
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	1	0.24
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	1	0.24
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	1	0.24
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	1	0.24
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	1	0.24
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	1	0.24
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	1	0.24
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	1	0.24
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	1	0.24
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	1	0.24
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	1	0.24
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	1	0.24
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	6	0.24
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	6	0.24
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	6	0.24
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	6	0.24
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	19	0.24
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	19	0.24
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	19	0.24
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	19	0.24
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	2	0.24
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	2	0.24
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	2	0.24
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	2	0.24
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	2	0.24
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	2	0.24
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	2	0.24
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	2	0.24
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	2	0.24
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	2	0.24
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	2	0.24
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	2	0.24
(1,1050)	1:155:A:ILE:HG13	1:167:A:LEU:HG	11	0.24
(1,1044)	1:155:A:ILE:HG22	1:182:A:PHE:HD2	19	0.24
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	1	0.24
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	1	0.24
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	3	0.24
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	3	0.24
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	17	0.24
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	17	0.24
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	13	0.24
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	13	0.24
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	4	0.24
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	4	0.24
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	4	0.24
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	4	0.24
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	4	0.24
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	4	0.24
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	4	0.24
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	4	0.24
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	4	0.24
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	4	0.24
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	4	0.24
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	20	0.24
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	20	0.24
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	20	0.24
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	20	0.24
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	20	0.24
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	20	0.24
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	20	0.24
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	20	0.24
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	20	0.24
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	20	0.24
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	20	0.24
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	20	0.24
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	16	0.24
(1,941)	1:120:A:GLU:HG2	1:183:A:PHE:HB2	12	0.24
(1,941)	1:120:A:GLU:HG2	1:183:A:PHE:HB3	12	0.24
(1,941)	1:120:A:GLU:HG3	1:183:A:PHE:HB2	12	0.24
(1,941)	1:120:A:GLU:HG3	1:183:A:PHE:HB3	12	0.24
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE1	7	0.24
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE2	7	0.24
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE1	7	0.24
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE2	7	0.24
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD1	18	0.24
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD2	18	0.24
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD1	18	0.24
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD2	18	0.24
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD1	18	0.24
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD2	18	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	9	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	9	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	9	0.24
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	9	0.24
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	9	0.24
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	9	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	9	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	9	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	9	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	12	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	12	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	12	0.24
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	12	0.24
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	12	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	12	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	12	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	12	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	13	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	13	0.24
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	13	0.24
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	13	0.24
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	13	0.24
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	13	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	13	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	13	0.24
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	13	0.24
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	19	0.24
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	19	0.24
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	19	0.24
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	19	0.24
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	19	0.24
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	19	0.24
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	14	0.24
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	14	0.24
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	12	0.24
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	12	0.24
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	12	0.24
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	12	0.24
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	12	0.24
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	12	0.24
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	12	0.24
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	12	0.24
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	12	0.24
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	12	0.24
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	12	0.24
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	12	0.24
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	2	0.24
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	2	0.24
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	2	0.24
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	2	0.24
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	2	0.24
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	2	0.24
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	2	0.24
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	2	0.24
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	2	0.24
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	2	0.24
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	2	0.24
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	12	0.24
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	12	0.24
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	12	0.24
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	12	0.24
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	16	0.24
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	16	0.24
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	16	0.24
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	17	0.24
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	17	0.24
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	17	0.24
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	7	0.24
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	16	0.24
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB2	20	0.24
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB3	20	0.24
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	10	0.24
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	11	0.24
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	20	0.24
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	20	0.24
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	20	0.24
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	20	0.24
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD11	15	0.24
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD12	15	0.24
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD13	15	0.24
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD21	15	0.24
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD22	15	0.24
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD23	15	0.24
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD11	15	0.24
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD12	15	0.24
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD13	15	0.24
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD21	15	0.24
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD22	15	0.24
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD23	15	0.24
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	3	0.24
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	3	0.24
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD11	20	0.24
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD12	20	0.24
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD13	20	0.24
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD21	20	0.24
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD22	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD23	20	0.24
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE1	5	0.24
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE2	5	0.24
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE1	5	0.24
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE2	5	0.24
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	19	0.24
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	19	0.24
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	19	0.24
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	19	0.24
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	19	0.24
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	19	0.24
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	10	0.24
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	11	0.24
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	12	0.24
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	16	0.24
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	10	0.24
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	10	0.24
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	13	0.24
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	13	0.24
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	20	0.24
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	20	0.24
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	19	0.24
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	19	0.24
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	4	0.24
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	4	0.24
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	7	0.24
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	7	0.24
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	16	0.24
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	16	0.24
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	20	0.24
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	20	0.24
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	19	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	3	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	5	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	9	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	10	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	12	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	13	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	15	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	17	0.24
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	19	0.24
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	15	0.23
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	17	0.23
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	1	0.23
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	8	0.23
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	11	0.23
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	13	0.23
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	18	0.23
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	14	0.23
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	15	0.23
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	4	0.23
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	16	0.23
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	9	0.23
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	11	0.23
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB2	12	0.23
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB3	12	0.23
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB2	12	0.23
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB3	12	0.23
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB2	12	0.23
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB3	12	0.23
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB2	12	0.23
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB3	12	0.23
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB2	12	0.23
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB3	12	0.23
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB2	12	0.23
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB3	12	0.23
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	1	0.23
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	1	0.23
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	1	0.23
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	1	0.23
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	5	0.23
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	5	0.23
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	5	0.23
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	5	0.23
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE1	6	0.23
(1,1047)	1:155:A:ILE:HD11	1:183:A:PHE:HE2	6	0.23
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE1	6	0.23
(1,1047)	1:155:A:ILE:HD12	1:183:A:PHE:HE2	6	0.23
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE1	6	0.23
(1,1047)	1:155:A:ILE:HD13	1:183:A:PHE:HE2	6	0.23
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	12	0.23
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	12	0.23
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	20	0.23
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	8	0.23
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	8	0.23
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	7	0.23
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	7	0.23
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	7	0.23
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	7	0.23
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	7	0.23
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	7	0.23
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	7	0.23
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	7	0.23
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	7	0.23
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	7	0.23
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	7	0.23
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	7	0.23
(1,970)	1:124:A:LEU:HD11	1:153:A:THR:HG21	2	0.23
(1,970)	1:124:A:LEU:HD11	1:153:A:THR:HG22	2	0.23
(1,970)	1:124:A:LEU:HD11	1:153:A:THR:HG23	2	0.23
(1,970)	1:124:A:LEU:HD12	1:153:A:THR:HG21	2	0.23
(1,970)	1:124:A:LEU:HD12	1:153:A:THR:HG22	2	0.23
(1,970)	1:124:A:LEU:HD12	1:153:A:THR:HG23	2	0.23
(1,970)	1:124:A:LEU:HD13	1:153:A:THR:HG21	2	0.23
(1,970)	1:124:A:LEU:HD13	1:153:A:THR:HG22	2	0.23
(1,970)	1:124:A:LEU:HD13	1:153:A:THR:HG23	2	0.23
(1,970)	1:124:A:LEU:HD21	1:153:A:THR:HG21	2	0.23
(1,970)	1:124:A:LEU:HD21	1:153:A:THR:HG22	2	0.23
(1,970)	1:124:A:LEU:HD21	1:153:A:THR:HG23	2	0.23
(1,970)	1:124:A:LEU:HD22	1:153:A:THR:HG21	2	0.23
(1,970)	1:124:A:LEU:HD22	1:153:A:THR:HG22	2	0.23
(1,970)	1:124:A:LEU:HD22	1:153:A:THR:HG23	2	0.23
(1,970)	1:124:A:LEU:HD23	1:153:A:THR:HG21	2	0.23
(1,970)	1:124:A:LEU:HD23	1:153:A:THR:HG22	2	0.23
(1,970)	1:124:A:LEU:HD23	1:153:A:THR:HG23	2	0.23
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	14	0.23
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	14	0.23
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	14	0.23
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	14	0.23
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	14	0.23
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	14	0.23
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	14	0.23
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	14	0.23
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	14	0.23
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	14	0.23
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	14	0.23
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	12	0.23
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	4	0.23
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	15	0.23
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	16	0.23
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	16	0.23
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	18	0.23
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	18	0.23
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD1	19	0.23
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD2	19	0.23
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD1	19	0.23
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD2	19	0.23
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD1	19	0.23
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD2	19	0.23
(1,935)	1:117:A:PHE:HE1	1:174:A:ILE:HB	7	0.23
(1,935)	1:117:A:PHE:HE2	1:174:A:ILE:HB	7	0.23
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD1	3	0.23
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD2	3	0.23
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD1	13	0.23
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD2	13	0.23
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD1	13	0.23
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD2	13	0.23
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD1	13	0.23
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD2	13	0.23
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	18	0.23
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	18	0.23
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	18	0.23
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	18	0.23
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	18	0.23
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	18	0.23
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	18	0.23
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	18	0.23
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	18	0.23
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	16	0.23
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	16	0.23
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	16	0.23
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	16	0.23
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	16	0.23
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	16	0.23
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	9	0.23
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	10	0.23
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	10	0.23
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB1	6	0.23
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB2	6	0.23
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB3	6	0.23
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	2	0.23
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	2	0.23
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	2	0.23
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	2	0.23
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	2	0.23
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	2	0.23
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	2	0.23
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	2	0.23
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	2	0.23
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	2	0.23
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	2	0.23
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	2	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	6	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	6	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	6	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	6	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	6	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	6	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	6	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	6	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	6	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	6	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	6	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	6	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	6	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	6	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	6	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	6	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	6	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	6	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	6	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	6	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	6	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	6	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	6	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	6	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	6	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	6	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	6	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	6	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	6	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	6	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	6	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	6	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	6	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	6	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	6	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	11	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	11	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	11	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	11	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	11	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	11	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	11	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	11	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	11	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	11	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	11	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	11	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	11	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	11	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	11	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	11	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	11	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	11	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	11	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	11	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	11	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	11	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	11	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	11	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	11	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	11	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	11	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	11	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	11	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	11	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	11	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	11	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	11	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	11	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	11	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	17	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	17	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	17	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	17	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	17	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	17	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	17	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	17	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	17	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	17	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	17	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	17	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	17	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	17	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	17	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	17	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	17	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	17	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	17	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	17	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	17	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	17	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	17	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	17	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	17	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	17	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	17	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	17	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	17	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	17	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	17	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	17	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	17	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	17	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	17	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	20	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	20	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	20	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	20	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	20	0.23
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	20	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	20	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	20	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	20	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	20	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	20	0.23
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	20	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	20	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	20	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	20	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	20	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	20	0.23
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	20	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	20	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	20	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	20	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	20	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	20	0.23
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	20	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	20	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	20	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	20	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	20	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	20	0.23
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	20	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	20	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	20	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	20	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	20	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	20	0.23
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	20	0.23
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	5	0.23
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	5	0.23
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	5	0.23
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	8	0.23
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	8	0.23
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	17	0.23
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	17	0.23
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	17	0.23
(1,815)	1:76:A:ILE:HG13	1:87:A:TRP:HD1	11	0.23
(1,815)	1:76:A:ILE:HG13	1:87:A:TRP:HD1	13	0.23
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	19	0.23
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	19	0.23
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	3	0.23
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	3	0.23
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	3	0.23
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	3	0.23
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	3	0.23
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	3	0.23
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	3	0.23
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	3	0.23
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	3	0.23
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	3	0.23
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	3	0.23
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	3	0.23
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	3	0.23
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	3	0.23
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	3	0.23
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	3	0.23
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	3	0.23
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	3	0.23
(1,749)	1:58:A:ASP:HB3	1:69:A:ILE:HG13	19	0.23
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD11	2	0.23
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD12	2	0.23
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD13	2	0.23
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD21	2	0.23
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD22	2	0.23
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD23	2	0.23
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	5	0.23
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	17	0.23
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	7	0.23
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB2	6	0.23
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB3	6	0.23
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	13	0.23
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	13	0.23
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	8	0.23
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	8	0.23
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	10	0.23
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	10	0.23
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	10	0.23
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	10	0.23
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	10	0.23
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	17	0.23
(1,552)	1:151:A:GLU:HG2	1:153:A:THR:H	12	0.23
(1,552)	1:151:A:GLU:HG3	1:153:A:THR:H	12	0.23
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	1	0.23
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	4	0.23
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	18	0.23
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB2	4	0.23
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB3	4	0.23
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	9	0.23
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	9	0.23
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	10	0.23
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	10	0.23
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	15	0.23
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	15	0.23
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	12	0.23
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	12	0.23
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	5	0.23
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	4	0.23
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	8	0.23
(1,174)	1:130:A:LEU:HA	1:131:A:SER:H	18	0.23
(3,76)	1:126:A:SER:H	1:198:A:CYS:O	20	0.22
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	4	0.22
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	5	0.22
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	8	0.22
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	12	0.22
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	13	0.22
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	5	0.22
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	3	0.22
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	5	0.22
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	7	0.22
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	17	0.22
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	15	0.22
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	18	0.22
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD11	9	0.22
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD12	9	0.22
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD13	9	0.22
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD11	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD12	9	0.22
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD13	9	0.22
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD11	9	0.22
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD12	9	0.22
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD13	9	0.22
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD11	9	0.22
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD12	9	0.22
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD13	9	0.22
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD11	9	0.22
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD12	9	0.22
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD13	9	0.22
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD11	9	0.22
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD12	9	0.22
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD13	9	0.22
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	2	0.22
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	2	0.22
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	2	0.22
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	2	0.22
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	18	0.22
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	18	0.22
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	18	0.22
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	18	0.22
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	2	0.22
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	2	0.22
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	15	0.22
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	15	0.22
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	18	0.22
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	18	0.22
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	4	0.22
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	4	0.22
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	10	0.22
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	10	0.22
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	10	0.22
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	10	0.22
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	10	0.22
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	10	0.22
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	10	0.22
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	10	0.22
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	10	0.22
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	10	0.22
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	10	0.22
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	17	0.22
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	17	0.22
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	17	0.22
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	17	0.22
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	17	0.22
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	17	0.22
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	17	0.22
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	17	0.22
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	17	0.22
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	17	0.22
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	17	0.22
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	17	0.22
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	10	0.22
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD11	1	0.22
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD12	1	0.22
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD13	1	0.22
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD21	1	0.22
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD22	1	0.22
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD23	1	0.22
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD11	1	0.22
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD12	1	0.22
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD13	1	0.22
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD21	1	0.22
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD22	1	0.22
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD23	1	0.22
(1,940)	1:117:A:PHE:HD1	1:183:A:PHE:HE1	3	0.22
(1,940)	1:117:A:PHE:HD1	1:183:A:PHE:HE2	3	0.22
(1,940)	1:117:A:PHE:HD2	1:183:A:PHE:HE1	3	0.22
(1,940)	1:117:A:PHE:HD2	1:183:A:PHE:HE2	3	0.22
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE1	1	0.22
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE2	1	0.22
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE1	1	0.22
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE2	1	0.22
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE1	5	0.22
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE2	5	0.22
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE1	5	0.22
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE2	5	0.22
(1,935)	1:117:A:PHE:HE1	1:174:A:ILE:HB	1	0.22
(1,935)	1:117:A:PHE:HE2	1:174:A:ILE:HB	1	0.22
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD1	17	0.22
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD2	17	0.22
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD1	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD2	17	0.22
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD1	17	0.22
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD2	17	0.22
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD1	9	0.22
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD2	9	0.22
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD1	9	0.22
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD2	9	0.22
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD1	9	0.22
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD2	9	0.22
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	16	0.22
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	16	0.22
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	16	0.22
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	16	0.22
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	16	0.22
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	16	0.22
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	16	0.22
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	16	0.22
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	16	0.22
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	15	0.22
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	15	0.22
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	17	0.22
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	17	0.22
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	12	0.22
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	12	0.22
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	12	0.22
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	12	0.22
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	12	0.22
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	12	0.22
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	12	0.22
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	12	0.22
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	12	0.22
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	12	0.22
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	12	0.22
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	12	0.22
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	12	0.22
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	12	0.22
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	12	0.22
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	12	0.22
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	12	0.22
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	12	0.22
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	12	0.22
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	12	0.22
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	12	0.22
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	12	0.22
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	12	0.22
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	12	0.22
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	12	0.22
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	12	0.22
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	12	0.22
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	12	0.22
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	12	0.22
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	12	0.22
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	12	0.22
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	12	0.22
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	12	0.22
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	12	0.22
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	12	0.22
(1,793)	1:73:A:LEU:HD11	1:90:A:LEU:HG	15	0.22
(1,793)	1:73:A:LEU:HD12	1:90:A:LEU:HG	15	0.22
(1,793)	1:73:A:LEU:HD13	1:90:A:LEU:HG	15	0.22
(1,793)	1:73:A:LEU:HD21	1:90:A:LEU:HG	15	0.22
(1,793)	1:73:A:LEU:HD22	1:90:A:LEU:HG	15	0.22
(1,793)	1:73:A:LEU:HD23	1:90:A:LEU:HG	15	0.22
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	12	0.22
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	12	0.22
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	12	0.22
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	14	0.22
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	14	0.22
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	14	0.22
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	14	0.22
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	14	0.22
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	14	0.22
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	14	0.22
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	14	0.22
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	14	0.22
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	14	0.22
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	14	0.22
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	14	0.22
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	14	0.22
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	14	0.22
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	14	0.22
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	14	0.22
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	14	0.22
(1,740)	1:156:A:PHE:H	1:167:A:LEU:HG	20	0.22
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	19	0.22
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	18	0.22
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	15	0.22
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB2	9	0.22
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB3	9	0.22
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB2	17	0.22
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB3	17	0.22
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	8	0.22
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	17	0.22
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	17	0.22
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	17	0.22
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	10	0.22
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	10	0.22
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	9	0.22
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	9	0.22
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	9	0.22
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	9	0.22
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	9	0.22
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	9	0.22
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	17	0.22
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	17	0.22
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	17	0.22
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	17	0.22
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	17	0.22
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	17	0.22
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	2	0.22
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	15	0.22
(1,540)	1:115:A:LEU:HD11	1:118:A:GLN:H	7	0.22
(1,540)	1:115:A:LEU:HD12	1:118:A:GLN:H	7	0.22
(1,540)	1:115:A:LEU:HD13	1:118:A:GLN:H	7	0.22
(1,540)	1:115:A:LEU:HD21	1:118:A:GLN:H	7	0.22
(1,540)	1:115:A:LEU:HD22	1:118:A:GLN:H	7	0.22
(1,540)	1:115:A:LEU:HD23	1:118:A:GLN:H	7	0.22
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	8	0.22
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	16	0.22
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	16	0.22
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	16	0.22
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	9	0.22
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	9	0.22
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	18	0.22
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	20	0.22
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	20	0.22
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	11	0.22
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	11	0.22
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	7	0.22
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	7	0.22
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	2	0.22
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	2	0.22
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	6	0.22
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	6	0.22
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	19	0.22
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	19	0.22
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	8	0.22
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	8	0.22
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	15	0.22
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	15	0.22
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	18	0.22
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	18	0.22
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	6	0.22
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	6	0.22
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	1	0.22
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	2	0.22
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	6	0.22
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	11	0.22
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	17	0.22
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	10	0.21
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	11	0.21
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	20	0.21
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	5	0.21
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	7	0.21
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	15	0.21
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	12	0.21
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	16	0.21
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	6	0.21
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	16	0.21
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	1	0.21
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	3	0.21
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	3	0.21
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	3	0.21
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	3	0.21
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	10	0.21
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	10	0.21
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	10	0.21
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	16	0.21
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	16	0.21
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	16	0.21
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	16	0.21
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	6	0.21
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	6	0.21
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	19	0.21
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	19	0.21
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	8	0.21
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	8	0.21
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	8	0.21
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	8	0.21
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	8	0.21
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	8	0.21
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	8	0.21
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	8	0.21
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	8	0.21
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	8	0.21
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	8	0.21
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	8	0.21
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	8	0.21
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	8	0.21
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	5	0.21
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	5	0.21
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	10	0.21
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	10	0.21
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	3	0.21
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	4	0.21
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	20	0.21
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	1	0.21
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	5	0.21
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	8	0.21
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	8	0.21
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	15	0.21
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	15	0.21
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	19	0.21
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	19	0.21
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	8	0.21
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	8	0.21
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	8	0.21
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	8	0.21
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	8	0.21
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB1	2	0.21
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB2	2	0.21
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB3	2	0.21
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB1	2	0.21
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB2	2	0.21
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB3	2	0.21
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB1	5	0.21
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB2	5	0.21
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB3	5	0.21
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB1	5	0.21
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB2	5	0.21
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB3	5	0.21
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD1	18	0.21
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD2	18	0.21
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD1	20	0.21
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD2	20	0.21
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD1	20	0.21
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD2	20	0.21
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD1	20	0.21
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD2	20	0.21
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB2	9	0.21
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB3	9	0.21
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB2	9	0.21
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB3	9	0.21
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB2	9	0.21
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB3	9	0.21
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	12	0.21
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	12	0.21
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG2	2	0.21
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG3	2	0.21
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG2	2	0.21
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG3	2	0.21
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG2	2	0.21
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG3	2	0.21
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG2	2	0.21
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG3	2	0.21
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG2	2	0.21
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG3	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG2	2	0.21
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG3	2	0.21
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	20	0.21
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	20	0.21
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	20	0.21
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	20	0.21
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	20	0.21
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	20	0.21
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	20	0.21
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	20	0.21
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	20	0.21
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	20	0.21
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	20	0.21
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	20	0.21
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	11	0.21
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	14	0.21
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	14	0.21
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	20	0.21
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	20	0.21
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	20	0.21
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	18	0.21
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	18	0.21
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	18	0.21
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	18	0.21
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	7	0.21
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	7	0.21
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	7	0.21
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	7	0.21
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	7	0.21
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	7	0.21
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	7	0.21
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	7	0.21
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	7	0.21
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	7	0.21
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	7	0.21
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	7	0.21
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	7	0.21
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	7	0.21
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	7	0.21
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	7	0.21
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	7	0.21
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD11	12	0.21
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD12	12	0.21
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD13	12	0.21
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD21	12	0.21
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD22	12	0.21
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD23	12	0.21
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	14	0.21
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	11	0.21
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	9	0.21
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	9	0.21
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	9	0.21
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	13	0.21
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	13	0.21
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	13	0.21
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	3	0.21
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	7	0.21
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	16	0.21
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	19	0.21
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	19	0.21
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	19	0.21
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	7	0.21
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	7	0.21
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	12	0.21
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	12	0.21
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	14	0.21
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	14	0.21
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD11	20	0.21
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD12	20	0.21
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD13	20	0.21
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD21	20	0.21
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD22	20	0.21
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD23	20	0.21
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD11	20	0.21
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD12	20	0.21
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD13	20	0.21
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD21	20	0.21
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD22	20	0.21
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD23	20	0.21
(1,605)	1:155:A:ILE:HG22	1:160:A:TRP:HE1	13	0.21
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	4	0.21
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	4	0.21
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	4	0.21
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	4	0.21
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	4	0.21
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	7	0.21
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	7	0.21
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	7	0.21
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	7	0.21
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	7	0.21
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	7	0.21
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	14	0.21
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	14	0.21
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	14	0.21
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	14	0.21
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	14	0.21
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	14	0.21
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	1	0.21
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	7	0.21
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	9	0.21
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	13	0.21
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	14	0.21
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	17	0.21
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	18	0.21
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	4	0.21
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	9	0.21
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	14	0.21
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	20	0.21
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB2	8	0.21
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB3	8	0.21
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	18	0.21
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	18	0.21
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	5	0.21
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	5	0.21
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	14	0.21
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	14	0.21
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	15	0.21
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	15	0.21
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	17	0.21
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	17	0.21
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	8	0.21
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	8	0.21
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	9	0.21
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	18	0.21
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	18	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	1	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	1	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	3	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	3	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	4	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	4	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	5	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	5	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	7	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	7	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	11	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	11	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	12	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	12	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	13	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	13	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	16	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	16	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	17	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	17	0.21
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	20	0.21
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	20	0.21
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	2	0.21
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	2	0.21
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	3	0.21
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	3	0.21
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	4	0.21
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	4	0.21
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	5	0.21
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	5	0.21
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	12	0.21
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	12	0.21
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	13	0.21
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	13	0.21
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	16	0.21
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	16	0.21
(1,261)	1:83:A:ASP:HB3	1:84:A:SER:H	17	0.21
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	5	0.21
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	5	0.21
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	8	0.21
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	14	0.21
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	14	0.21
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	17	0.21
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	17	0.21
(3,74)	1:124:A:LEU:H	1:198:A:CYS:O	1	0.2
(3,20)	1:94:A:ILE:H	1:136:A:SER:O	2	0.2
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	1	0.2
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	6	0.2
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	14	0.2
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	4	0.2
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	5	0.2
(2,101)	1:165:A:ARG:O	1:169:A:VAL:H	2	0.2
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	15	0.2
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	12	0.2
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	13	0.2
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	2	0.2
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	15	0.2
(1,1100)	1:173:A:LEU:HD11	1:179:A:ALA:HB1	18	0.2
(1,1100)	1:173:A:LEU:HD11	1:179:A:ALA:HB2	18	0.2
(1,1100)	1:173:A:LEU:HD11	1:179:A:ALA:HB3	18	0.2
(1,1100)	1:173:A:LEU:HD12	1:179:A:ALA:HB1	18	0.2
(1,1100)	1:173:A:LEU:HD12	1:179:A:ALA:HB2	18	0.2
(1,1100)	1:173:A:LEU:HD12	1:179:A:ALA:HB3	18	0.2
(1,1100)	1:173:A:LEU:HD13	1:179:A:ALA:HB1	18	0.2
(1,1100)	1:173:A:LEU:HD13	1:179:A:ALA:HB2	18	0.2
(1,1100)	1:173:A:LEU:HD13	1:179:A:ALA:HB3	18	0.2
(1,1100)	1:173:A:LEU:HD21	1:179:A:ALA:HB1	18	0.2
(1,1100)	1:173:A:LEU:HD21	1:179:A:ALA:HB2	18	0.2
(1,1100)	1:173:A:LEU:HD21	1:179:A:ALA:HB3	18	0.2
(1,1100)	1:173:A:LEU:HD22	1:179:A:ALA:HB1	18	0.2
(1,1100)	1:173:A:LEU:HD22	1:179:A:ALA:HB2	18	0.2
(1,1100)	1:173:A:LEU:HD22	1:179:A:ALA:HB3	18	0.2
(1,1100)	1:173:A:LEU:HD23	1:179:A:ALA:HB1	18	0.2
(1,1100)	1:173:A:LEU:HD23	1:179:A:ALA:HB2	18	0.2
(1,1100)	1:173:A:LEU:HD23	1:179:A:ALA:HB3	18	0.2
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB2	11	0.2
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB3	11	0.2
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB2	11	0.2
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB3	11	0.2
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB2	11	0.2
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB2	11	0.2
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB3	11	0.2
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB2	11	0.2
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB3	11	0.2
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB2	11	0.2
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB3	11	0.2
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	12	0.2
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	12	0.2
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	12	0.2
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	12	0.2
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	12	0.2
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	12	0.2
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	12	0.2
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	12	0.2
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	12	0.2
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	12	0.2
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	12	0.2
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	12	0.2
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	12	0.2
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	12	0.2
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	12	0.2
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	12	0.2
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	12	0.2
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	12	0.2
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD11	1	0.2
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD12	1	0.2
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD13	1	0.2
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD21	1	0.2
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD22	1	0.2
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD23	1	0.2
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	8	0.2
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	8	0.2
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	8	0.2
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	8	0.2
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	12	0.2
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	12	0.2
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	12	0.2
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	12	0.2
(1,1034)	1:155:A:ILE:HG21	1:170:A:VAL:HB	9	0.2
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	4	0.2
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	4	0.2
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	4	0.2
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	4	0.2
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	4	0.2
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	4	0.2
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	4	0.2
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	4	0.2
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	4	0.2
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	4	0.2
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	4	0.2
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	11	0.2
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	11	0.2
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	11	0.2
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	11	0.2
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	11	0.2
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	11	0.2
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	11	0.2
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	11	0.2
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	11	0.2
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	11	0.2
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	11	0.2
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	11	0.2
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	13	0.2
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	13	0.2
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	13	0.2
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	13	0.2
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	13	0.2
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	13	0.2
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	13	0.2
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	13	0.2
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	13	0.2
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	13	0.2
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	13	0.2
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	13	0.2
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	8	0.2
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	8	0.2
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	8	0.2
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	8	0.2
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	8	0.2
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	8	0.2
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	8	0.2
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	8	0.2
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	8	0.2
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	8	0.2
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	8	0.2
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	16	0.2
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	16	0.2
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	16	0.2
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	16	0.2
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	16	0.2
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	16	0.2
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	16	0.2
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	16	0.2
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	16	0.2
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	16	0.2
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	16	0.2
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	16	0.2
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	14	0.2
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	14	0.2
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	19	0.2
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	19	0.2
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	1	0.2
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	1	0.2
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	1	0.2
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	1	0.2
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	1	0.2
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	1	0.2
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	1	0.2
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	1	0.2
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	1	0.2
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	1	0.2
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	1	0.2
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	1	0.2
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	4	0.2
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	4	0.2
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	5	0.2
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	5	0.2
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	2	0.2
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	2	0.2
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	2	0.2
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	2	0.2
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	2	0.2
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	2	0.2
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	2	0.2
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	2	0.2
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	14	0.2
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	14	0.2
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	14	0.2
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	14	0.2
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	14	0.2
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	14	0.2
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD1	10	0.2
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD2	10	0.2
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD1	10	0.2
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD2	10	0.2
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD1	10	0.2
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD2	10	0.2
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE1	19	0.2
(1,938)	1:117:A:PHE:HB2	1:183:A:PHE:HE2	19	0.2
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE1	19	0.2
(1,938)	1:117:A:PHE:HB3	1:183:A:PHE:HE2	19	0.2
(1,934)	1:117:A:PHE:HE1	1:182:A:PHE:HE1	2	0.2
(1,934)	1:117:A:PHE:HE1	1:182:A:PHE:HE2	2	0.2
(1,934)	1:117:A:PHE:HE2	1:182:A:PHE:HE1	2	0.2
(1,934)	1:117:A:PHE:HE2	1:182:A:PHE:HE2	2	0.2
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB1	1	0.2
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB2	1	0.2
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB3	1	0.2
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB1	1	0.2
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB2	1	0.2
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB3	1	0.2
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD1	2	0.2
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD2	2	0.2
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD1	2	0.2
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD2	2	0.2
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD1	2	0.2
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD2	2	0.2
(1,904)	1:111:A:ILE:HG13	1:182:A:PHE:HD2	3	0.2
(1,902)	1:111:A:ILE:HD11	1:155:A:ILE:HG13	13	0.2
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	1	0.2
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	1	0.2
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	1	0.2
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	1	0.2
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	1	0.2
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	1	0.2
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	1	0.2
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	1	0.2
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	1	0.2
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	1	0.2
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	1	0.2
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	1	0.2
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	1	0.2
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	1	0.2
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	1	0.2
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	1	0.2
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	1	0.2
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	1	0.2
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	1	0.2
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	1	0.2
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	1	0.2
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	1	0.2
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	1	0.2
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	1	0.2
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	1	0.2
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	1	0.2
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	1	0.2
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	1	0.2
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	1	0.2
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	1	0.2
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	1	0.2
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	1	0.2
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	1	0.2
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	1	0.2
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	1	0.2
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	11	0.2
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	11	0.2
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD11	14	0.2
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD12	14	0.2
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD13	14	0.2
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD21	14	0.2
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD22	14	0.2
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD23	14	0.2
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD11	14	0.2
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD12	14	0.2
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD13	14	0.2
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD21	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD22	14	0.2
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD23	14	0.2
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD11	14	0.2
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD12	14	0.2
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD13	14	0.2
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD21	14	0.2
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD22	14	0.2
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD23	14	0.2
(1,842)	1:99:A:GLN:HG2	1:139:A:THR:HA	6	0.2
(1,842)	1:99:A:GLN:HG3	1:139:A:THR:HA	6	0.2
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	3	0.2
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB2	17	0.2
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB3	17	0.2
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	5	0.2
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	5	0.2
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	5	0.2
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	5	0.2
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	5	0.2
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	5	0.2
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	5	0.2
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	5	0.2
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	5	0.2
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	5	0.2
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	5	0.2
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	5	0.2
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	8	0.2
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	8	0.2
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	8	0.2
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	8	0.2
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	8	0.2
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	8	0.2
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	8	0.2
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	8	0.2
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	8	0.2
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	8	0.2
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	8	0.2
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	8	0.2
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	14	0.2
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	14	0.2
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	14	0.2
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	14	0.2
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	14	0.2
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	14	0.2
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	14	0.2
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	14	0.2
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	14	0.2
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	14	0.2
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	14	0.2
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	1	0.2
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	1	0.2
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	2	0.2
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	2	0.2
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	8	0.2
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	8	0.2
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	18	0.2
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	18	0.2
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	19	0.2
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	19	0.2
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	3	0.2
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	3	0.2
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	3	0.2
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	9	0.2
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	9	0.2
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	9	0.2
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	15	0.2
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	7	0.2
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	7	0.2
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	7	0.2
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	10	0.2
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	10	0.2
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	10	0.2
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	15	0.2
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	15	0.2
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	15	0.2
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	6	0.2
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	9	0.2
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	11	0.2
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	17	0.2
(1,670)	1:100:A:ILE:HD11	1:143:A:ARG:H	2	0.2
(1,670)	1:100:A:ILE:HD12	1:143:A:ARG:H	2	0.2
(1,670)	1:100:A:ILE:HD13	1:143:A:ARG:H	2	0.2
(1,670)	1:100:A:ILE:HD11	1:143:A:ARG:H	9	0.2
(1,670)	1:100:A:ILE:HD12	1:143:A:ARG:H	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:100:A:ILE:HD13	1:143:A:ARG:H	9	0.2
(1,658)	1:77:A:ARG:HB2	1:87:A:TRP:H	14	0.2
(1,658)	1:77:A:ARG:HB3	1:87:A:TRP:H	14	0.2
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	18	0.2
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	18	0.2
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	15	0.2
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	20	0.2
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	13	0.2
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	13	0.2
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	13	0.2
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	11	0.2
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	14	0.2
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	10	0.2
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	19	0.2
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	7	0.2
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	8	0.2
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	8	0.2
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	8	0.2
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	6	0.2
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	6	0.2
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	4	0.2
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	4	0.2
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	8	0.2
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	8	0.2
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	14	0.2
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	14	0.2
(1,268)	1:88:A:GLN:HB2	1:89:A:ARG:H	18	0.2
(1,268)	1:88:A:GLN:HB3	1:89:A:ARG:H	18	0.2
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	1	0.2
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	1	0.2
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	6	0.2
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	6	0.2
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	7	0.2
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	7	0.2
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	9	0.2
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	9	0.2
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	10	0.2
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	10	0.2
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	17	0.2
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	17	0.2
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	20	0.2
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:83:A:ASP:HB3	1:84:A:SER:H	4	0.2
(1,256)	1:80:A:GLN:HG2	1:81:A:THR:H	19	0.2
(1,256)	1:80:A:GLN:HG3	1:81:A:THR:H	19	0.2
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	11	0.2
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	11	0.2
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	19	0.19
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	9	0.19
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	10	0.19
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	19	0.19
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	20	0.19
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	7	0.19
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	4	0.19
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	6	0.19
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	8	0.19
(2,75)	1:118:A:GLN:O	1:122:A:ASP:H	2	0.19
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	4	0.19
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	7	0.19
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	8	0.19
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	15	0.19
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	6	0.19
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	13	0.19
(2,12)	1:70:A:LEU:O	1:74:A:ILE:N	13	0.19
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	16	0.19
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	16	0.19
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	16	0.19
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	16	0.19
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	16	0.19
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	16	0.19
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	16	0.19
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	16	0.19
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	16	0.19
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	16	0.19
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	16	0.19
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	16	0.19
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	16	0.19
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	16	0.19
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	16	0.19
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	16	0.19
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	16	0.19
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	16	0.19
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	11	0.19
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	11	0.19
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	11	0.19
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE1	7	0.19
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE2	7	0.19
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE1	7	0.19
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE2	7	0.19
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE1	7	0.19
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE2	7	0.19
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	2	0.19
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	2	0.19
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	6	0.19
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	6	0.19
(1,1009)	1:149:A:LEU:HD11	1:160:A:TRP:HE1	2	0.19
(1,1009)	1:149:A:LEU:HD12	1:160:A:TRP:HE1	2	0.19
(1,1009)	1:149:A:LEU:HD13	1:160:A:TRP:HE1	2	0.19
(1,1009)	1:149:A:LEU:HD21	1:160:A:TRP:HE1	2	0.19
(1,1009)	1:149:A:LEU:HD22	1:160:A:TRP:HE1	2	0.19
(1,1009)	1:149:A:LEU:HD23	1:160:A:TRP:HE1	2	0.19
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	7	0.19
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	7	0.19
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	9	0.19
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	9	0.19
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	2	0.19
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	2	0.19
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	2	0.19
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	2	0.19
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	2	0.19
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	2	0.19
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	2	0.19
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	2	0.19
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	2	0.19
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	2	0.19
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	2	0.19
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	2	0.19
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	3	0.19
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	3	0.19
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	3	0.19
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	3	0.19
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	3	0.19
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	3	0.19
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	3	0.19
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	3	0.19
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	3	0.19
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	3	0.19
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	3	0.19
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	14	0.19
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	14	0.19
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	18	0.19
(1,922)	1:112:A:LEU:HB2	1:183:A:PHE:HE1	6	0.19
(1,922)	1:112:A:LEU:HB2	1:183:A:PHE:HE2	6	0.19
(1,922)	1:112:A:LEU:HB3	1:183:A:PHE:HE1	6	0.19
(1,922)	1:112:A:LEU:HB3	1:183:A:PHE:HE2	6	0.19
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD1	17	0.19
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD2	17	0.19
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD1	17	0.19
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD2	17	0.19
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD1	17	0.19
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD2	17	0.19
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	5	0.19
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	5	0.19
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	5	0.19
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	5	0.19
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	5	0.19
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	5	0.19
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	5	0.19
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	5	0.19
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	5	0.19
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	12	0.19
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	12	0.19
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	12	0.19
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	12	0.19
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	12	0.19
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	12	0.19
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	6	0.19
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	6	0.19
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	6	0.19
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	6	0.19
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	6	0.19
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	6	0.19
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	6	0.19
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	6	0.19
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	6	0.19
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	6	0.19
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	6	0.19
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	11	0.19
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	11	0.19
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	11	0.19
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	11	0.19
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	11	0.19
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	11	0.19
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	11	0.19
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	11	0.19
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	11	0.19
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	11	0.19
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	11	0.19
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	11	0.19
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB2	3	0.19
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB3	3	0.19
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	11	0.19
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	11	0.19
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	11	0.19
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	11	0.19
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	11	0.19
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	11	0.19
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	11	0.19
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	11	0.19
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	11	0.19
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	11	0.19
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	11	0.19
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	11	0.19
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	18	0.19
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	18	0.19
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	18	0.19
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	18	0.19
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	18	0.19
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	18	0.19
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	18	0.19
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	18	0.19
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	18	0.19
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	18	0.19
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	18	0.19
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	18	0.19
(1,813)	1:76:A:ILE:HG13	1:87:A:TRP:HE3	14	0.19
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	5	0.19
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	15	0.19
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	15	0.19
(1,781)	1:70:A:LEU:HG	1:94:A:ILE:HG13	13	0.19
(1,778)	1:70:A:LEU:HD13	1:94:A:ILE:HG13	13	0.19
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	5	0.19
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	5	0.19
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	5	0.19
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	5	0.19
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	5	0.19
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	5	0.19
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	5	0.19
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	5	0.19
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	5	0.19
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	5	0.19
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	5	0.19
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	5	0.19
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	5	0.19
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	5	0.19
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	5	0.19
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	5	0.19
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	5	0.19
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	5	0.19
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	13	0.19
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	13	0.19
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	13	0.19
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	13	0.19
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	13	0.19
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	13	0.19
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	13	0.19
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	13	0.19
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	13	0.19
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	13	0.19
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	13	0.19
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	13	0.19
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	13	0.19
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	13	0.19
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	13	0.19
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	13	0.19
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	13	0.19
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	13	0.19
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	14	0.19
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	14	0.19
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	14	0.19
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	14	0.19
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	14	0.19
(1,749)	1:58:A:ASP:HB3	1:69:A:ILE:HG13	9	0.19
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	6	0.19
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	10	0.19
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	8	0.19
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	19	0.19
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	16	0.19
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	16	0.19
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	16	0.19
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	1	0.19
(1,670)	1:100:A:ILE:HD11	1:143:A:ARG:H	15	0.19
(1,670)	1:100:A:ILE:HD12	1:143:A:ARG:H	15	0.19
(1,670)	1:100:A:ILE:HD13	1:143:A:ARG:H	15	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD11	10	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD12	10	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD13	10	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD21	10	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD22	10	0.19
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD23	10	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD11	10	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD12	10	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD13	10	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD21	10	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD22	10	0.19
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD23	10	0.19
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	8	0.19
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	8	0.19
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	6	0.19
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	6	0.19
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	6	0.19
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	6	0.19
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	6	0.19
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	6	0.19
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	2	0.19
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	3	0.19
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	5	0.19
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	12	0.19
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	17	0.19
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	17	0.19
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	8	0.19
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	6	0.19
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	17	0.19
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	20	0.19
(1,552)	1:151:A:GLU:HG2	1:153:A:THR:H	7	0.19
(1,552)	1:151:A:GLU:HG3	1:153:A:THR:H	7	0.19
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB2	13	0.19
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB3	13	0.19
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	4	0.19
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	4	0.19
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	4	0.19
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	15	0.19
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	15	0.19
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	15	0.19
(1,316)	1:124:A:LEU:HG	1:125:A:LEU:H	18	0.19
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	4	0.19
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	4	0.19
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	6	0.19
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	6	0.19
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	7	0.19
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	7	0.19
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	8	0.19
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	8	0.19
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	16	0.19
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	16	0.19
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	19	0.19
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	19	0.19
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	17	0.19
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	17	0.19
(1,265)	1:86:A:GLU:HB2	1:87:A:TRP:H	11	0.19
(1,265)	1:86:A:GLU:HB3	1:87:A:TRP:H	11	0.19
(1,261)	1:83:A:ASP:HB3	1:84:A:SER:H	6	0.19
(1,261)	1:83:A:ASP:HB3	1:84:A:SER:H	8	0.19
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	4	0.19
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	4	0.19
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	11	0.19
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	11	0.19
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	14	0.19
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	14	0.19
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	16	0.19
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	17	0.19
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	17	0.19
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	2	0.18
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	8	0.18
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	14	0.18
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	18	0.18
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	2	0.18
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	5	0.18
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	8	0.18
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	15	0.18
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	16	0.18
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	20	0.18
(2,45)	1:96:A:THR:O	1:100:A:ILE:H	5	0.18
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	13	0.18
(2,12)	1:70:A:LEU:O	1:74:A:ILE:N	2	0.18
(2,11)	1:70:A:LEU:O	1:74:A:ILE:H	10	0.18
(2,11)	1:70:A:LEU:O	1:74:A:ILE:H	19	0.18
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE1	10	0.18
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE2	10	0.18
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE1	10	0.18
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE2	10	0.18
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE1	10	0.18
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE2	10	0.18
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE1	10	0.18
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE2	10	0.18
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE1	10	0.18
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE2	10	0.18
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE1	10	0.18
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE2	10	0.18
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	3	0.18
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	3	0.18
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	3	0.18
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	3	0.18
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	3	0.18
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	3	0.18
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	3	0.18
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	3	0.18
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	3	0.18
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	3	0.18
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	3	0.18
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	3	0.18
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	3	0.18
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	3	0.18
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	3	0.18
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	3	0.18
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	3	0.18
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	4	0.18
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	4	0.18
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	4	0.18
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	4	0.18
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	4	0.18
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	4	0.18
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	4	0.18
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	4	0.18
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	4	0.18
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	4	0.18
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	4	0.18
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	4	0.18
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	4	0.18
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	4	0.18
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	4	0.18
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	4	0.18
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	4	0.18
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	4	0.18
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD11	17	0.18
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD12	17	0.18
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD13	17	0.18
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD11	17	0.18
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD12	17	0.18
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD13	17	0.18
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD11	17	0.18
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD12	17	0.18
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD13	17	0.18
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD11	17	0.18
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD12	17	0.18
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD13	17	0.18
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD11	17	0.18
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD12	17	0.18
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD13	17	0.18
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD11	17	0.18
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD12	17	0.18
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD13	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD11	14	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD12	14	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD13	14	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD21	14	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD22	14	0.18
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD23	14	0.18
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	15	0.18
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	15	0.18
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	15	0.18
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	15	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	13	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	13	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	13	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	13	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	13	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	13	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	13	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	13	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	13	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	13	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	13	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	13	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	17	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	17	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	17	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	17	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	17	0.18
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	17	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	17	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	17	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	17	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	17	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	17	0.18
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	17	0.18
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	10	0.18
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	10	0.18
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	9	0.18
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	9	0.18
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	7	0.18
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	7	0.18
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	3	0.18
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	3	0.18
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	3	0.18
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	3	0.18
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	3	0.18
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	3	0.18
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	3	0.18
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	3	0.18
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	3	0.18
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	3	0.18
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	3	0.18
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	5	0.18
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	5	0.18
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	5	0.18
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	5	0.18
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	5	0.18
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	5	0.18
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	5	0.18
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	5	0.18
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	5	0.18
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	5	0.18
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	5	0.18
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	5	0.18
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	14	0.18
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	14	0.18
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	14	0.18
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	14	0.18
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	14	0.18
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	14	0.18
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	14	0.18
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	14	0.18
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	14	0.18
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	14	0.18
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	14	0.18
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	14	0.18
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	1	0.18
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	7	0.18
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	15	0.18
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	12	0.18
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	6	0.18
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	16	0.18
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	17	0.18
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	2	0.18
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	3	0.18
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	11	0.18
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	4	0.18
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	4	0.18
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	4	0.18
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	4	0.18
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	4	0.18
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	4	0.18
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	7	0.18
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	7	0.18
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	7	0.18
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	7	0.18
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	7	0.18
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	7	0.18
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD1	14	0.18
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD2	14	0.18
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD1	14	0.18
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD2	14	0.18
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD1	14	0.18
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD2	14	0.18
(1,941)	1:120:A:GLU:HG2	1:183:A:PHE:HB2	11	0.18
(1,941)	1:120:A:GLU:HG2	1:183:A:PHE:HB3	11	0.18
(1,941)	1:120:A:GLU:HG3	1:183:A:PHE:HB2	11	0.18
(1,941)	1:120:A:GLU:HG3	1:183:A:PHE:HB3	11	0.18
(1,940)	1:117:A:PHE:HD1	1:183:A:PHE:HE1	18	0.18
(1,940)	1:117:A:PHE:HD1	1:183:A:PHE:HE2	18	0.18
(1,940)	1:117:A:PHE:HD2	1:183:A:PHE:HE1	18	0.18
(1,940)	1:117:A:PHE:HD2	1:183:A:PHE:HE2	18	0.18
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD1	1	0.18
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD2	1	0.18
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD1	1	0.18
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD2	1	0.18
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD1	1	0.18
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD2	1	0.18
(1,902)	1:111:A:ILE:HD13	1:155:A:ILE:HG13	16	0.18
(1,894)	1:109:A:ARG:HG2	1:127:A:VAL:HB	11	0.18
(1,894)	1:109:A:ARG:HG3	1:127:A:VAL:HB	11	0.18
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	4	0.18
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	4	0.18
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	16	0.18
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	12	0.18
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	12	0.18
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	12	0.18
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	12	0.18
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	12	0.18
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	12	0.18
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	17	0.18
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	17	0.18
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	17	0.18
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	17	0.18
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	17	0.18
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	17	0.18
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	13	0.18
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	16	0.18
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	16	0.18
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	16	0.18
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	16	0.18
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	16	0.18
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	16	0.18
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	16	0.18
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	16	0.18
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	16	0.18
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	16	0.18
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	16	0.18
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	16	0.18
(1,822)	1:76:A:ILE:HG23	1:90:A:LEU:HD13	3	0.18
(1,816)	1:76:A:ILE:HD11	1:87:A:TRP:HD1	19	0.18
(1,816)	1:76:A:ILE:HD12	1:87:A:TRP:HD1	19	0.18
(1,816)	1:76:A:ILE:HD13	1:87:A:TRP:HD1	19	0.18
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB2	15	0.18
(1,812)	1:74:A:ILE:HB	1:87:A:TRP:HB3	15	0.18
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	16	0.18
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	10	0.18
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	10	0.18
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	11	0.18
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	11	0.18
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	13	0.18
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	13	0.18
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB2	12	0.18
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB3	12	0.18
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB2	12	0.18
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB3	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	10	0.18
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	10	0.18
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	10	0.18
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	10	0.18
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	8	0.18
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	8	0.18
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	8	0.18
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	8	0.18
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	8	0.18
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	8	0.18
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	8	0.18
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	8	0.18
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	8	0.18
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	8	0.18
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	8	0.18
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	8	0.18
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	8	0.18
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	8	0.18
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	8	0.18
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	8	0.18
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	8	0.18
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	8	0.18
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	8	0.18
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	6	0.18
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	10	0.18
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	12	0.18
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	13	0.18
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	14	0.18
(1,708)	1:125:A:LEU:H	1:146:A:LEU:HA	2	0.18
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	16	0.18
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	20	0.18
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	20	0.18
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	4	0.18
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	12	0.18
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	15	0.18
(1,670)	1:100:A:ILE:HD11	1:143:A:ARG:H	5	0.18
(1,670)	1:100:A:ILE:HD12	1:143:A:ARG:H	5	0.18
(1,670)	1:100:A:ILE:HD13	1:143:A:ARG:H	5	0.18
(1,664)	1:97:A:LEU:HB2	1:140:A:ARG:H	10	0.18
(1,664)	1:97:A:LEU:HB3	1:140:A:ARG:H	10	0.18
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	10	0.18
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	10	0.18
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	13	0.18
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	13	0.18
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	9	0.18
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	9	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD11	8	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD12	8	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD13	8	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD21	8	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD22	8	0.18
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD23	8	0.18
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	8	0.18
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	8	0.18
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	8	0.18
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	8	0.18
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	8	0.18
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	8	0.18
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	8	0.18
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	8	0.18
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	8	0.18
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	8	0.18
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	8	0.18
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	8	0.18
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE1	14	0.18
(1,593)	1:112:A:LEU:HB2	1:117:A:PHE:HE2	14	0.18
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE1	14	0.18
(1,593)	1:112:A:LEU:HB3	1:117:A:PHE:HE2	14	0.18
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	6	0.18
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	6	0.18
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB2	1	0.18
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB3	1	0.18
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB2	1	0.18
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB3	1	0.18
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB2	1	0.18
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB3	1	0.18
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB2	1	0.18
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB3	1	0.18
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB2	1	0.18
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB3	1	0.18
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB2	1	0.18
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB3	1	0.18
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB2	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB3	2	0.18
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB2	2	0.18
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB3	2	0.18
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB2	2	0.18
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB3	2	0.18
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB2	2	0.18
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB3	2	0.18
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB2	2	0.18
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB3	2	0.18
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB2	2	0.18
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB3	2	0.18
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	12	0.18
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	12	0.18
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	12	0.18
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	12	0.18
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	12	0.18
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	12	0.18
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	18	0.18
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	6	0.18
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	19	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	9	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	9	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	9	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	18	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	18	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	18	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	20	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	20	0.18
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	20	0.18
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	7	0.18
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	1	0.18
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	10	0.18
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	13	0.18
(1,540)	1:115:A:LEU:HD11	1:118:A:GLN:H	10	0.18
(1,540)	1:115:A:LEU:HD12	1:118:A:GLN:H	10	0.18
(1,540)	1:115:A:LEU:HD13	1:118:A:GLN:H	10	0.18
(1,540)	1:115:A:LEU:HD21	1:118:A:GLN:H	10	0.18
(1,540)	1:115:A:LEU:HD22	1:118:A:GLN:H	10	0.18
(1,540)	1:115:A:LEU:HD23	1:118:A:GLN:H	10	0.18
(1,540)	1:115:A:LEU:HD11	1:118:A:GLN:H	14	0.18
(1,540)	1:115:A:LEU:HD12	1:118:A:GLN:H	14	0.18
(1,540)	1:115:A:LEU:HD13	1:118:A:GLN:H	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:115:A:LEU:HD21	1:118:A:GLN:H	14	0.18
(1,540)	1:115:A:LEU:HD22	1:118:A:GLN:H	14	0.18
(1,540)	1:115:A:LEU:HD23	1:118:A:GLN:H	14	0.18
(1,540)	1:115:A:LEU:HD11	1:118:A:GLN:H	19	0.18
(1,540)	1:115:A:LEU:HD12	1:118:A:GLN:H	19	0.18
(1,540)	1:115:A:LEU:HD13	1:118:A:GLN:H	19	0.18
(1,540)	1:115:A:LEU:HD21	1:118:A:GLN:H	19	0.18
(1,540)	1:115:A:LEU:HD22	1:118:A:GLN:H	19	0.18
(1,540)	1:115:A:LEU:HD23	1:118:A:GLN:H	19	0.18
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	9	0.18
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	13	0.18
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	17	0.18
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB2	11	0.18
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB3	11	0.18
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	12	0.18
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	12	0.18
(1,316)	1:124:A:LEU:HG	1:125:A:LEU:H	6	0.18
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	3	0.18
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	3	0.18
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	9	0.18
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	9	0.18
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB2	2	0.18
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB3	2	0.18
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB2	2	0.18
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB3	2	0.18
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	16	0.18
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	16	0.18
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	1	0.18
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	1	0.18
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	6	0.18
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	6	0.18
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	12	0.18
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	12	0.18
(1,261)	1:83:A:ASP:HB3	1:84:A:SER:H	16	0.18
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	13	0.18
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	13	0.18
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	18	0.18
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	18	0.18
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	19	0.18
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	19	0.18
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	20	0.18
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	9	0.18
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	12	0.18
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	16	0.18
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	14	0.18
(2,127)	1:185:A:ILE:O	1:189:A:MET:H	19	0.17
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	10	0.17
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	17	0.17
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	1	0.17
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	5	0.17
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	12	0.17
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	13	0.17
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	4	0.17
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	18	0.17
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	19	0.17
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	3	0.17
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	10	0.17
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	18	0.17
(2,45)	1:96:A:THR:O	1:100:A:ILE:H	10	0.17
(2,17)	1:73:A:LEU:O	1:77:A:ARG:H	14	0.17
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	19	0.17
(2,11)	1:70:A:LEU:O	1:74:A:ILE:H	1	0.17
(2,11)	1:70:A:LEU:O	1:74:A:ILE:H	18	0.17
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB2	1	0.17
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB3	1	0.17
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB2	1	0.17
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB3	1	0.17
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB2	1	0.17
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB3	1	0.17
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB2	1	0.17
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB3	1	0.17
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB2	1	0.17
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB3	1	0.17
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB2	1	0.17
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB3	1	0.17
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE1	4	0.17
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE2	4	0.17
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE1	4	0.17
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE2	4	0.17
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE1	4	0.17
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE2	4	0.17
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	17	0.17
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	16	0.17
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	16	0.17
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	14	0.17
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	18	0.17
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	9	0.17
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	17	0.17
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	1	0.17
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	5	0.17
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	5	0.17
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	7	0.17
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	7	0.17
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	9	0.17
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	9	0.17
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	9	0.17
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	9	0.17
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	9	0.17
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	9	0.17
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	9	0.17
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	9	0.17
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	9	0.17
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	9	0.17
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	9	0.17
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	9	0.17
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	18	0.17
(1,934)	1:117:A:PHE:HE1	1:182:A:PHE:HE1	1	0.17
(1,934)	1:117:A:PHE:HE1	1:182:A:PHE:HE2	1	0.17
(1,934)	1:117:A:PHE:HE2	1:182:A:PHE:HE1	1	0.17
(1,934)	1:117:A:PHE:HE2	1:182:A:PHE:HE2	1	0.17
(1,930)	1:112:A:LEU:HA	1:118:A:GLN:HG2	7	0.17
(1,930)	1:112:A:LEU:HA	1:118:A:GLN:HG3	7	0.17
(1,904)	1:111:A:ILE:HG21	1:182:A:PHE:HD2	2	0.17
(1,903)	1:111:A:ILE:HG21	1:155:A:ILE:HG13	11	0.17
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	7	0.17
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	7	0.17
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	7	0.17
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	7	0.17
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	7	0.17
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	7	0.17
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	13	0.17
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	13	0.17
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG2	5	0.17
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG3	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG2	5	0.17
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG3	5	0.17
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG2	5	0.17
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG3	5	0.17
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG2	5	0.17
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG3	5	0.17
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG2	5	0.17
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG3	5	0.17
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG2	5	0.17
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG3	5	0.17
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	10	0.17
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	10	0.17
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	10	0.17
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	10	0.17
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	10	0.17
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	10	0.17
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	10	0.17
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	10	0.17
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	10	0.17
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	10	0.17
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	10	0.17
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	10	0.17
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	10	0.17
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	10	0.17
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	10	0.17
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	10	0.17
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	10	0.17
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	10	0.17
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	10	0.17
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	10	0.17
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	10	0.17
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	10	0.17
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	10	0.17
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	10	0.17
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	10	0.17
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	10	0.17
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	10	0.17
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	10	0.17
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	10	0.17
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	10	0.17
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	10	0.17
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	10	0.17
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	10	0.17
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	10	0.17
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	10	0.17
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG2	18	0.17
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG3	18	0.17
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG2	18	0.17
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG3	18	0.17
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG2	18	0.17
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG3	18	0.17
(1,847)	1:100:A:ILE:HG13	1:143:A:ARG:HA	14	0.17
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB2	10	0.17
(1,827)	1:97:A:LEU:HD11	1:143:A:ARG:HB3	10	0.17
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB2	10	0.17
(1,827)	1:97:A:LEU:HD12	1:143:A:ARG:HB3	10	0.17
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB2	10	0.17
(1,827)	1:97:A:LEU:HD13	1:143:A:ARG:HB3	10	0.17
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB2	10	0.17
(1,827)	1:97:A:LEU:HD21	1:143:A:ARG:HB3	10	0.17
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB2	10	0.17
(1,827)	1:97:A:LEU:HD22	1:143:A:ARG:HB3	10	0.17
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB2	10	0.17
(1,827)	1:97:A:LEU:HD23	1:143:A:ARG:HB3	10	0.17
(1,808)	1:74:A:ILE:HG12	1:90:A:LEU:HG	14	0.17
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	16	0.17
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	16	0.17
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	17	0.17
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	17	0.17
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	9	0.17
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	9	0.17
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	9	0.17
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	9	0.17
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	19	0.17
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	19	0.17
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	19	0.17
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	19	0.17
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	1	0.17
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	1	0.17
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	1	0.17
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	1	0.17
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	1	0.17
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	1	0.17
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	1	0.17
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	1	0.17
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	1	0.17
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	1	0.17
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	1	0.17
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	1	0.17
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	1	0.17
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	1	0.17
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	1	0.17
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	1	0.17
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	1	0.17
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	5	0.17
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	5	0.17
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	5	0.17
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	5	0.17
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	5	0.17
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	5	0.17
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	11	0.17
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	11	0.17
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	11	0.17
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	11	0.17
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	11	0.17
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	11	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD11	19	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD12	19	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD13	19	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD21	19	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD22	19	0.17
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD23	19	0.17
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	1	0.17
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	5	0.17
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	13	0.17
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	15	0.17
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	16	0.17
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	1	0.17
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	12	0.17
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	12	0.17
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	4	0.17
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	4	0.17
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	4	0.17
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	8	0.17
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	8	0.17
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	11	0.17
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	11	0.17
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	11	0.17
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	6	0.17
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	6	0.17
(1,660)	1:95:A:TYR:HB2	1:139:A:THR:H	14	0.17
(1,660)	1:95:A:TYR:HB3	1:139:A:THR:H	14	0.17
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	1	0.17
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	1	0.17
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	5	0.17
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	5	0.17
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	11	0.17
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	11	0.17
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	7	0.17
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	7	0.17
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	8	0.17
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	8	0.17
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	8	0.17
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	8	0.17
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	8	0.17
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	8	0.17
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	8	0.17
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	8	0.17
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	8	0.17
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	8	0.17
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	8	0.17
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	8	0.17
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	8	0.17
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	8	0.17
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	8	0.17
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	8	0.17
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	8	0.17
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	8	0.17
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	8	0.17
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	8	0.17
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	8	0.17
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	8	0.17
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	8	0.17
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	8	0.17
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	8	0.17
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	8	0.17
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	8	0.17
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	8	0.17
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	8	0.17
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	8	0.17
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	8	0.17
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	8	0.17
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	8	0.17
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	8	0.17
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	8	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	3	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	3	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	3	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	3	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	3	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	3	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	3	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	3	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	3	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	3	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	3	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	3	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	12	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	12	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	12	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	12	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	12	0.17
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	12	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	12	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	12	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	12	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	12	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	12	0.17
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	12	0.17
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB2	19	0.17
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB3	19	0.17
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB2	19	0.17
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB3	19	0.17
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB2	19	0.17
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB3	19	0.17
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB2	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB3	19	0.17
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB2	19	0.17
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB3	19	0.17
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB2	19	0.17
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB3	19	0.17
(1,588)	1:80:A:GLN:HB2	1:84:A:SER:HG	9	0.17
(1,588)	1:80:A:GLN:HB3	1:84:A:SER:HG	9	0.17
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	5	0.17
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	5	0.17
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	5	0.17
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	5	0.17
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	5	0.17
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	5	0.17
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	19	0.17
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	4	0.17
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	8	0.17
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	6	0.17
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	6	0.17
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	6	0.17
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	6	0.17
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	11	0.17
(1,517)	1:182:A:PHE:HA	1:185:A:ILE:HB	6	0.17
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	8	0.17
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	8	0.17
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	17	0.17
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	17	0.17
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	1	0.17
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	1	0.17
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	6	0.17
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	6	0.17
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	7	0.17
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	7	0.17
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	10	0.17
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	10	0.17
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	15	0.17
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	15	0.17
(1,226)	1:205:A:LYS:HA	1:206:A:LEU:H	10	0.17
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	6	0.17
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	19	0.17
(3,85)	1:154:A:SER:H	1:198:A:CYS:O	12	0.16
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	1	0.16
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	9	0.16
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	9	0.16
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	2	0.16
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	4	0.16
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	8	0.16
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	15	0.16
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	1	0.16
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	5	0.16
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	11	0.16
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	14	0.16
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	4	0.16
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	8	0.16
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	14	0.16
(2,45)	1:96:A:THR:O	1:100:A:ILE:H	2	0.16
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	1	0.16
(2,11)	1:70:A:LEU:O	1:74:A:ILE:H	15	0.16
(2,9)	1:69:A:ILE:O	1:73:A:LEU:H	13	0.16
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	4	0.16
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	12	0.16
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	15	0.16
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	2	0.16
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	2	0.16
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	2	0.16
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	2	0.16
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	2	0.16
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	2	0.16
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	2	0.16
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	2	0.16
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	2	0.16
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	2	0.16
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	2	0.16
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	2	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	5	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	5	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	5	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	5	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	5	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	5	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	5	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	5	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	5	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	5	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	5	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	5	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	5	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	5	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	5	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	5	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	5	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	8	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	8	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	8	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	8	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	8	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	8	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	8	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	8	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	8	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	8	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	8	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	8	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	8	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	8	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	8	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	8	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	8	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	8	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	19	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	19	0.16
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	19	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	19	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	19	0.16
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	19	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	19	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	19	0.16
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	19	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	19	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	19	0.16
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	19	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	19	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	19	0.16
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	19	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	19	0.16
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	19	0.16
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB1	17	0.16
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB2	17	0.16
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB3	17	0.16
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB1	17	0.16
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB2	17	0.16
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB3	17	0.16
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB1	17	0.16
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB2	17	0.16
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB3	17	0.16
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB1	17	0.16
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB2	17	0.16
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB3	17	0.16
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB1	17	0.16
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB2	17	0.16
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB3	17	0.16
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB1	17	0.16
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB2	17	0.16
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB3	17	0.16
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	4	0.16
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	4	0.16
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	4	0.16
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	4	0.16
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	14	0.16
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	14	0.16
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	14	0.16
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	14	0.16
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD11	2	0.16
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD12	2	0.16
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD13	2	0.16
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD21	2	0.16
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD22	2	0.16
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD23	2	0.16
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD11	2	0.16
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD12	2	0.16
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD13	2	0.16
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD21	2	0.16
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD22	2	0.16
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD23	2	0.16
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	10	0.16
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	10	0.16
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	10	0.16
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	10	0.16
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	10	0.16
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	10	0.16
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	10	0.16
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	10	0.16
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	10	0.16
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	10	0.16
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	10	0.16
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	5	0.16
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	5	0.16
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	7	0.16
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	7	0.16
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	15	0.16
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	15	0.16
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	11	0.16
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	11	0.16
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	20	0.16
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	20	0.16
(1,1009)	1:149:A:LEU:HD11	1:160:A:TRP:HE1	19	0.16
(1,1009)	1:149:A:LEU:HD12	1:160:A:TRP:HE1	19	0.16
(1,1009)	1:149:A:LEU:HD13	1:160:A:TRP:HE1	19	0.16
(1,1009)	1:149:A:LEU:HD21	1:160:A:TRP:HE1	19	0.16
(1,1009)	1:149:A:LEU:HD22	1:160:A:TRP:HE1	19	0.16
(1,1009)	1:149:A:LEU:HD23	1:160:A:TRP:HE1	19	0.16
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	15	0.16
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	15	0.16
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	12	0.16
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	12	0.16
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	12	0.16
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	12	0.16
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	12	0.16
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	12	0.16
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	12	0.16
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	12	0.16
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	12	0.16
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	12	0.16
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	12	0.16
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	12	0.16
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB2	4	0.16
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB2	4	0.16
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB3	4	0.16
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB2	4	0.16
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB3	4	0.16
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB2	4	0.16
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB3	4	0.16
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB2	4	0.16
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB3	4	0.16
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB2	4	0.16
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB3	4	0.16
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB2	8	0.16
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB3	8	0.16
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB2	8	0.16
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB3	8	0.16
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB2	8	0.16
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB3	8	0.16
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB2	8	0.16
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB3	8	0.16
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB2	8	0.16
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB3	8	0.16
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB2	8	0.16
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB3	8	0.16
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	12	0.16
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	12	0.16
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	16	0.16
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	9	0.16
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	11	0.16
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	17	0.16
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	20	0.16
(1,976)	1:124:A:LEU:HG	1:152:A:GLU:HG2	6	0.16
(1,976)	1:124:A:LEU:HG	1:152:A:GLU:HG3	6	0.16
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	20	0.16
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	20	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD11	14	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD12	14	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD13	14	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD21	14	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD22	14	0.16
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD23	14	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD11	14	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD12	14	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD13	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD21	14	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD22	14	0.16
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD23	14	0.16
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	5	0.16
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	11	0.16
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	11	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	9	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	9	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	9	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	9	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	9	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	9	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	9	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	9	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	9	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	10	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	10	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	10	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	10	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	10	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	10	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	10	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	10	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	10	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	14	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	14	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	14	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	14	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	14	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	14	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	14	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	14	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	14	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	20	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	20	0.16
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	20	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	20	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	20	0.16
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	20	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	20	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	20	0.16
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	10	0.16
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	10	0.16
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	10	0.16
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	10	0.16
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	10	0.16
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	10	0.16
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	15	0.16
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	15	0.16
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	15	0.16
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	15	0.16
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	15	0.16
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	15	0.16
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB2	17	0.16
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB3	17	0.16
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB2	17	0.16
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB3	17	0.16
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB2	17	0.16
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB3	17	0.16
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB2	20	0.16
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB3	20	0.16
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB2	20	0.16
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB3	20	0.16
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB2	20	0.16
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB3	20	0.16
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	6	0.16
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	6	0.16
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	6	0.16
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	6	0.16
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	6	0.16
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	6	0.16
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	6	0.16
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	6	0.16
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	6	0.16
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	5	0.16
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	5	0.16
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	7	0.16
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	7	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG11	11	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG12	11	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG13	11	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG21	11	0.16
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG22	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG23	11	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG11	11	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG12	11	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG13	11	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG21	11	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG22	11	0.16
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG23	11	0.16
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	14	0.16
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	14	0.16
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG2	13	0.16
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG3	13	0.16
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG2	13	0.16
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG3	13	0.16
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG2	13	0.16
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG3	13	0.16
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	7	0.16
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	14	0.16
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB2	7	0.16
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB3	7	0.16
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	7	0.16
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	7	0.16
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	7	0.16
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	7	0.16
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	16	0.16
(1,793)	1:73:A:LEU:HD11	1:90:A:LEU:HG	1	0.16
(1,793)	1:73:A:LEU:HD12	1:90:A:LEU:HG	1	0.16
(1,793)	1:73:A:LEU:HD13	1:90:A:LEU:HG	1	0.16
(1,793)	1:73:A:LEU:HD21	1:90:A:LEU:HG	1	0.16
(1,793)	1:73:A:LEU:HD22	1:90:A:LEU:HG	1	0.16
(1,793)	1:73:A:LEU:HD23	1:90:A:LEU:HG	1	0.16
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	6	0.16
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	6	0.16
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	12	0.16
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	12	0.16
(1,779)	1:70:A:LEU:HD11	1:94:A:ILE:HB	13	0.16
(1,779)	1:70:A:LEU:HD12	1:94:A:ILE:HB	13	0.16
(1,779)	1:70:A:LEU:HD13	1:94:A:ILE:HB	13	0.16
(1,779)	1:70:A:LEU:HD21	1:94:A:ILE:HB	13	0.16
(1,779)	1:70:A:LEU:HD22	1:94:A:ILE:HB	13	0.16
(1,779)	1:70:A:LEU:HD23	1:94:A:ILE:HB	13	0.16
(1,775)	1:70:A:LEU:HG	1:90:A:LEU:HB2	2	0.16
(1,775)	1:70:A:LEU:HG	1:90:A:LEU:HB3	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:61:A:HIS:HB3	1:69:A:ILE:HG13	18	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	4	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	4	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	4	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	4	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	4	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	4	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	8	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	8	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	8	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	8	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	8	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	8	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	17	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	17	0.16
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	17	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	17	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	17	0.16
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	17	0.16
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	2	0.16
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	4	0.16
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	11	0.16
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	18	0.16
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	20	0.16
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD11	19	0.16
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD12	19	0.16
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD13	19	0.16
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD21	19	0.16
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD22	19	0.16
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD23	19	0.16
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG2	7	0.16
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG3	7	0.16
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB2	18	0.16
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB3	18	0.16
(1,692)	1:121:A:ALA:H	1:155:A:ILE:HG12	11	0.16
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	9	0.16
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	9	0.16
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	12	0.16
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	12	0.16
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	12	0.16
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	18	0.16
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	18	0.16
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	5	0.16
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	10	0.16
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	20	0.16
(1,670)	1:100:A:ILE:HD11	1:143:A:ARG:H	10	0.16
(1,670)	1:100:A:ILE:HD12	1:143:A:ARG:H	10	0.16
(1,670)	1:100:A:ILE:HD13	1:143:A:ARG:H	10	0.16
(1,667)	1:98:A:ARG:HB2	1:143:A:ARG:H	14	0.16
(1,667)	1:98:A:ARG:HB3	1:143:A:ARG:H	14	0.16
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	11	0.16
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	11	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB1	3	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB2	3	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB3	3	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB1	3	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB2	3	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB3	3	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB1	3	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB2	3	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB3	3	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB1	15	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB2	15	0.16
(1,633)	1:174:A:ILE:HD11	1:179:A:ALA:HB3	15	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB1	15	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB2	15	0.16
(1,633)	1:174:A:ILE:HD12	1:179:A:ALA:HB3	15	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB1	15	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB2	15	0.16
(1,633)	1:174:A:ILE:HD13	1:179:A:ALA:HB3	15	0.16
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	13	0.16
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	13	0.16
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	7	0.16
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	7	0.16
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	7	0.16
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	7	0.16
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	7	0.16
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	7	0.16
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	7	0.16
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	7	0.16
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	7	0.16
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	7	0.16
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	7	0.16
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	7	0.16
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	7	0.16
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	7	0.16
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	7	0.16
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	7	0.16
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	7	0.16
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	7	0.16
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	7	0.16
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	7	0.16
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	7	0.16
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	7	0.16
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	7	0.16
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	7	0.16
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	7	0.16
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	7	0.16
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	7	0.16
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	7	0.16
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	7	0.16
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	7	0.16
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	7	0.16
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	7	0.16
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	7	0.16
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	7	0.16
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	7	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	4	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	4	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	4	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	4	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	4	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	4	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	4	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	4	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	4	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	4	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	4	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	4	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	5	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	5	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	5	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	5	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	5	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	5	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	5	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	5	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	5	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	5	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	5	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	10	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	10	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	10	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	10	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	10	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	10	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	10	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	10	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	10	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	10	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	10	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	10	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	15	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	15	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	15	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	15	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	15	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	15	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	15	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	15	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	15	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	15	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	15	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	15	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	19	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	19	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	19	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	19	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	19	0.16
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	19	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	19	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	19	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	19	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	19	0.16
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	19	0.16
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	4	0.16
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	4	0.16
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	1	0.16
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	1	0.16
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	1	0.16
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	1	0.16
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	1	0.16
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	1	0.16
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	2	0.16
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	2	0.16
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	2	0.16
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	2	0.16
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	2	0.16
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	2	0.16
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	14	0.16
(1,574)	1:162:A:LEU:HD11	1:167:A:LEU:H	20	0.16
(1,574)	1:162:A:LEU:HD12	1:167:A:LEU:H	20	0.16
(1,574)	1:162:A:LEU:HD13	1:167:A:LEU:H	20	0.16
(1,574)	1:162:A:LEU:HD21	1:167:A:LEU:H	20	0.16
(1,574)	1:162:A:LEU:HD22	1:167:A:LEU:H	20	0.16
(1,574)	1:162:A:LEU:HD23	1:167:A:LEU:H	20	0.16
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	17	0.16
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	11	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	2	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	2	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	2	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	3	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	3	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	3	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	8	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	8	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	8	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	10	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	10	0.16
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	10	0.16
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	14	0.16
(1,551)	1:149:A:LEU:HD11	1:154:A:SER:HA	11	0.16
(1,551)	1:149:A:LEU:HD12	1:154:A:SER:HA	11	0.16
(1,551)	1:149:A:LEU:HD13	1:154:A:SER:HA	11	0.16
(1,551)	1:149:A:LEU:HD21	1:154:A:SER:HA	11	0.16
(1,551)	1:149:A:LEU:HD22	1:154:A:SER:HA	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:149:A:LEU:HD23	1:154:A:SER:HA	11	0.16
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	15	0.16
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	15	0.16
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	10	0.16
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG21	11	0.16
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG22	11	0.16
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG23	11	0.16
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	5	0.16
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	5	0.16
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	17	0.16
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	17	0.16
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	20	0.16
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	20	0.16
(1,330)	1:145:A:MET:HB2	1:146:A:LEU:H	2	0.16
(1,330)	1:145:A:MET:HB3	1:146:A:LEU:H	2	0.16
(1,316)	1:124:A:LEU:HG	1:125:A:LEU:H	20	0.16
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	4	0.16
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	4	0.16
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	17	0.16
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	17	0.16
(1,293)	1:110:A:ARG:HB2	1:111:A:ILE:H	9	0.16
(1,293)	1:110:A:ARG:HB3	1:111:A:ILE:H	9	0.16
(1,293)	1:110:A:ARG:HB2	1:111:A:ILE:H	17	0.16
(1,293)	1:110:A:ARG:HB3	1:111:A:ILE:H	17	0.16
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	2	0.16
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	2	0.16
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	5	0.16
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	5	0.16
(1,272)	1:90:A:LEU:HB2	1:91:A:ASN:H	10	0.16
(1,272)	1:90:A:LEU:HB3	1:91:A:ASN:H	10	0.16
(1,272)	1:90:A:LEU:HB2	1:91:A:ASN:H	18	0.16
(1,272)	1:90:A:LEU:HB3	1:91:A:ASN:H	18	0.16
(1,272)	1:90:A:LEU:HB2	1:91:A:ASN:H	19	0.16
(1,272)	1:90:A:LEU:HB3	1:91:A:ASN:H	19	0.16
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	10	0.16
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	10	0.16
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	5	0.16
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	5	0.16
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	13	0.16
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	6	0.16
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	11	0.16
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	14	0.16
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	9	0.16
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	11	0.16
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	15	0.16
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	5	0.15
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	15	0.15
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	2	0.15
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	10	0.15
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	14	0.15
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	7	0.15
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	10	0.15
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	14	0.15
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	20	0.15
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	13	0.15
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	3	0.15
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	7	0.15
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	5	0.15
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	17	0.15
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	18	0.15
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	3	0.15
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	18	0.15
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	6	0.15
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	9	0.15
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	3	0.15
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	18	0.15
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	6	0.15
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	13	0.15
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	1	0.15
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	8	0.15
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	9	0.15
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	11	0.15
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	12	0.15
(2,13)	1:71:A:TYR:O	1:75:A:VAL:H	2	0.15
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE1	15	0.15
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE2	15	0.15
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE1	15	0.15
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE2	15	0.15
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE1	15	0.15
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE2	15	0.15
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE1	15	0.15
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE2	15	0.15
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE1	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE2	15	0.15
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE1	15	0.15
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE2	15	0.15
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	20	0.15
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	20	0.15
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	20	0.15
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	20	0.15
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	20	0.15
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	20	0.15
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	20	0.15
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	20	0.15
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	20	0.15
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	20	0.15
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	20	0.15
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	20	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	6	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	6	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	6	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	6	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	6	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	6	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	6	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	6	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	6	0.15
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	6	0.15
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	6	0.15
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	6	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	6	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	6	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	6	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	6	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	6	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	6	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	11	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	11	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	11	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	11	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	11	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	11	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	11	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	11	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	11	0.15
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	11	0.15
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	11	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	11	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	11	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	11	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	11	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	11	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	11	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	18	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	18	0.15
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	18	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	18	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	18	0.15
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	18	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	18	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	18	0.15
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	18	0.15
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	18	0.15
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	18	0.15
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	18	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	18	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	18	0.15
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	18	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	18	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	18	0.15
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	18	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD11	6	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD12	6	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD13	6	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD11	6	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD12	6	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD13	6	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD11	6	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD12	6	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD13	6	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD11	6	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD12	6	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD13	6	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD11	6	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD12	6	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD13	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD11	6	0.15
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD12	6	0.15
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD13	6	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD11	12	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD12	12	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD13	12	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD11	12	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD12	12	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD13	12	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD11	12	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD12	12	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD13	12	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD11	12	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD12	12	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD13	12	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD11	12	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD12	12	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD13	12	0.15
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD11	12	0.15
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD12	12	0.15
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD13	12	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD11	13	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD12	13	0.15
(1,1091)	1:170:A:VAL:HG11	1:185:A:ILE:HD13	13	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD11	13	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD12	13	0.15
(1,1091)	1:170:A:VAL:HG12	1:185:A:ILE:HD13	13	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD11	13	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD12	13	0.15
(1,1091)	1:170:A:VAL:HG13	1:185:A:ILE:HD13	13	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD11	13	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD12	13	0.15
(1,1091)	1:170:A:VAL:HG21	1:185:A:ILE:HD13	13	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD11	13	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD12	13	0.15
(1,1091)	1:170:A:VAL:HG22	1:185:A:ILE:HD13	13	0.15
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD11	13	0.15
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD12	13	0.15
(1,1091)	1:170:A:VAL:HG23	1:185:A:ILE:HD13	13	0.15
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD11	3	0.15
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD12	3	0.15
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD13	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD21	3	0.15
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD22	3	0.15
(1,1085)	1:160:A:TRP:HE1	1:167:A:LEU:HD23	3	0.15
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG2	7	0.15
(1,1068)	1:157:A:PRO:HB2	1:189:A:MET:HG3	7	0.15
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG2	7	0.15
(1,1068)	1:157:A:PRO:HB3	1:189:A:MET:HG3	7	0.15
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	9	0.15
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	9	0.15
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	9	0.15
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	9	0.15
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	9	0.15
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	9	0.15
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	17	0.15
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	17	0.15
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	17	0.15
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	17	0.15
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	17	0.15
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	17	0.15
(1,1063)	1:156:A:PHE:HE1	1:170:A:VAL:HB	2	0.15
(1,1063)	1:156:A:PHE:HE2	1:170:A:VAL:HB	2	0.15
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD11	5	0.15
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD12	5	0.15
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD13	5	0.15
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD21	5	0.15
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD22	5	0.15
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD23	5	0.15
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD11	5	0.15
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD12	5	0.15
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD13	5	0.15
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD21	5	0.15
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD22	5	0.15
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD23	5	0.15
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE1	8	0.15
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE2	8	0.15
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE1	8	0.15
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE2	8	0.15
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE1	8	0.15
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE2	8	0.15
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	3	0.15
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	3	0.15
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	9	0.15
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	16	0.15
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	16	0.15
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	12	0.15
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	12	0.15
(1,1009)	1:149:A:LEU:HD11	1:160:A:TRP:HE1	5	0.15
(1,1009)	1:149:A:LEU:HD12	1:160:A:TRP:HE1	5	0.15
(1,1009)	1:149:A:LEU:HD13	1:160:A:TRP:HE1	5	0.15
(1,1009)	1:149:A:LEU:HD21	1:160:A:TRP:HE1	5	0.15
(1,1009)	1:149:A:LEU:HD22	1:160:A:TRP:HE1	5	0.15
(1,1009)	1:149:A:LEU:HD23	1:160:A:TRP:HE1	5	0.15
(1,1009)	1:149:A:LEU:HD11	1:160:A:TRP:HE1	18	0.15
(1,1009)	1:149:A:LEU:HD12	1:160:A:TRP:HE1	18	0.15
(1,1009)	1:149:A:LEU:HD13	1:160:A:TRP:HE1	18	0.15
(1,1009)	1:149:A:LEU:HD21	1:160:A:TRP:HE1	18	0.15
(1,1009)	1:149:A:LEU:HD22	1:160:A:TRP:HE1	18	0.15
(1,1009)	1:149:A:LEU:HD23	1:160:A:TRP:HE1	18	0.15
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	1	0.15
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	1	0.15
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	1	0.15
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	1	0.15
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	1	0.15
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	1	0.15
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	1	0.15
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	1	0.15
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	1	0.15
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	1	0.15
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	1	0.15
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	1	0.15
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB2	3	0.15
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB3	3	0.15
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB2	3	0.15
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB3	3	0.15
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB2	3	0.15
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB3	3	0.15
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB2	3	0.15
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB3	3	0.15
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB2	3	0.15
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB3	3	0.15
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB2	3	0.15
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB3	3	0.15
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB3	10	0.15
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB2	10	0.15
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB3	10	0.15
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB2	10	0.15
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB3	10	0.15
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB2	10	0.15
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB3	10	0.15
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB2	10	0.15
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB3	10	0.15
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB2	10	0.15
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB3	10	0.15
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	13	0.15
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	5	0.15
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	10	0.15
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	13	0.15
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	4	0.15
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	12	0.15
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	12	0.15
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	12	0.15
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	12	0.15
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	12	0.15
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	12	0.15
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	12	0.15
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	12	0.15
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	12	0.15
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	12	0.15
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	12	0.15
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	12	0.15
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	7	0.15
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	13	0.15
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	16	0.15
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	16	0.15
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	16	0.15
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	16	0.15
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	16	0.15
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	16	0.15
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	16	0.15
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	16	0.15
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	16	0.15
(1,935)	1:117:A:PHE:HE1	1:174:A:ILE:HB	2	0.15
(1,935)	1:117:A:PHE:HE2	1:174:A:ILE:HB	2	0.15
(1,935)	1:117:A:PHE:HE1	1:174:A:ILE:HB	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:117:A:PHE:HE2	1:174:A:ILE:HB	14	0.15
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB2	9	0.15
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB3	9	0.15
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB2	9	0.15
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB3	9	0.15
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB2	9	0.15
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB3	9	0.15
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD1	19	0.15
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD2	19	0.15
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD1	19	0.15
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD2	19	0.15
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD1	19	0.15
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD2	19	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	1	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	1	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	1	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	1	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	1	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	1	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	1	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	1	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	1	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	2	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	2	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	2	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	2	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	2	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	2	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	2	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	2	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	2	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	15	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	15	0.15
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	15	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	15	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	15	0.15
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	15	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	15	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	15	0.15
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	15	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	2	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	2	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	2	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	2	0.15
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	2	0.15
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	20	0.15
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	20	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	2	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	2	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	2	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	2	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	2	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	2	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	2	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	2	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	2	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	2	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	2	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	2	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	17	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	17	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	17	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	17	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	17	0.15
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	17	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	17	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	17	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	17	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	17	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	17	0.15
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	17	0.15
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	9	0.15
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	9	0.15
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG2	17	0.15
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG3	17	0.15
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG2	17	0.15
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG3	17	0.15
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG2	17	0.15
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG3	17	0.15
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD11	12	0.15
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD12	12	0.15
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD13	12	0.15
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD21	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD22	12	0.15
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD23	12	0.15
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD11	12	0.15
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD12	12	0.15
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD13	12	0.15
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD21	12	0.15
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD22	12	0.15
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD23	12	0.15
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD11	12	0.15
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD12	12	0.15
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD13	12	0.15
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD21	12	0.15
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD22	12	0.15
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD23	12	0.15
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	20	0.15
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	9	0.15
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	9	0.15
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	9	0.15
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	9	0.15
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	9	0.15
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	9	0.15
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	13	0.15
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	13	0.15
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	13	0.15
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	13	0.15
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	13	0.15
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	13	0.15
(1,822)	1:76:A:ILE:HG22	1:90:A:LEU:HD13	20	0.15
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	14	0.15
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	3	0.15
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	3	0.15
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	4	0.15
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	4	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	4	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	4	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	4	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	13	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	13	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	13	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	18	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	18	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	19	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	19	0.15
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	19	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	9	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	9	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	9	0.15
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	9	0.15
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	9	0.15
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	9	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	9	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	9	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	9	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	9	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	9	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	9	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	9	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	9	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	9	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	9	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	9	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	9	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	11	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	11	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	11	0.15
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	11	0.15
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	11	0.15
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	11	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	11	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	11	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	11	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	11	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	11	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	11	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	11	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	11	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	11	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	11	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	11	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	11	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	15	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	15	0.15
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	15	0.15
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	15	0.15
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	15	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	15	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	15	0.15
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	15	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	15	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	15	0.15
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	15	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	15	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	15	0.15
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	15	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	15	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	15	0.15
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	15	0.15
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	15	0.15
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	15	0.15
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	15	0.15
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	15	0.15
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	15	0.15
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	15	0.15
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	12	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD11	7	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD12	7	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD13	7	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD21	7	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD22	7	0.15
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD23	7	0.15
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	16	0.15
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	16	0.15
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	17	0.15
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	17	0.15
(1,675)	1:101:A:ARG:H	1:164:A:GLU:HG2	17	0.15
(1,675)	1:101:A:ARG:H	1:164:A:GLU:HG3	17	0.15
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	13	0.15
(1,660)	1:95:A:TYR:HB2	1:139:A:THR:H	17	0.15
(1,660)	1:95:A:TYR:HB3	1:139:A:THR:H	17	0.15
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	1	0.15
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	1	0.15
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	1	0.15
(1,605)	1:155:A:ILE:HG22	1:160:A:TRP:HE1	6	0.15
(1,605)	1:155:A:ILE:HG21	1:160:A:TRP:HE1	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:155:A:ILE:HG22	1:160:A:TRP:HE1	18	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	4	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	4	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	4	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	4	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	4	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	4	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	4	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	4	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	4	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	4	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	4	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	4	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	4	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	4	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	4	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	4	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	4	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	4	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	4	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	4	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	4	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	4	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	4	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	4	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	4	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	4	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	4	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	4	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	4	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	4	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	4	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	4	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	4	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	4	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	4	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	4	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	9	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	9	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	9	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	9	0.15
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	9	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	9	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	9	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	9	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	9	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	9	0.15
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	9	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	9	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	9	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	9	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	9	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	9	0.15
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	9	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	9	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	9	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	9	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	9	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	9	0.15
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	9	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	9	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	9	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	9	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	9	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	9	0.15
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	9	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	9	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	9	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	9	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	9	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	9	0.15
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	9	0.15
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE1	6	0.15
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE2	6	0.15
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE1	6	0.15
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE2	6	0.15
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE1	6	0.15
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE2	6	0.15
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE1	6	0.15
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE2	6	0.15
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE1	6	0.15
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE2	6	0.15
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE1	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE2	6	0.15
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE1	12	0.15
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE2	12	0.15
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE1	12	0.15
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE2	12	0.15
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE1	12	0.15
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE2	12	0.15
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE1	12	0.15
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE2	12	0.15
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE1	12	0.15
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE2	12	0.15
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE1	12	0.15
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE2	12	0.15
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	15	0.15
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	15	0.15
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	15	0.15
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	15	0.15
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	15	0.15
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	15	0.15
(1,560)	1:153:A:THR:H	1:158:A:ALA:HA	16	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	1	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	1	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	1	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	11	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	11	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	11	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	16	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	16	0.15
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	16	0.15
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	3	0.15
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	5	0.15
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	12	0.15
(1,534)	1:80:A:GLN:HG2	1:82:A:LYS:H	11	0.15
(1,534)	1:80:A:GLN:HG3	1:82:A:LYS:H	11	0.15
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	6	0.15
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	17	0.15
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	13	0.15
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	13	0.15
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	19	0.15
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	19	0.15
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	1	0.15
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG21	16	0.15
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG22	16	0.15
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG23	16	0.15
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	1	0.15
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	1	0.15
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	2	0.15
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	2	0.15
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	6	0.15
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	6	0.15
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	14	0.15
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	14	0.15
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	16	0.15
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	16	0.15
(1,330)	1:145:A:MET:HB2	1:146:A:LEU:H	16	0.15
(1,330)	1:145:A:MET:HB3	1:146:A:LEU:H	16	0.15
(1,314)	1:122:A:ASP:HB2	1:123:A:SER:H	10	0.15
(1,314)	1:122:A:ASP:HB3	1:123:A:SER:H	10	0.15
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	7	0.15
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	7	0.15
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	4	0.15
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	4	0.15
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	11	0.15
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	11	0.15
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	20	0.15
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	20	0.15
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	3	0.15
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	3	0.15
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	15	0.15
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	15	0.15
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	16	0.15
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	16	0.15
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	19	0.15
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	19	0.15
(1,266)	1:87:A:TRP:HB2	1:88:A:GLN:H	14	0.15
(1,266)	1:87:A:TRP:HB3	1:88:A:GLN:H	14	0.15
(1,261)	1:83:A:ASP:HB3	1:84:A:SER:H	15	0.15
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	15	0.15
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	15	0.15
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	8	0.15
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	8	0.15
(1,226)	1:205:A:LYS:HA	1:206:A:LEU:H	3	0.15
(1,226)	1:205:A:LYS:HA	1:206:A:LEU:H	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:205:A:LYS:HA	1:206:A:LEU:H	19	0.15
(1,226)	1:205:A:LYS:HA	1:206:A:LEU:H	20	0.15
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	3	0.15
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	10	0.15
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	14	0.15
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	10	0.15
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	8	0.15
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	9	0.15
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	17	0.15
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	4	0.15
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	5	0.15
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	8	0.15
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	12	0.15
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	16	0.15
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	5	0.14
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	11	0.14
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	12	0.14
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	16	0.14
(2,113)	1:171:A:ASP:O	1:175:A:ALA:H	9	0.14
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	14	0.14
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	15	0.14
(2,101)	1:165:A:ARG:O	1:169:A:VAL:H	5	0.14
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	3	0.14
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	17	0.14
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	1	0.14
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	2	0.14
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	17	0.14
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	1	0.14
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	9	0.14
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	17	0.14
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	1	0.14
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	7	0.14
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	9	0.14
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	12	0.14
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	19	0.14
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	7	0.14
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	16	0.14
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	12	0.14
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	17	0.14
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	7	0.14
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	10	0.14
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:97:A:LEU:O	1:101:A:ARG:H	5	0.14
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	16	0.14
(2,19)	1:74:A:ILE:O	1:78:A:ASN:H	14	0.14
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	4	0.14
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	6	0.14
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	17	0.14
(2,9)	1:69:A:ILE:O	1:73:A:LEU:H	10	0.14
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	6	0.14
(1,1098)	1:173:A:LEU:HD11	1:182:A:PHE:HE1	15	0.14
(1,1098)	1:173:A:LEU:HD11	1:182:A:PHE:HE2	15	0.14
(1,1098)	1:173:A:LEU:HD12	1:182:A:PHE:HE1	15	0.14
(1,1098)	1:173:A:LEU:HD12	1:182:A:PHE:HE2	15	0.14
(1,1098)	1:173:A:LEU:HD13	1:182:A:PHE:HE1	15	0.14
(1,1098)	1:173:A:LEU:HD13	1:182:A:PHE:HE2	15	0.14
(1,1098)	1:173:A:LEU:HD21	1:182:A:PHE:HE1	15	0.14
(1,1098)	1:173:A:LEU:HD21	1:182:A:PHE:HE2	15	0.14
(1,1098)	1:173:A:LEU:HD22	1:182:A:PHE:HE1	15	0.14
(1,1098)	1:173:A:LEU:HD22	1:182:A:PHE:HE2	15	0.14
(1,1098)	1:173:A:LEU:HD23	1:182:A:PHE:HE1	15	0.14
(1,1098)	1:173:A:LEU:HD23	1:182:A:PHE:HE2	15	0.14
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	16	0.14
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	16	0.14
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	16	0.14
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	16	0.14
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	16	0.14
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	16	0.14
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	16	0.14
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	16	0.14
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	16	0.14
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	16	0.14
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	16	0.14
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	16	0.14
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	2	0.14
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	2	0.14
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	2	0.14
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	2	0.14
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	2	0.14
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	2	0.14
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	2	0.14
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	2	0.14
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	2	0.14
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	2	0.14
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	2	0.14
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	2	0.14
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	2	0.14
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	2	0.14
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	2	0.14
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	2	0.14
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	2	0.14
(1,1086)	1:160:A:TRP:HZ2	1:167:A:LEU:HB2	7	0.14
(1,1086)	1:160:A:TRP:HZ2	1:167:A:LEU:HB3	7	0.14
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB2	19	0.14
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB3	19	0.14
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB2	19	0.14
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB3	19	0.14
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB2	19	0.14
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB3	19	0.14
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	20	0.14
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	20	0.14
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	20	0.14
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	20	0.14
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	20	0.14
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	20	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	18	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	18	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	18	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	18	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	18	0.14
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	18	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	18	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	18	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	18	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	18	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	18	0.14
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	18	0.14
(1,1056)	1:156:A:PHE:HA	1:185:A:ILE:HB	2	0.14
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	11	0.14
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	11	0.14
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	17	0.14
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	17	0.14
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	18	0.14
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	18	0.14
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:151:A:GLU:HA	1:189:A:MET:HG3	14	0.14
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	13	0.14
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	13	0.14
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	4	0.14
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	4	0.14
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	5	0.14
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	5	0.14
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	1	0.14
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	1	0.14
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG2	15	0.14
(1,998)	1:146:A:LEU:HD11	1:164:A:GLU:HG3	15	0.14
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG2	15	0.14
(1,998)	1:146:A:LEU:HD12	1:164:A:GLU:HG3	15	0.14
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG2	15	0.14
(1,998)	1:146:A:LEU:HD13	1:164:A:GLU:HG3	15	0.14
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG2	15	0.14
(1,998)	1:146:A:LEU:HD21	1:164:A:GLU:HG3	15	0.14
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG2	15	0.14
(1,998)	1:146:A:LEU:HD22	1:164:A:GLU:HG3	15	0.14
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG2	15	0.14
(1,998)	1:146:A:LEU:HD23	1:164:A:GLU:HG3	15	0.14
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	12	0.14
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	4	0.14
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	1	0.14
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	1	0.14
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	13	0.14
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	13	0.14
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	13	0.14
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	13	0.14
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	13	0.14
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	13	0.14
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	13	0.14
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	13	0.14
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	13	0.14
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	13	0.14
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	13	0.14
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	13	0.14
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	17	0.14
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	17	0.14
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	17	0.14
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	17	0.14
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	17	0.14
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	17	0.14
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	17	0.14
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	17	0.14
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	17	0.14
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	17	0.14
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	17	0.14
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	19	0.14
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	12	0.14
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	12	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	13	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	13	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	13	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	13	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	13	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	13	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	13	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	13	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	13	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	17	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	17	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	17	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	17	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	17	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	17	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	17	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	17	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	17	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	18	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	18	0.14
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	18	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	18	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	18	0.14
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	18	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	18	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	18	0.14
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	18	0.14
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD1	8	0.14
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD2	8	0.14
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD1	8	0.14
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD2	8	0.14
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD1	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD2	8	0.14
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB2	19	0.14
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB3	19	0.14
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB2	19	0.14
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB3	19	0.14
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB2	19	0.14
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB3	19	0.14
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB2	17	0.14
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB3	17	0.14
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB2	17	0.14
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB3	17	0.14
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB2	17	0.14
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB3	17	0.14
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB2	18	0.14
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB3	18	0.14
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB2	18	0.14
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB3	18	0.14
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB2	18	0.14
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB3	18	0.14
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD1	10	0.14
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD2	10	0.14
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD1	10	0.14
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD2	10	0.14
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD1	10	0.14
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD2	10	0.14
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	10	0.14
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	10	0.14
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	10	0.14
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	10	0.14
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	10	0.14
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	10	0.14
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	10	0.14
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	10	0.14
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	10	0.14
(1,894)	1:109:A:ARG:HG2	1:127:A:VAL:HB	15	0.14
(1,894)	1:109:A:ARG:HG3	1:127:A:VAL:HB	15	0.14
(1,891)	1:108:A:TRP:HD1	1:170:A:VAL:HB	2	0.14
(1,882)	1:108:A:TRP:HD1	1:155:A:ILE:HG13	3	0.14
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	2	0.14
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	2	0.14
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	4	0.14
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	4	0.14
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	4	0.14
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	4	0.14
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	4	0.14
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	4	0.14
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	4	0.14
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	4	0.14
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	4	0.14
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	4	0.14
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	4	0.14
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	5	0.14
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	5	0.14
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	5	0.14
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	5	0.14
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	5	0.14
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	5	0.14
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	5	0.14
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	5	0.14
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	5	0.14
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	5	0.14
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	5	0.14
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	5	0.14
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	8	0.14
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	8	0.14
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	8	0.14
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	8	0.14
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	8	0.14
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	8	0.14
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	8	0.14
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	8	0.14
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	8	0.14
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	8	0.14
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	8	0.14
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	8	0.14
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	10	0.14
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	10	0.14
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	10	0.14
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	10	0.14
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	10	0.14
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	10	0.14
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	10	0.14
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	10	0.14
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	10	0.14
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	10	0.14
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	10	0.14
(1,857)	1:101:A:ARG:HG2	1:142:A:ALA:HA	19	0.14
(1,857)	1:101:A:ARG:HG3	1:142:A:ALA:HA	19	0.14
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG2	12	0.14
(1,851)	1:100:A:ILE:HD11	1:165:A:ARG:HG3	12	0.14
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG2	12	0.14
(1,851)	1:100:A:ILE:HD12	1:165:A:ARG:HG3	12	0.14
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG2	12	0.14
(1,851)	1:100:A:ILE:HD13	1:165:A:ARG:HG3	12	0.14
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	18	0.14
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	18	0.14
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	18	0.14
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	18	0.14
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	18	0.14
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	18	0.14
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	20	0.14
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	20	0.14
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	20	0.14
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	20	0.14
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	20	0.14
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	20	0.14
(1,847)	1:100:A:ILE:HG12	1:143:A:ARG:HA	2	0.14
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	2	0.14
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	17	0.14
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	19	0.14
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	12	0.14
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	12	0.14
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	12	0.14
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	12	0.14
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	12	0.14
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	12	0.14
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	15	0.14
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	15	0.14
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	15	0.14
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	15	0.14
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	15	0.14
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	15	0.14
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB2	13	0.14
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB3	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	6	0.14
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	17	0.14
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	7	0.14
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	7	0.14
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	9	0.14
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	9	0.14
(1,783)	1:70:A:LEU:HG	1:93:A:ASP:HA	12	0.14
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB2	3	0.14
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB3	3	0.14
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB2	3	0.14
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB3	3	0.14
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB2	9	0.14
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB3	9	0.14
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB2	9	0.14
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB3	9	0.14
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	3	0.14
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	3	0.14
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	3	0.14
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	3	0.14
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	19	0.14
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	19	0.14
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	19	0.14
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	19	0.14
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	19	0.14
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	19	0.14
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	19	0.14
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	19	0.14
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	19	0.14
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	19	0.14
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	19	0.14
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	19	0.14
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	19	0.14
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	19	0.14
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	19	0.14
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	19	0.14
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	19	0.14
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	19	0.14
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	13	0.14
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	13	0.14
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	13	0.14
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	13	0.14
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	13	0.14
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	4	0.14
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	4	0.14
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	4	0.14
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	14	0.14
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	14	0.14
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	14	0.14
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD11	17	0.14
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD12	17	0.14
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD13	17	0.14
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD21	17	0.14
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD22	17	0.14
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD23	17	0.14
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	3	0.14
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD11	3	0.14
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD12	3	0.14
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD13	3	0.14
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD21	3	0.14
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD22	3	0.14
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD23	3	0.14
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	10	0.14
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	12	0.14
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG2	5	0.14
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG3	5	0.14
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG2	15	0.14
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG3	15	0.14
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG2	16	0.14
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG3	16	0.14
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	6	0.14
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	6	0.14
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	6	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG11	20	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG12	20	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG13	20	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG21	20	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG22	20	0.14
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG23	20	0.14
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	5	0.14
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	5	0.14
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	14	0.14
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	14	0.14
(1,677)	1:104:A:VAL:H	1:168:A:LEU:HD11	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:104:A:VAL:H	1:168:A:LEU:HD12	3	0.14
(1,677)	1:104:A:VAL:H	1:168:A:LEU:HD13	3	0.14
(1,677)	1:104:A:VAL:H	1:168:A:LEU:HD21	3	0.14
(1,677)	1:104:A:VAL:H	1:168:A:LEU:HD22	3	0.14
(1,677)	1:104:A:VAL:H	1:168:A:LEU:HD23	3	0.14
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	14	0.14
(1,671)	1:100:A:ILE:HG13	1:143:A:ARG:H	14	0.14
(1,670)	1:100:A:ILE:HD11	1:143:A:ARG:H	1	0.14
(1,670)	1:100:A:ILE:HD12	1:143:A:ARG:H	1	0.14
(1,670)	1:100:A:ILE:HD13	1:143:A:ARG:H	1	0.14
(1,660)	1:95:A:TYR:HB2	1:139:A:THR:H	19	0.14
(1,660)	1:95:A:TYR:HB3	1:139:A:THR:H	19	0.14
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	8	0.14
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	8	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD11	4	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD12	4	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD13	4	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD21	4	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD22	4	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD23	4	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD11	4	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD12	4	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD13	4	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD21	4	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD22	4	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD23	4	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD11	7	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD12	7	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD13	7	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD21	7	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD22	7	0.14
(1,627)	1:162:A:LEU:HB2	1:167:A:LEU:HD23	7	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD11	7	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD12	7	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD13	7	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD21	7	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD22	7	0.14
(1,627)	1:162:A:LEU:HB3	1:167:A:LEU:HD23	7	0.14
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD11	4	0.14
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD12	4	0.14
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD13	4	0.14
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD21	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD22	4	0.14
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD23	4	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	10	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	10	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	10	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	10	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	10	0.14
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	10	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	10	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	10	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	10	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	10	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	10	0.14
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	10	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	10	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	10	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	10	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	10	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	10	0.14
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	10	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	10	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	10	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	10	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	10	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	10	0.14
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	10	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	10	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	10	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	10	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	10	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	10	0.14
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	10	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	10	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	10	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	10	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	10	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	10	0.14
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	10	0.14
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	7	0.14
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	7	0.14
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	7	0.14
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	7	0.14
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	7	0.14
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	7	0.14
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	7	0.14
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	7	0.14
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	7	0.14
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	7	0.14
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	7	0.14
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	15	0.14
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	15	0.14
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB2	5	0.14
(1,590)	1:112:A:LEU:HD11	1:117:A:PHE:HB3	5	0.14
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB2	5	0.14
(1,590)	1:112:A:LEU:HD12	1:117:A:PHE:HB3	5	0.14
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB2	5	0.14
(1,590)	1:112:A:LEU:HD13	1:117:A:PHE:HB3	5	0.14
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB2	5	0.14
(1,590)	1:112:A:LEU:HD21	1:117:A:PHE:HB3	5	0.14
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB2	5	0.14
(1,590)	1:112:A:LEU:HD22	1:117:A:PHE:HB3	5	0.14
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB2	5	0.14
(1,590)	1:112:A:LEU:HD23	1:117:A:PHE:HB3	5	0.14
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	8	0.14
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	8	0.14
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	8	0.14
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	8	0.14
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	8	0.14
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	8	0.14
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB2	14	0.14
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB3	14	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	5	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	5	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	5	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	15	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	15	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	15	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	19	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	19	0.14
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	19	0.14
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	19	0.14
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	2	0.14
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:84:A:SER:H	1:87:A:TRP:HB2	6	0.14
(1,537)	1:84:A:SER:H	1:87:A:TRP:HB3	6	0.14
(1,534)	1:80:A:GLN:HG2	1:82:A:LYS:H	9	0.14
(1,534)	1:80:A:GLN:HG3	1:82:A:LYS:H	9	0.14
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB2	6	0.14
(1,504)	1:149:A:LEU:HA	1:152:A:GLU:HB3	6	0.14
(1,406)	1:118:A:GLN:HA	1:121:A:ALA:H	6	0.14
(1,405)	1:117:A:PHE:HA	1:120:A:GLU:H	3	0.14
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	12	0.14
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	11	0.14
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	11	0.14
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	16	0.14
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	16	0.14
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	5	0.14
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	5	0.14
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	5	0.14
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	7	0.14
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	7	0.14
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	7	0.14
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	4	0.14
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	4	0.14
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	7	0.14
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	7	0.14
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	9	0.14
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	9	0.14
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	15	0.14
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	15	0.14
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	18	0.14
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	18	0.14
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	19	0.14
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	19	0.14
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	3	0.14
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	3	0.14
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	15	0.14
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	15	0.14
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	11	0.14
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	11	0.14
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB2	14	0.14
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB3	14	0.14
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB2	14	0.14
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB3	14	0.14
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	9	0.14
(1,293)	1:110:A:ARG:HB2	1:111:A:ILE:H	12	0.14
(1,293)	1:110:A:ARG:HB3	1:111:A:ILE:H	12	0.14
(1,293)	1:110:A:ARG:HB2	1:111:A:ILE:H	13	0.14
(1,293)	1:110:A:ARG:HB3	1:111:A:ILE:H	13	0.14
(1,293)	1:110:A:ARG:HB2	1:111:A:ILE:H	20	0.14
(1,293)	1:110:A:ARG:HB3	1:111:A:ILE:H	20	0.14
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	11	0.14
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	11	0.14
(1,266)	1:87:A:TRP:HB2	1:88:A:GLN:H	20	0.14
(1,266)	1:87:A:TRP:HB3	1:88:A:GLN:H	20	0.14
(1,256)	1:80:A:GLN:HG2	1:81:A:THR:H	2	0.14
(1,256)	1:80:A:GLN:HG3	1:81:A:THR:H	2	0.14
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	18	0.14
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	18	0.14
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	19	0.14
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	19	0.14
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	9	0.14
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	9	0.14
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	12	0.14
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	12	0.14
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	15	0.14
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	15	0.14
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	20	0.14
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	16	0.14
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	1	0.14
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	2	0.14
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	5	0.14
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	15	0.14
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	20	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	1	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	2	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	3	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	6	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	7	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	13	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	17	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	18	0.14
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	20	0.14
(2,117)	1:180:A:GLU:O	1:184:A:LYS:H	6	0.13
(2,117)	1:180:A:GLU:O	1:184:A:LYS:H	9	0.13
(2,117)	1:180:A:GLU:O	1:184:A:LYS:H	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	4	0.13
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	7	0.13
(2,108)	1:168:A:LEU:O	1:172:A:ARG:N	5	0.13
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	9	0.13
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	8	0.13
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	16	0.13
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	12	0.13
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	13	0.13
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	20	0.13
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	13	0.13
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	20	0.13
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	19	0.13
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	6	0.13
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	1	0.13
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	5	0.13
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	15	0.13
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	19	0.13
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	1	0.13
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	19	0.13
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	2	0.13
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	5	0.13
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	7	0.13
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	18	0.13
(2,12)	1:70:A:LEU:O	1:74:A:ILE:N	10	0.13
(2,12)	1:70:A:LEU:O	1:74:A:ILE:N	19	0.13
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	1	0.13
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	11	0.13
(2,3)	1:66:A:ASP:O	1:70:A:LEU:H	12	0.13
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	18	0.13
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	18	0.13
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	18	0.13
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	18	0.13
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	18	0.13
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	18	0.13
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	18	0.13
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	18	0.13
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	18	0.13
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	18	0.13
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	18	0.13
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	18	0.13
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB1	13	0.13
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB2	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1092)	1:170:A:VAL:HG11	1:186:A:ALA:HB3	13	0.13
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB1	13	0.13
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB2	13	0.13
(1,1092)	1:170:A:VAL:HG12	1:186:A:ALA:HB3	13	0.13
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB1	13	0.13
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB2	13	0.13
(1,1092)	1:170:A:VAL:HG13	1:186:A:ALA:HB3	13	0.13
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB1	13	0.13
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB2	13	0.13
(1,1092)	1:170:A:VAL:HG21	1:186:A:ALA:HB3	13	0.13
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB1	13	0.13
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB2	13	0.13
(1,1092)	1:170:A:VAL:HG22	1:186:A:ALA:HB3	13	0.13
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB1	13	0.13
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB2	13	0.13
(1,1092)	1:170:A:VAL:HG23	1:186:A:ALA:HB3	13	0.13
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB2	12	0.13
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB3	12	0.13
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB2	12	0.13
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB3	12	0.13
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB2	12	0.13
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB3	12	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD11	12	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD12	12	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD13	12	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD21	12	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD22	12	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD23	12	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD11	12	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD12	12	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD13	12	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD21	12	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD22	12	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD23	12	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD11	17	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD12	17	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD13	17	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD21	17	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD22	17	0.13
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD23	17	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD11	17	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD12	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD13	17	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD21	17	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD22	17	0.13
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD23	17	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	7	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	7	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	7	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	7	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	7	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	7	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	7	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	7	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	7	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	7	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	7	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	7	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	8	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	8	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	8	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	8	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	8	0.13
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	8	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	8	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	8	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	8	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	8	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	8	0.13
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	8	0.13
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE1	15	0.13
(1,1046)	1:155:A:ILE:HD11	1:182:A:PHE:HE2	15	0.13
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE1	15	0.13
(1,1046)	1:155:A:ILE:HD12	1:182:A:PHE:HE2	15	0.13
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE1	15	0.13
(1,1046)	1:155:A:ILE:HD13	1:182:A:PHE:HE2	15	0.13
(1,1043)	1:155:A:ILE:HB	1:186:A:ALA:HB1	14	0.13
(1,1043)	1:155:A:ILE:HB	1:186:A:ALA:HB2	14	0.13
(1,1043)	1:155:A:ILE:HB	1:186:A:ALA:HB3	14	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	4	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	4	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	8	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	8	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	10	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	12	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	12	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	14	0.13
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	14	0.13
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	10	0.13
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	10	0.13
(1,1012)	1:150:A:ALA:HB1	1:159:A:SER:HA	7	0.13
(1,1012)	1:150:A:ALA:HB2	1:159:A:SER:HA	7	0.13
(1,1012)	1:150:A:ALA:HB3	1:159:A:SER:HA	7	0.13
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	6	0.13
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	6	0.13
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB2	20	0.13
(1,1006)	1:149:A:LEU:HD11	1:161:A:GLU:HB3	20	0.13
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB2	20	0.13
(1,1006)	1:149:A:LEU:HD12	1:161:A:GLU:HB3	20	0.13
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB2	20	0.13
(1,1006)	1:149:A:LEU:HD13	1:161:A:GLU:HB3	20	0.13
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB2	20	0.13
(1,1006)	1:149:A:LEU:HD21	1:161:A:GLU:HB3	20	0.13
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB2	20	0.13
(1,1006)	1:149:A:LEU:HD22	1:161:A:GLU:HB3	20	0.13
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB2	20	0.13
(1,1006)	1:149:A:LEU:HD23	1:161:A:GLU:HB3	20	0.13
(1,1000)	1:146:A:LEU:HG	1:164:A:GLU:HB2	2	0.13
(1,1000)	1:146:A:LEU:HG	1:164:A:GLU:HB3	2	0.13
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	2	0.13
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	8	0.13
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	20	0.13
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	17	0.13
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	17	0.13
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	10	0.13
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	10	0.13
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	15	0.13
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	15	0.13
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD11	10	0.13
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD12	10	0.13
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD13	10	0.13
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD21	10	0.13
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD22	10	0.13
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD23	10	0.13
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD11	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD12	10	0.13
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD13	10	0.13
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD21	10	0.13
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD22	10	0.13
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD23	10	0.13
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	6	0.13
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	6	0.13
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	6	0.13
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	6	0.13
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	6	0.13
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	6	0.13
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	6	0.13
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	6	0.13
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	6	0.13
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	6	0.13
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	6	0.13
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	6	0.13
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	14	0.13
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	15	0.13
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	16	0.13
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	20	0.13
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	10	0.13
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	10	0.13
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	20	0.13
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	20	0.13
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	4	0.13
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	4	0.13
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	4	0.13
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	4	0.13
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	4	0.13
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	4	0.13
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	4	0.13
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	4	0.13
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	4	0.13
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB2	8	0.13
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB3	8	0.13
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB2	8	0.13
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB3	8	0.13
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB2	8	0.13
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB3	8	0.13
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD1	20	0.13
(1,906)	1:111:A:ILE:HD11	1:182:A:PHE:HD2	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD1	20	0.13
(1,906)	1:111:A:ILE:HD12	1:182:A:PHE:HD2	20	0.13
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD1	20	0.13
(1,906)	1:111:A:ILE:HD13	1:182:A:PHE:HD2	20	0.13
(1,894)	1:109:A:ARG:HG2	1:127:A:VAL:HB	13	0.13
(1,894)	1:109:A:ARG:HG3	1:127:A:VAL:HB	13	0.13
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	8	0.13
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	8	0.13
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	8	0.13
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	8	0.13
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	8	0.13
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	8	0.13
(1,881)	1:108:A:TRP:HD1	1:125:A:LEU:HB2	13	0.13
(1,881)	1:108:A:TRP:HD1	1:125:A:LEU:HB3	13	0.13
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	16	0.13
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	16	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	9	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	9	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	9	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	9	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	9	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	9	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	9	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	9	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	9	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	9	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	9	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	9	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	18	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	18	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	18	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	18	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	18	0.13
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	18	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	18	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	18	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	18	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	18	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	18	0.13
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	18	0.13
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG2	6	0.13
(1,865)	1:104:A:VAL:HG11	1:164:A:GLU:HG3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG2	6	0.13
(1,865)	1:104:A:VAL:HG12	1:164:A:GLU:HG3	6	0.13
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG2	6	0.13
(1,865)	1:104:A:VAL:HG13	1:164:A:GLU:HG3	6	0.13
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG2	6	0.13
(1,865)	1:104:A:VAL:HG21	1:164:A:GLU:HG3	6	0.13
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG2	6	0.13
(1,865)	1:104:A:VAL:HG22	1:164:A:GLU:HG3	6	0.13
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG2	6	0.13
(1,865)	1:104:A:VAL:HG23	1:164:A:GLU:HG3	6	0.13
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD11	4	0.13
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD12	4	0.13
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD13	4	0.13
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD21	4	0.13
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD22	4	0.13
(1,862)	1:104:A:VAL:HG11	1:146:A:LEU:HD23	4	0.13
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD11	4	0.13
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD12	4	0.13
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD13	4	0.13
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD21	4	0.13
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD22	4	0.13
(1,862)	1:104:A:VAL:HG12	1:146:A:LEU:HD23	4	0.13
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD11	4	0.13
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD12	4	0.13
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD13	4	0.13
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD21	4	0.13
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD22	4	0.13
(1,862)	1:104:A:VAL:HG13	1:146:A:LEU:HD23	4	0.13
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD11	4	0.13
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD12	4	0.13
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD13	4	0.13
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD21	4	0.13
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD22	4	0.13
(1,862)	1:104:A:VAL:HG21	1:146:A:LEU:HD23	4	0.13
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD11	4	0.13
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD12	4	0.13
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD13	4	0.13
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD21	4	0.13
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD22	4	0.13
(1,862)	1:104:A:VAL:HG22	1:146:A:LEU:HD23	4	0.13
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD11	4	0.13
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD12	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD13	4	0.13
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD21	4	0.13
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD22	4	0.13
(1,862)	1:104:A:VAL:HG23	1:146:A:LEU:HD23	4	0.13
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	4	0.13
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	4	0.13
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	4	0.13
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	4	0.13
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	4	0.13
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	4	0.13
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	13	0.13
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	13	0.13
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	13	0.13
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	13	0.13
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	13	0.13
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	13	0.13
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD11	17	0.13
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD12	17	0.13
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD13	17	0.13
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD21	17	0.13
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD22	17	0.13
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD23	17	0.13
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD11	17	0.13
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD12	17	0.13
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD13	17	0.13
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD21	17	0.13
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD22	17	0.13
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD23	17	0.13
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD11	17	0.13
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD12	17	0.13
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD13	17	0.13
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD21	17	0.13
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD22	17	0.13
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD23	17	0.13
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB1	18	0.13
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB2	18	0.13
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB3	18	0.13
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB1	18	0.13
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB2	18	0.13
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB3	18	0.13
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	1	0.13
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	1	0.13
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	1	0.13
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	1	0.13
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	1	0.13
(1,826)	1:77:A:ARG:HB2	1:87:A:TRP:HB2	6	0.13
(1,826)	1:77:A:ARG:HB2	1:87:A:TRP:HB3	6	0.13
(1,826)	1:77:A:ARG:HB3	1:87:A:TRP:HB2	6	0.13
(1,826)	1:77:A:ARG:HB3	1:87:A:TRP:HB3	6	0.13
(1,816)	1:76:A:ILE:HD11	1:87:A:TRP:HD1	14	0.13
(1,816)	1:76:A:ILE:HD12	1:87:A:TRP:HD1	14	0.13
(1,816)	1:76:A:ILE:HD13	1:87:A:TRP:HD1	14	0.13
(1,816)	1:76:A:ILE:HD11	1:87:A:TRP:HD1	15	0.13
(1,816)	1:76:A:ILE:HD12	1:87:A:TRP:HD1	15	0.13
(1,816)	1:76:A:ILE:HD13	1:87:A:TRP:HD1	15	0.13
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	3	0.13
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	3	0.13
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	3	0.13
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	3	0.13
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	14	0.13
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	14	0.13
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	14	0.13
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	14	0.13
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	5	0.13
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	8	0.13
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	9	0.13
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	20	0.13
(1,788)	1:71:A:TYR:HE1	1:90:A:LEU:HG	20	0.13
(1,788)	1:71:A:TYR:HE2	1:90:A:LEU:HG	20	0.13
(1,783)	1:70:A:LEU:HG	1:93:A:ASP:HA	11	0.13
(1,783)	1:70:A:LEU:HG	1:93:A:ASP:HA	14	0.13
(1,779)	1:70:A:LEU:HD11	1:94:A:ILE:HB	2	0.13
(1,779)	1:70:A:LEU:HD12	1:94:A:ILE:HB	2	0.13
(1,779)	1:70:A:LEU:HD13	1:94:A:ILE:HB	2	0.13
(1,779)	1:70:A:LEU:HD21	1:94:A:ILE:HB	2	0.13
(1,779)	1:70:A:LEU:HD22	1:94:A:ILE:HB	2	0.13
(1,779)	1:70:A:LEU:HD23	1:94:A:ILE:HB	2	0.13
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	1	0.13
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	1	0.13
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	1	0.13
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	10	0.13
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	10	0.13
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB2	7	0.13
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB3	7	0.13
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB2	7	0.13
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB3	7	0.13
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	12	0.13
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	12	0.13
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	12	0.13
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	12	0.13
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	12	0.13
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	12	0.13
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	12	0.13
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	12	0.13
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	12	0.13
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	12	0.13
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	12	0.13
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	12	0.13
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	12	0.13
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	12	0.13
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	12	0.13
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	12	0.13
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	12	0.13
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	12	0.13
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	1	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	1	0.13
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	1	0.13
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	7	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	7	0.13
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	7	0.13
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	8	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	8	0.13
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	8	0.13
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	9	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	9	0.13
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	9	0.13
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	10	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	10	0.13
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	10	0.13
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	11	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	11	0.13
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	11	0.13
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	15	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	15	0.13
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	16	0.13
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	16	0.13
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	16	0.13
(1,742)	1:157:A:PRO:HG2	1:186:A:ALA:H	7	0.13
(1,742)	1:157:A:PRO:HG3	1:186:A:ALA:H	7	0.13
(1,740)	1:156:A:PHE:H	1:167:A:LEU:HG	1	0.13
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	4	0.13
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG2	4	0.13
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG3	4	0.13
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG2	8	0.13
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG3	8	0.13
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	8	0.13
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	8	0.13
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	14	0.13
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	14	0.13
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	14	0.13
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	2	0.13
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	2	0.13
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	4	0.13
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	4	0.13
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	7	0.13
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	7	0.13
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	11	0.13
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	11	0.13
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	2	0.13
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	2	0.13
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	2	0.13
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG2	15	0.13
(1,639)	1:59:A:VAL:H	1:68:A:ARG:HG3	15	0.13
(1,637)	1:58:A:ASP:HB2	1:69:A:ILE:H	1	0.13
(1,637)	1:58:A:ASP:HB3	1:69:A:ILE:H	1	0.13
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	15	0.13
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	15	0.13
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD11	7	0.13
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD12	7	0.13
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD13	7	0.13
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD21	7	0.13
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD22	7	0.13
(1,623)	1:162:A:LEU:HG	1:167:A:LEU:HD23	7	0.13
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	17	0.13
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	17	0.13
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	17	0.13
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	17	0.13
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	17	0.13
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	17	0.13
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	17	0.13
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	17	0.13
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	17	0.13
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	17	0.13
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	17	0.13
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	17	0.13
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	17	0.13
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	17	0.13
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	17	0.13
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	17	0.13
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	17	0.13
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	17	0.13
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	17	0.13
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	17	0.13
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	17	0.13
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	17	0.13
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	17	0.13
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	17	0.13
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	17	0.13
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	17	0.13
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	17	0.13
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	17	0.13
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	17	0.13
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	17	0.13
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	17	0.13
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	17	0.13
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	17	0.13
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	17	0.13
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	17	0.13
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	16	0.13
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	16	0.13
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	9	0.13
(1,557)	1:153:A:THR:HA	1:155:A:ILE:H	2	0.13
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	5	0.13
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	4	0.13
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	8	0.13
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	12	0.13
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	12	0.13
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	12	0.13
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	14	0.13
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	14	0.13
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	14	0.13
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	19	0.13
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	19	0.13
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	19	0.13
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	7	0.13
(1,540)	1:115:A:LEU:HD11	1:118:A:GLN:H	2	0.13
(1,540)	1:115:A:LEU:HD12	1:118:A:GLN:H	2	0.13
(1,540)	1:115:A:LEU:HD13	1:118:A:GLN:H	2	0.13
(1,540)	1:115:A:LEU:HD21	1:118:A:GLN:H	2	0.13
(1,540)	1:115:A:LEU:HD22	1:118:A:GLN:H	2	0.13
(1,540)	1:115:A:LEU:HD23	1:118:A:GLN:H	2	0.13
(1,537)	1:84:A:SER:H	1:87:A:TRP:HB2	7	0.13
(1,537)	1:84:A:SER:H	1:87:A:TRP:HB3	7	0.13
(1,406)	1:118:A:GLN:HA	1:121:A:ALA:H	1	0.13
(1,406)	1:118:A:GLN:HA	1:121:A:ALA:H	10	0.13
(1,406)	1:118:A:GLN:HA	1:121:A:ALA:H	19	0.13
(1,405)	1:117:A:PHE:HA	1:120:A:GLU:H	18	0.13
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	1	0.13
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	13	0.13
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	20	0.13
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	2	0.13
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	2	0.13
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	5	0.13
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	5	0.13
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	20	0.13
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG21	8	0.13
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG22	8	0.13
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG23	8	0.13
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG21	15	0.13
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG22	15	0.13
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG23	15	0.13
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	14	0.13
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	14	0.13
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	10	0.13
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	10	0.13
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	12	0.13
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:123:A:SER:HB2	1:124:A:LEU:H	2	0.13
(1,315)	1:123:A:SER:HB3	1:124:A:LEU:H	2	0.13
(1,315)	1:123:A:SER:HB2	1:124:A:LEU:H	10	0.13
(1,315)	1:123:A:SER:HB3	1:124:A:LEU:H	10	0.13
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	1	0.13
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	1	0.13
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	19	0.13
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	19	0.13
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	13	0.13
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	13	0.13
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	18	0.13
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	18	0.13
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	2	0.13
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	2	0.13
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	7	0.13
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	7	0.13
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	14	0.13
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	14	0.13
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	18	0.13
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	18	0.13
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	1	0.13
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	1	0.13
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	15	0.13
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	15	0.13
(1,266)	1:87:A:TRP:HB2	1:88:A:GLN:H	3	0.13
(1,266)	1:87:A:TRP:HB3	1:88:A:GLN:H	3	0.13
(1,262)	1:84:A:SER:H	1:85:A:GLU:HG2	9	0.13
(1,262)	1:84:A:SER:H	1:85:A:GLU:HG3	9	0.13
(1,256)	1:80:A:GLN:HG2	1:81:A:THR:H	17	0.13
(1,256)	1:80:A:GLN:HG3	1:81:A:THR:H	17	0.13
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	1	0.13
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	1	0.13
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	13	0.13
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	13	0.13
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	4	0.13
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	4	0.13
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	9	0.13
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	9	0.13
(1,222)	1:200:A:VAL:HA	1:201:A:ASP:H	4	0.13
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	5	0.13
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	6	0.13
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	9	0.13
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	11	0.13
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	12	0.13
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	13	0.13
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	2	0.13
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	12	0.13
(1,22)	1:80:A:GLN:H	1:81:A:THR:H	10	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	2	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	4	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	9	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	13	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	15	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	16	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	17	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	18	0.13
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	19	0.13
(3,82)	1:151:A:GLU:H	1:198:A:CYS:O	2	0.12
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	8	0.12
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	3	0.12
(2,109)	1:169:A:VAL:O	1:173:A:LEU:H	7	0.12
(2,108)	1:168:A:LEU:O	1:172:A:ARG:N	2	0.12
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	3	0.12
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	4	0.12
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	11	0.12
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	15	0.12
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	2	0.12
(2,79)	1:120:A:GLU:O	1:124:A:LEU:H	3	0.12
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	10	0.12
(2,73)	1:110:A:ARG:O	1:114:A:ASP:H	2	0.12
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	13	0.12
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	11	0.12
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	16	0.12
(2,59)	1:103:A:GLU:O	1:107:A:ARG:H	4	0.12
(2,59)	1:103:A:GLU:O	1:107:A:ARG:H	20	0.12
(2,47)	1:97:A:LEU:O	1:101:A:ARG:H	2	0.12
(2,45)	1:96:A:THR:O	1:100:A:ILE:H	1	0.12
(2,45)	1:96:A:THR:O	1:100:A:ILE:H	15	0.12
(2,43)	1:95:A:TYR:O	1:99:A:GLN:H	1	0.12
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	4	0.12
(2,39)	1:93:A:ASP:O	1:97:A:LEU:H	17	0.12
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	2	0.12
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	18	0.12
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	10	0.12
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	16	0.12
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	20	0.12
(2,13)	1:71:A:TYR:O	1:75:A:VAL:H	13	0.12
(2,12)	1:70:A:LEU:O	1:74:A:ILE:N	18	0.12
(2,9)	1:69:A:ILE:O	1:73:A:LEU:H	17	0.12
(2,9)	1:69:A:ILE:O	1:73:A:LEU:H	18	0.12
(2,9)	1:69:A:ILE:O	1:73:A:LEU:H	19	0.12
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	3	0.12
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	5	0.12
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	14	0.12
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	17	0.12
(2,3)	1:66:A:ASP:O	1:70:A:LEU:H	16	0.12
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE1	8	0.12
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE2	8	0.12
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE1	8	0.12
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE2	8	0.12
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE1	8	0.12
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE2	8	0.12
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE1	8	0.12
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE2	8	0.12
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE1	8	0.12
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE2	8	0.12
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE1	8	0.12
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE2	8	0.12
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB1	9	0.12
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB2	9	0.12
(1,1090)	1:167:A:LEU:HD11	1:186:A:ALA:HB3	9	0.12
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB1	9	0.12
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB2	9	0.12
(1,1090)	1:167:A:LEU:HD12	1:186:A:ALA:HB3	9	0.12
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB1	9	0.12
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB2	9	0.12
(1,1090)	1:167:A:LEU:HD13	1:186:A:ALA:HB3	9	0.12
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB1	9	0.12
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB2	9	0.12
(1,1090)	1:167:A:LEU:HD21	1:186:A:ALA:HB3	9	0.12
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB1	9	0.12
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB2	9	0.12
(1,1090)	1:167:A:LEU:HD22	1:186:A:ALA:HB3	9	0.12
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB1	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB2	9	0.12
(1,1090)	1:167:A:LEU:HD23	1:186:A:ALA:HB3	9	0.12
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD11	19	0.12
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD12	19	0.12
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD13	19	0.12
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD21	19	0.12
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD22	19	0.12
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD23	19	0.12
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD11	19	0.12
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD12	19	0.12
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD13	19	0.12
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD21	19	0.12
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD22	19	0.12
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD23	19	0.12
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	11	0.12
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	11	0.12
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	11	0.12
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	11	0.12
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	11	0.12
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	11	0.12
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	11	0.12
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	11	0.12
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	11	0.12
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	11	0.12
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	11	0.12
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	11	0.12
(1,1056)	1:156:A:PHE:HA	1:185:A:ILE:HB	7	0.12
(1,1050)	1:155:A:ILE:HG21	1:167:A:LEU:HG	5	0.12
(1,1034)	1:155:A:ILE:HG21	1:170:A:VAL:HB	5	0.12
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB2	9	0.12
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB3	9	0.12
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB2	9	0.12
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB3	9	0.12
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB2	10	0.12
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB3	10	0.12
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB2	10	0.12
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB3	10	0.12
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB2	11	0.12
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB3	11	0.12
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB2	11	0.12
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB3	11	0.12
(1,1020)	1:152:A:GLU:HG2	1:190:A:TYR:HD1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:152:A:GLU:HG2	1:190:A:TYR:HD2	8	0.12
(1,1020)	1:152:A:GLU:HG3	1:190:A:TYR:HD1	8	0.12
(1,1020)	1:152:A:GLU:HG3	1:190:A:TYR:HD2	8	0.12
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	6	0.12
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	6	0.12
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	13	0.12
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	13	0.12
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	1	0.12
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	1	0.12
(1,1012)	1:150:A:ALA:HB1	1:159:A:SER:HA	18	0.12
(1,1012)	1:150:A:ALA:HB2	1:159:A:SER:HA	18	0.12
(1,1012)	1:150:A:ALA:HB3	1:159:A:SER:HA	18	0.12
(1,1009)	1:149:A:LEU:HD11	1:160:A:TRP:HE1	16	0.12
(1,1009)	1:149:A:LEU:HD12	1:160:A:TRP:HE1	16	0.12
(1,1009)	1:149:A:LEU:HD13	1:160:A:TRP:HE1	16	0.12
(1,1009)	1:149:A:LEU:HD21	1:160:A:TRP:HE1	16	0.12
(1,1009)	1:149:A:LEU:HD22	1:160:A:TRP:HE1	16	0.12
(1,1009)	1:149:A:LEU:HD23	1:160:A:TRP:HE1	16	0.12
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	20	0.12
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	20	0.12
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB2	20	0.12
(1,1004)	1:146:A:LEU:HD11	1:162:A:LEU:HB3	20	0.12
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB2	20	0.12
(1,1004)	1:146:A:LEU:HD12	1:162:A:LEU:HB3	20	0.12
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB2	20	0.12
(1,1004)	1:146:A:LEU:HD13	1:162:A:LEU:HB3	20	0.12
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB2	20	0.12
(1,1004)	1:146:A:LEU:HD21	1:162:A:LEU:HB3	20	0.12
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB2	20	0.12
(1,1004)	1:146:A:LEU:HD22	1:162:A:LEU:HB3	20	0.12
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB2	20	0.12
(1,1004)	1:146:A:LEU:HD23	1:162:A:LEU:HB3	20	0.12
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	6	0.12
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	6	0.12
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	19	0.12
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	15	0.12
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	19	0.12
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	12	0.12
(1,984)	1:125:A:LEU:HD11	1:145:A:MET:HB2	17	0.12
(1,984)	1:125:A:LEU:HD11	1:145:A:MET:HB3	17	0.12
(1,984)	1:125:A:LEU:HD12	1:145:A:MET:HB2	17	0.12
(1,984)	1:125:A:LEU:HD12	1:145:A:MET:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,984)	1:125:A:LEU:HD13	1:145:A:MET:HB2	17	0.12
(1,984)	1:125:A:LEU:HD13	1:145:A:MET:HB3	17	0.12
(1,984)	1:125:A:LEU:HD21	1:145:A:MET:HB2	17	0.12
(1,984)	1:125:A:LEU:HD21	1:145:A:MET:HB3	17	0.12
(1,984)	1:125:A:LEU:HD22	1:145:A:MET:HB2	17	0.12
(1,984)	1:125:A:LEU:HD22	1:145:A:MET:HB3	17	0.12
(1,984)	1:125:A:LEU:HD23	1:145:A:MET:HB2	17	0.12
(1,984)	1:125:A:LEU:HD23	1:145:A:MET:HB3	17	0.12
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	15	0.12
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	15	0.12
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	16	0.12
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	16	0.12
(1,976)	1:124:A:LEU:HG	1:152:A:GLU:HG2	10	0.12
(1,976)	1:124:A:LEU:HG	1:152:A:GLU:HG3	10	0.12
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	8	0.12
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	8	0.12
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	6	0.12
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	3	0.12
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	6	0.12
(1,941)	1:120:A:GLU:HG2	1:183:A:PHE:HB2	8	0.12
(1,941)	1:120:A:GLU:HG2	1:183:A:PHE:HB3	8	0.12
(1,941)	1:120:A:GLU:HG3	1:183:A:PHE:HB2	8	0.12
(1,941)	1:120:A:GLU:HG3	1:183:A:PHE:HB3	8	0.12
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB2	6	0.12
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB3	6	0.12
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB2	6	0.12
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB3	6	0.12
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB2	6	0.12
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB3	6	0.12
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB2	6	0.12
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB3	6	0.12
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB2	6	0.12
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB3	6	0.12
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB2	6	0.12
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB3	6	0.12
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	3	0.12
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	3	0.12
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	3	0.12
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	3	0.12
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	3	0.12
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	3	0.12
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	3	0.12
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	3	0.12
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	4	0.12
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	4	0.12
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	4	0.12
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	4	0.12
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	4	0.12
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	4	0.12
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	8	0.12
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	8	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	6	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	6	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	6	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	6	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	6	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	6	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	6	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	6	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	6	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	6	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	6	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	6	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	20	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	20	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	20	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	20	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	20	0.12
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	20	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	20	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	20	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	20	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	20	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	20	0.12
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	20	0.12
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE1	3	0.12
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE2	3	0.12
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE3	3	0.12
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE1	3	0.12
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE2	3	0.12
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE3	3	0.12
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	6	0.12
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	15	0.12
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	15	0.12
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	1	0.12
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	1	0.12
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	1	0.12
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	1	0.12
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	1	0.12
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	1	0.12
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	14	0.12
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	14	0.12
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	14	0.12
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	14	0.12
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	14	0.12
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	14	0.12
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	19	0.12
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	19	0.12
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	19	0.12
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	19	0.12
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	19	0.12
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	19	0.12
(1,846)	1:100:A:ILE:HD11	1:143:A:ARG:HB2	20	0.12
(1,846)	1:100:A:ILE:HD11	1:143:A:ARG:HB3	20	0.12
(1,846)	1:100:A:ILE:HD12	1:143:A:ARG:HB2	20	0.12
(1,846)	1:100:A:ILE:HD12	1:143:A:ARG:HB3	20	0.12
(1,846)	1:100:A:ILE:HD13	1:143:A:ARG:HB2	20	0.12
(1,846)	1:100:A:ILE:HD13	1:143:A:ARG:HB3	20	0.12
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD11	20	0.12
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD12	20	0.12
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD13	20	0.12
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD21	20	0.12
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD22	20	0.12
(1,844)	1:100:A:ILE:HD11	1:146:A:LEU:HD23	20	0.12
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD11	20	0.12
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD12	20	0.12
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD13	20	0.12
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD21	20	0.12
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD22	20	0.12
(1,844)	1:100:A:ILE:HD12	1:146:A:LEU:HD23	20	0.12
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD11	20	0.12
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD12	20	0.12
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD13	20	0.12
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD21	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD22	20	0.12
(1,844)	1:100:A:ILE:HD13	1:146:A:LEU:HD23	20	0.12
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB1	8	0.12
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB2	8	0.12
(1,835)	1:98:A:ARG:HG2	1:142:A:ALA:HB3	8	0.12
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB1	8	0.12
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB2	8	0.12
(1,835)	1:98:A:ARG:HG3	1:142:A:ALA:HB3	8	0.12
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	11	0.12
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	16	0.12
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	18	0.12
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	3	0.12
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	3	0.12
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	3	0.12
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	3	0.12
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	3	0.12
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	3	0.12
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	4	0.12
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	4	0.12
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	4	0.12
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	4	0.12
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	4	0.12
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	4	0.12
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	17	0.12
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	17	0.12
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	17	0.12
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	17	0.12
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	17	0.12
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	17	0.12
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	19	0.12
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	19	0.12
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	19	0.12
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	19	0.12
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	19	0.12
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	19	0.12
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB2	19	0.12
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB3	19	0.12
(1,826)	1:77:A:ARG:HB2	1:87:A:TRP:HB2	7	0.12
(1,826)	1:77:A:ARG:HB2	1:87:A:TRP:HB3	7	0.12
(1,826)	1:77:A:ARG:HB3	1:87:A:TRP:HB2	7	0.12
(1,826)	1:77:A:ARG:HB3	1:87:A:TRP:HB3	7	0.12
(1,822)	1:76:A:ILE:HG22	1:90:A:LEU:HD11	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	19	0.12
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	19	0.12
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	19	0.12
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	3	0.12
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	4	0.12
(1,793)	1:73:A:LEU:HD11	1:90:A:LEU:HG	2	0.12
(1,793)	1:73:A:LEU:HD12	1:90:A:LEU:HG	2	0.12
(1,793)	1:73:A:LEU:HD13	1:90:A:LEU:HG	2	0.12
(1,793)	1:73:A:LEU:HD21	1:90:A:LEU:HG	2	0.12
(1,793)	1:73:A:LEU:HD22	1:90:A:LEU:HG	2	0.12
(1,793)	1:73:A:LEU:HD23	1:90:A:LEU:HG	2	0.12
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD11	15	0.12
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD12	15	0.12
(1,770)	1:68:A:ARG:HA	1:94:A:ILE:HD13	15	0.12
(1,763)	1:67:A:ASP:HB2	1:94:A:ILE:HD11	10	0.12
(1,763)	1:67:A:ASP:HB2	1:94:A:ILE:HD12	10	0.12
(1,763)	1:67:A:ASP:HB2	1:94:A:ILE:HD13	10	0.12
(1,763)	1:67:A:ASP:HB3	1:94:A:ILE:HD11	10	0.12
(1,763)	1:67:A:ASP:HB3	1:94:A:ILE:HD12	10	0.12
(1,763)	1:67:A:ASP:HB3	1:94:A:ILE:HD13	10	0.12
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	6	0.12
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	6	0.12
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	6	0.12
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	6	0.12
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	6	0.12
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	6	0.12
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	6	0.12
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	6	0.12
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	6	0.12
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	6	0.12
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	6	0.12
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	6	0.12
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	6	0.12
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	6	0.12
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	6	0.12
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	6	0.12
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	6	0.12
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	6	0.12
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD11	12	0.12
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD12	12	0.12
(1,751)	1:58:A:ASP:HB2	1:69:A:ILE:HD13	12	0.12
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD11	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD12	12	0.12
(1,751)	1:58:A:ASP:HB3	1:69:A:ILE:HD13	12	0.12
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	2	0.12
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	2	0.12
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	2	0.12
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	19	0.12
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	19	0.12
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	19	0.12
(1,742)	1:157:A:PRO:HG2	1:186:A:ALA:H	4	0.12
(1,742)	1:157:A:PRO:HG3	1:186:A:ALA:H	4	0.12
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD11	18	0.12
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD12	18	0.12
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD13	18	0.12
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD21	18	0.12
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD22	18	0.12
(1,735)	1:155:A:ILE:H	1:167:A:LEU:HD23	18	0.12
(1,732)	1:155:A:ILE:HB	1:186:A:ALA:H	7	0.12
(1,728)	1:154:A:SER:H	1:189:A:MET:HB2	11	0.12
(1,728)	1:154:A:SER:H	1:189:A:MET:HB3	11	0.12
(1,718)	1:152:A:GLU:HA	1:190:A:TYR:H	11	0.12
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD11	18	0.12
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD12	18	0.12
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD13	18	0.12
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD21	18	0.12
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD22	18	0.12
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD23	18	0.12
(1,702)	1:124:A:LEU:HG	1:153:A:THR:H	14	0.12
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG2	19	0.12
(1,700)	1:124:A:LEU:H	1:152:A:GLU:HG3	19	0.12
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	15	0.12
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	15	0.12
(1,689)	1:117:A:PHE:HB2	1:180:A:GLU:H	17	0.12
(1,689)	1:117:A:PHE:HB3	1:180:A:GLU:H	17	0.12
(1,686)	1:111:A:ILE:HG13	1:182:A:PHE:H	13	0.12
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	5	0.12
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	5	0.12
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	5	0.12
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	19	0.12
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	19	0.12
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	19	0.12
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	1	0.12
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	10	0.12
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	10	0.12
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	12	0.12
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	12	0.12
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	15	0.12
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	15	0.12
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	19	0.12
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	19	0.12
(1,675)	1:101:A:ARG:H	1:164:A:GLU:HG2	13	0.12
(1,675)	1:101:A:ARG:H	1:164:A:GLU:HG3	13	0.12
(1,674)	1:101:A:ARG:HA	1:143:A:ARG:H	19	0.12
(1,671)	1:100:A:ILE:HG12	1:143:A:ARG:H	2	0.12
(1,660)	1:95:A:TYR:HB2	1:139:A:THR:H	2	0.12
(1,660)	1:95:A:TYR:HB3	1:139:A:THR:H	2	0.12
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	12	0.12
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	12	0.12
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	12	0.12
(1,653)	1:74:A:ILE:HD11	1:88:A:GLN:H	1	0.12
(1,653)	1:74:A:ILE:HD12	1:88:A:GLN:H	1	0.12
(1,653)	1:74:A:ILE:HD13	1:88:A:GLN:H	1	0.12
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	17	0.12
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	17	0.12
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD11	7	0.12
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD12	7	0.12
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD13	7	0.12
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD21	7	0.12
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD22	7	0.12
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD23	7	0.12
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	18	0.12
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	18	0.12
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	18	0.12
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	18	0.12
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	18	0.12
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	18	0.12
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	18	0.12
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	18	0.12
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	18	0.12
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	18	0.12
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	18	0.12
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	18	0.12
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	18	0.12
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	18	0.12
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	18	0.12
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	18	0.12
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	18	0.12
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	18	0.12
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	18	0.12
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	18	0.12
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	18	0.12
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	18	0.12
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	18	0.12
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	18	0.12
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	18	0.12
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	18	0.12
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	18	0.12
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	18	0.12
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	18	0.12
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	18	0.12
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	18	0.12
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	18	0.12
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	18	0.12
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	18	0.12
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	18	0.12
(1,585)	1:76:A:ILE:HD11	1:80:A:GLN:HG2	15	0.12
(1,585)	1:76:A:ILE:HD11	1:80:A:GLN:HG3	15	0.12
(1,585)	1:76:A:ILE:HD12	1:80:A:GLN:HG2	15	0.12
(1,585)	1:76:A:ILE:HD12	1:80:A:GLN:HG3	15	0.12
(1,585)	1:76:A:ILE:HD13	1:80:A:GLN:HG2	15	0.12
(1,585)	1:76:A:ILE:HD13	1:80:A:GLN:HG3	15	0.12
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	1	0.12
(1,574)	1:162:A:LEU:HD11	1:167:A:LEU:H	15	0.12
(1,574)	1:162:A:LEU:HD12	1:167:A:LEU:H	15	0.12
(1,574)	1:162:A:LEU:HD13	1:167:A:LEU:H	15	0.12
(1,574)	1:162:A:LEU:HD21	1:167:A:LEU:H	15	0.12
(1,574)	1:162:A:LEU:HD22	1:167:A:LEU:H	15	0.12
(1,574)	1:162:A:LEU:HD23	1:167:A:LEU:H	15	0.12
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	2	0.12
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	5	0.12
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	11	0.12
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	4	0.12
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	4	0.12
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	4	0.12
(1,557)	1:153:A:THR:HA	1:155:A:ILE:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	9	0.12
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	20	0.12
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	15	0.12
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	8	0.12
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	8	0.12
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	8	0.12
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	13	0.12
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	13	0.12
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	13	0.12
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	15	0.12
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	15	0.12
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	15	0.12
(1,536)	1:82:A:LYS:HG2	1:84:A:SER:H	6	0.12
(1,536)	1:82:A:LYS:HG3	1:84:A:SER:H	6	0.12
(1,534)	1:80:A:GLN:HG2	1:82:A:LYS:H	3	0.12
(1,534)	1:80:A:GLN:HG3	1:82:A:LYS:H	3	0.12
(1,534)	1:80:A:GLN:HG2	1:82:A:LYS:H	13	0.12
(1,534)	1:80:A:GLN:HG3	1:82:A:LYS:H	13	0.12
(1,526)	1:61:A:HIS:HB2	1:63:A:GLU:H	8	0.12
(1,526)	1:61:A:HIS:HB3	1:63:A:GLU:H	8	0.12
(1,523)	1:57:A:HIS:HB2	1:60:A:SER:H	16	0.12
(1,523)	1:57:A:HIS:HB3	1:60:A:SER:H	16	0.12
(1,488)	1:109:A:ARG:HA	1:112:A:LEU:HB2	14	0.12
(1,488)	1:109:A:ARG:HA	1:112:A:LEU:HB3	14	0.12
(1,405)	1:117:A:PHE:HA	1:120:A:GLU:H	11	0.12
(1,353)	1:167:A:LEU:HB2	1:168:A:LEU:H	17	0.12
(1,353)	1:167:A:LEU:HB3	1:168:A:LEU:H	17	0.12
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	2	0.12
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	2	0.12
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	2	0.12
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	19	0.12
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	19	0.12
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	19	0.12
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG21	4	0.12
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG22	4	0.12
(1,341)	1:152:A:GLU:H	1:153:A:THR:HG23	4	0.12
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	2	0.12
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	2	0.12
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	5	0.12
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	5	0.12
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	3	0.12
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	11	0.12
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	11	0.12
(1,330)	1:145:A:MET:HB2	1:146:A:LEU:H	11	0.12
(1,330)	1:145:A:MET:HB3	1:146:A:LEU:H	11	0.12
(1,315)	1:123:A:SER:HB2	1:124:A:LEU:H	6	0.12
(1,315)	1:123:A:SER:HB3	1:124:A:LEU:H	6	0.12
(1,315)	1:123:A:SER:HB2	1:124:A:LEU:H	14	0.12
(1,315)	1:123:A:SER:HB3	1:124:A:LEU:H	14	0.12
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	2	0.12
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	2	0.12
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	5	0.12
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	5	0.12
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	14	0.12
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	14	0.12
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	17	0.12
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	17	0.12
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	8	0.12
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	8	0.12
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	16	0.12
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	16	0.12
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	5	0.12
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	5	0.12
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	10	0.12
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	10	0.12
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	15	0.12
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	15	0.12
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	2	0.12
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	2	0.12
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	5	0.12
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	5	0.12
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	13	0.12
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	13	0.12
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	17	0.12
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	17	0.12
(1,280)	1:98:A:ARG:HB2	1:99:A:GLN:H	6	0.12
(1,280)	1:98:A:ARG:HB3	1:99:A:GLN:H	6	0.12
(1,242)	1:73:A:LEU:HB2	1:74:A:ILE:H	2	0.12
(1,242)	1:73:A:LEU:HB3	1:74:A:ILE:H	2	0.12
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	6	0.12
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	6	0.12
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	11	0.12
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	14	0.12
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	14	0.12
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	18	0.12
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	18	0.12
(1,226)	1:205:A:LYS:HA	1:206:A:LEU:H	4	0.12
(1,193)	1:160:A:TRP:HA	1:161:A:GLU:H	5	0.12
(1,193)	1:160:A:TRP:HA	1:161:A:GLU:H	6	0.12
(1,193)	1:160:A:TRP:HA	1:161:A:GLU:H	11	0.12
(1,193)	1:160:A:TRP:HA	1:161:A:GLU:H	12	0.12
(1,193)	1:160:A:TRP:HA	1:161:A:GLU:H	13	0.12
(1,193)	1:160:A:TRP:HA	1:161:A:GLU:H	16	0.12
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	1	0.12
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	14	0.12
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	20	0.12
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	5	0.12
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	8	0.12
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	14	0.12
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	16	0.12
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	1	0.12
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	2	0.12
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	5	0.12
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	13	0.12
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	14	0.12
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	15	0.12
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	16	0.12
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	1	0.12
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	3	0.12
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	5	0.12
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	7	0.12
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	8	0.12
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	10	0.12
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	20	0.12
(3,104)	1:189:A:MET:H	1:198:A:CYS:O	13	0.11
(2,128)	1:185:A:ILE:O	1:189:A:MET:N	7	0.11
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	14	0.11
(2,116)	1:179:A:ALA:O	1:183:A:PHE:N	19	0.11
(2,115)	1:179:A:ALA:O	1:183:A:PHE:H	20	0.11
(2,113)	1:171:A:ASP:O	1:175:A:ALA:H	20	0.11
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	4	0.11
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	11	0.11
(2,105)	1:167:A:LEU:O	1:171:A:ASP:H	2	0.11
(2,105)	1:167:A:LEU:O	1:171:A:ASP:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	18	0.11
(2,95)	1:147:A:LEU:O	1:151:A:GLU:H	19	0.11
(2,80)	1:120:A:GLU:O	1:124:A:LEU:N	10	0.11
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	1	0.11
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	5	0.11
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	14	0.11
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	4	0.11
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	8	0.11
(2,57)	1:102:A:ARG:O	1:106:A:ASN:H	20	0.11
(2,51)	1:99:A:GLN:O	1:103:A:GLU:H	7	0.11
(2,51)	1:99:A:GLN:O	1:103:A:GLU:H	8	0.11
(2,47)	1:97:A:LEU:O	1:101:A:ARG:H	10	0.11
(2,45)	1:96:A:THR:O	1:100:A:ILE:H	16	0.11
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	15	0.11
(2,20)	1:74:A:ILE:O	1:78:A:ASN:N	19	0.11
(2,12)	1:70:A:LEU:O	1:74:A:ILE:N	1	0.11
(2,12)	1:70:A:LEU:O	1:74:A:ILE:N	15	0.11
(1,1098)	1:173:A:LEU:HD11	1:182:A:PHE:HE1	18	0.11
(1,1098)	1:173:A:LEU:HD11	1:182:A:PHE:HE2	18	0.11
(1,1098)	1:173:A:LEU:HD12	1:182:A:PHE:HE1	18	0.11
(1,1098)	1:173:A:LEU:HD12	1:182:A:PHE:HE2	18	0.11
(1,1098)	1:173:A:LEU:HD13	1:182:A:PHE:HE1	18	0.11
(1,1098)	1:173:A:LEU:HD13	1:182:A:PHE:HE2	18	0.11
(1,1098)	1:173:A:LEU:HD21	1:182:A:PHE:HE1	18	0.11
(1,1098)	1:173:A:LEU:HD21	1:182:A:PHE:HE2	18	0.11
(1,1098)	1:173:A:LEU:HD22	1:182:A:PHE:HE1	18	0.11
(1,1098)	1:173:A:LEU:HD22	1:182:A:PHE:HE2	18	0.11
(1,1098)	1:173:A:LEU:HD23	1:182:A:PHE:HE1	18	0.11
(1,1098)	1:173:A:LEU:HD23	1:182:A:PHE:HE2	18	0.11
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE1	3	0.11
(1,1095)	1:170:A:VAL:HG11	1:182:A:PHE:HE2	3	0.11
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE1	3	0.11
(1,1095)	1:170:A:VAL:HG12	1:182:A:PHE:HE2	3	0.11
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE1	3	0.11
(1,1095)	1:170:A:VAL:HG13	1:182:A:PHE:HE2	3	0.11
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE1	3	0.11
(1,1095)	1:170:A:VAL:HG21	1:182:A:PHE:HE2	3	0.11
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE1	3	0.11
(1,1095)	1:170:A:VAL:HG22	1:182:A:PHE:HE2	3	0.11
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE1	3	0.11
(1,1095)	1:170:A:VAL:HG23	1:182:A:PHE:HE2	3	0.11
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:170:A:VAL:HG11	1:182:A:PHE:HB3	2	0.11
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB2	2	0.11
(1,1094)	1:170:A:VAL:HG12	1:182:A:PHE:HB3	2	0.11
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB2	2	0.11
(1,1094)	1:170:A:VAL:HG13	1:182:A:PHE:HB3	2	0.11
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB2	2	0.11
(1,1094)	1:170:A:VAL:HG21	1:182:A:PHE:HB3	2	0.11
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB2	2	0.11
(1,1094)	1:170:A:VAL:HG22	1:182:A:PHE:HB3	2	0.11
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB2	2	0.11
(1,1094)	1:170:A:VAL:HG23	1:182:A:PHE:HB3	2	0.11
(1,1086)	1:160:A:TRP:HZ2	1:167:A:LEU:HB2	15	0.11
(1,1086)	1:160:A:TRP:HZ2	1:167:A:LEU:HB3	15	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB2	2	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB3	2	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB2	2	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB3	2	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB2	2	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB3	2	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB2	5	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB3	5	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB2	5	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB3	5	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB2	5	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB3	5	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB2	10	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB3	10	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB2	10	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB3	10	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB2	10	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB3	10	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB2	15	0.11
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB3	15	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB2	15	0.11
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB3	15	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB2	15	0.11
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB3	15	0.11
(1,1074)	1:158:A:ALA:HB1	1:189:A:MET:HG2	9	0.11
(1,1074)	1:158:A:ALA:HB1	1:189:A:MET:HG3	9	0.11
(1,1074)	1:158:A:ALA:HB2	1:189:A:MET:HG2	9	0.11
(1,1074)	1:158:A:ALA:HB2	1:189:A:MET:HG3	9	0.11
(1,1074)	1:158:A:ALA:HB3	1:189:A:MET:HG2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:158:A:ALA:HB3	1:189:A:MET:HG3	9	0.11
(1,1074)	1:158:A:ALA:HB1	1:189:A:MET:HG2	11	0.11
(1,1074)	1:158:A:ALA:HB1	1:189:A:MET:HG3	11	0.11
(1,1074)	1:158:A:ALA:HB2	1:189:A:MET:HG2	11	0.11
(1,1074)	1:158:A:ALA:HB2	1:189:A:MET:HG3	11	0.11
(1,1074)	1:158:A:ALA:HB3	1:189:A:MET:HG2	11	0.11
(1,1074)	1:158:A:ALA:HB3	1:189:A:MET:HG3	11	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	5	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	5	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	5	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	5	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	5	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	5	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	7	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	7	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	7	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	7	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	7	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	7	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	11	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	11	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	11	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	11	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	11	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	11	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	16	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	16	0.11
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	16	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	16	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	16	0.11
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	16	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD11	9	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD12	9	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD13	9	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD21	9	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD22	9	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD23	9	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD11	9	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD12	9	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD13	9	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD21	9	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD22	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD23	9	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD11	13	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD12	13	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD13	13	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD21	13	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD22	13	0.11
(1,1060)	1:156:A:PHE:HD1	1:167:A:LEU:HD23	13	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD11	13	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD12	13	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD13	13	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD21	13	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD22	13	0.11
(1,1060)	1:156:A:PHE:HD2	1:167:A:LEU:HD23	13	0.11
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	9	0.11
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	9	0.11
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	9	0.11
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	9	0.11
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	9	0.11
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	9	0.11
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	9	0.11
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	9	0.11
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	9	0.11
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	9	0.11
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	9	0.11
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	9	0.11
(1,1057)	1:156:A:PHE:HE1	1:166:A:TYR:HB2	6	0.11
(1,1057)	1:156:A:PHE:HE1	1:166:A:TYR:HB3	6	0.11
(1,1057)	1:156:A:PHE:HE2	1:166:A:TYR:HB2	6	0.11
(1,1057)	1:156:A:PHE:HE2	1:166:A:TYR:HB3	6	0.11
(1,1057)	1:156:A:PHE:HE1	1:166:A:TYR:HB2	9	0.11
(1,1057)	1:156:A:PHE:HE1	1:166:A:TYR:HB3	9	0.11
(1,1057)	1:156:A:PHE:HE2	1:166:A:TYR:HB2	9	0.11
(1,1057)	1:156:A:PHE:HE2	1:166:A:TYR:HB3	9	0.11
(1,1057)	1:156:A:PHE:HE1	1:166:A:TYR:HB2	11	0.11
(1,1057)	1:156:A:PHE:HE1	1:166:A:TYR:HB3	11	0.11
(1,1057)	1:156:A:PHE:HE2	1:166:A:TYR:HB2	11	0.11
(1,1057)	1:156:A:PHE:HE2	1:166:A:TYR:HB3	11	0.11
(1,1056)	1:156:A:PHE:HA	1:185:A:ILE:HB	9	0.11
(1,1056)	1:156:A:PHE:HA	1:185:A:ILE:HB	10	0.11
(1,1056)	1:156:A:PHE:HA	1:185:A:ILE:HB	20	0.11
(1,1020)	1:152:A:GLU:HG2	1:190:A:TYR:HD1	4	0.11
(1,1020)	1:152:A:GLU:HG2	1:190:A:TYR:HD2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:152:A:GLU:HG3	1:190:A:TYR:HD1	4	0.11
(1,1020)	1:152:A:GLU:HG3	1:190:A:TYR:HD2	4	0.11
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	1	0.11
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	1	0.11
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	19	0.11
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	19	0.11
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG2	20	0.11
(1,1018)	1:152:A:GLU:HA	1:189:A:MET:HG3	20	0.11
(1,1012)	1:150:A:ALA:HB1	1:159:A:SER:HA	8	0.11
(1,1012)	1:150:A:ALA:HB2	1:159:A:SER:HA	8	0.11
(1,1012)	1:150:A:ALA:HB3	1:159:A:SER:HA	8	0.11
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	4	0.11
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	4	0.11
(1,1000)	1:146:A:LEU:HG	1:164:A:GLU:HB2	11	0.11
(1,1000)	1:146:A:LEU:HG	1:164:A:GLU:HB3	11	0.11
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	5	0.11
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	9	0.11
(1,996)	1:146:A:LEU:HG	1:163:A:SER:HG	17	0.11
(1,995)	1:146:A:LEU:HD11	1:163:A:SER:HG	11	0.11
(1,995)	1:146:A:LEU:HD12	1:163:A:SER:HG	11	0.11
(1,995)	1:146:A:LEU:HD13	1:163:A:SER:HG	11	0.11
(1,995)	1:146:A:LEU:HD21	1:163:A:SER:HG	11	0.11
(1,995)	1:146:A:LEU:HD22	1:163:A:SER:HG	11	0.11
(1,995)	1:146:A:LEU:HD23	1:163:A:SER:HG	11	0.11
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	6	0.11
(1,989)	1:125:A:LEU:HG	1:146:A:LEU:HG	11	0.11
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	5	0.11
(1,987)	1:125:A:LEU:HA	1:146:A:LEU:HG	10	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	1	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	1	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	2	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	2	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	7	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	7	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	10	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	10	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	19	0.11
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	19	0.11
(1,976)	1:124:A:LEU:HG	1:152:A:GLU:HG2	11	0.11
(1,976)	1:124:A:LEU:HG	1:152:A:GLU:HG3	11	0.11
(1,969)	1:124:A:LEU:HB2	1:149:A:LEU:HG	4	0.11
(1,969)	1:124:A:LEU:HB3	1:149:A:LEU:HG	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD11	4	0.11
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD12	4	0.11
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD13	4	0.11
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD21	4	0.11
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD22	4	0.11
(1,968)	1:124:A:LEU:HB2	1:149:A:LEU:HD23	4	0.11
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD11	4	0.11
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD12	4	0.11
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD13	4	0.11
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD21	4	0.11
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD22	4	0.11
(1,968)	1:124:A:LEU:HB3	1:149:A:LEU:HD23	4	0.11
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	4	0.11
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	10	0.11
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	11	0.11
(1,954)	1:123:A:SER:HG	1:190:A:TYR:HB2	2	0.11
(1,954)	1:123:A:SER:HG	1:190:A:TYR:HB3	2	0.11
(1,953)	1:123:A:SER:HG	1:153:A:THR:HA	10	0.11
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	6	0.11
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	6	0.11
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	9	0.11
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	9	0.11
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE1	17	0.11
(1,952)	1:123:A:SER:HG	1:190:A:TYR:HE2	17	0.11
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	3	0.11
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	3	0.11
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	3	0.11
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	3	0.11
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	3	0.11
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	3	0.11
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	3	0.11
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	3	0.11
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	3	0.11
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	7	0.11
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	7	0.11
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	7	0.11
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	7	0.11
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	7	0.11
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	7	0.11
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	7	0.11
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	7	0.11
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE1	6	0.11
(1,948)	1:121:A:ALA:HB1	1:182:A:PHE:HE2	6	0.11
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE1	6	0.11
(1,948)	1:121:A:ALA:HB2	1:182:A:PHE:HE2	6	0.11
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE1	6	0.11
(1,948)	1:121:A:ALA:HB3	1:182:A:PHE:HE2	6	0.11
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD1	15	0.11
(1,946)	1:121:A:ALA:HB1	1:182:A:PHE:HD2	15	0.11
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD1	15	0.11
(1,946)	1:121:A:ALA:HB2	1:182:A:PHE:HD2	15	0.11
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD1	15	0.11
(1,946)	1:121:A:ALA:HB3	1:182:A:PHE:HD2	15	0.11
(1,935)	1:117:A:PHE:HE1	1:174:A:ILE:HB	10	0.11
(1,935)	1:117:A:PHE:HE2	1:174:A:ILE:HB	10	0.11
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB1	14	0.11
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB2	14	0.11
(1,933)	1:117:A:PHE:HE1	1:179:A:ALA:HB3	14	0.11
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB1	14	0.11
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB2	14	0.11
(1,933)	1:117:A:PHE:HE2	1:179:A:ALA:HB3	14	0.11
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD1	11	0.11
(1,923)	1:112:A:LEU:HG	1:183:A:PHE:HD2	11	0.11
(1,917)	1:111:A:ILE:HD11	1:185:A:ILE:HD11	17	0.11
(1,917)	1:111:A:ILE:HD11	1:185:A:ILE:HD12	17	0.11
(1,917)	1:111:A:ILE:HD11	1:185:A:ILE:HD13	17	0.11
(1,917)	1:111:A:ILE:HD12	1:185:A:ILE:HD11	17	0.11
(1,917)	1:111:A:ILE:HD12	1:185:A:ILE:HD12	17	0.11
(1,917)	1:111:A:ILE:HD12	1:185:A:ILE:HD13	17	0.11
(1,917)	1:111:A:ILE:HD13	1:185:A:ILE:HD11	17	0.11
(1,917)	1:111:A:ILE:HD13	1:185:A:ILE:HD12	17	0.11
(1,917)	1:111:A:ILE:HD13	1:185:A:ILE:HD13	17	0.11
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD1	13	0.11
(1,913)	1:111:A:ILE:HD11	1:156:A:PHE:HD2	13	0.11
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD1	13	0.11
(1,913)	1:111:A:ILE:HD12	1:156:A:PHE:HD2	13	0.11
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD1	13	0.11
(1,913)	1:111:A:ILE:HD13	1:156:A:PHE:HD2	13	0.11
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB2	7	0.11
(1,911)	1:111:A:ILE:HD11	1:183:A:PHE:HB3	7	0.11
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB2	7	0.11
(1,911)	1:111:A:ILE:HD12	1:183:A:PHE:HB3	7	0.11
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:111:A:ILE:HD13	1:183:A:PHE:HB3	7	0.11
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD1	5	0.11
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD2	5	0.11
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD1	5	0.11
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD2	5	0.11
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD1	5	0.11
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD2	5	0.11
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB2	2	0.11
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB3	2	0.11
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB2	2	0.11
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB3	2	0.11
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB2	2	0.11
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB3	2	0.11
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB2	11	0.11
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB3	11	0.11
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB2	11	0.11
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB3	11	0.11
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB2	11	0.11
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB3	11	0.11
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB2	13	0.11
(1,908)	1:111:A:ILE:HD11	1:182:A:PHE:HB3	13	0.11
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB2	13	0.11
(1,908)	1:111:A:ILE:HD12	1:182:A:PHE:HB3	13	0.11
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB2	13	0.11
(1,908)	1:111:A:ILE:HD13	1:182:A:PHE:HB3	13	0.11
(1,902)	1:111:A:ILE:HD13	1:155:A:ILE:HG21	5	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	7	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	7	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	7	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	7	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	7	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	7	0.11
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	7	0.11
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	7	0.11
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	7	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	8	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	8	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	8	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	8	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	8	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	8	0.11
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	8	0.11
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	8	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB1	19	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB2	19	0.11
(1,899)	1:111:A:ILE:HD11	1:186:A:ALA:HB3	19	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB1	19	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB2	19	0.11
(1,899)	1:111:A:ILE:HD12	1:186:A:ALA:HB3	19	0.11
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB1	19	0.11
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB2	19	0.11
(1,899)	1:111:A:ILE:HD13	1:186:A:ALA:HB3	19	0.11
(1,894)	1:109:A:ARG:HG2	1:127:A:VAL:HB	16	0.11
(1,894)	1:109:A:ARG:HG3	1:127:A:VAL:HB	16	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	11	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	11	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	11	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	11	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	11	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	11	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	13	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	13	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	13	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	13	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	13	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	13	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD11	15	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD12	15	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD13	15	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD21	15	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD22	15	0.11
(1,888)	1:108:A:TRP:HZ2	1:149:A:LEU:HD23	15	0.11
(1,887)	1:108:A:TRP:HZ2	1:167:A:LEU:HB2	2	0.11
(1,887)	1:108:A:TRP:HZ2	1:167:A:LEU:HB3	2	0.11
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	6	0.11
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	6	0.11
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	19	0.11
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	19	0.11
(1,876)	1:107:A:ARG:HB2	1:168:A:LEU:HG	3	0.11
(1,876)	1:107:A:ARG:HB3	1:168:A:LEU:HG	3	0.11
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG11	1	0.11
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG12	1	0.11
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG13	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG21	1	0.11
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG22	1	0.11
(1,874)	1:105:A:ARG:HG2	1:127:A:VAL:HG23	1	0.11
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG11	1	0.11
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG12	1	0.11
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG13	1	0.11
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG21	1	0.11
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG22	1	0.11
(1,874)	1:105:A:ARG:HG3	1:127:A:VAL:HG23	1	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	8	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	8	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	8	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	8	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	8	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	8	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	8	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	8	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	8	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	8	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	8	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	8	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	11	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	11	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	11	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	11	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	11	0.11
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	11	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	11	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	11	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	11	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	11	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	11	0.11
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	11	0.11
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB2	19	0.11
(1,866)	1:104:A:VAL:HG11	1:165:A:ARG:HB3	19	0.11
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB2	19	0.11
(1,866)	1:104:A:VAL:HG12	1:165:A:ARG:HB3	19	0.11
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB2	19	0.11
(1,866)	1:104:A:VAL:HG13	1:165:A:ARG:HB3	19	0.11
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB2	19	0.11
(1,866)	1:104:A:VAL:HG21	1:165:A:ARG:HB3	19	0.11
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:104:A:VAL:HG22	1:165:A:ARG:HB3	19	0.11
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB2	19	0.11
(1,866)	1:104:A:VAL:HG23	1:165:A:ARG:HB3	19	0.11
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	5	0.11
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	5	0.11
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	10	0.11
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	10	0.11
(1,858)	1:101:A:ARG:HB2	1:142:A:ALA:HA	20	0.11
(1,858)	1:101:A:ARG:HB3	1:142:A:ALA:HA	20	0.11
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG2	16	0.11
(1,849)	1:100:A:ILE:HD11	1:164:A:GLU:HG3	16	0.11
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG2	16	0.11
(1,849)	1:100:A:ILE:HD12	1:164:A:GLU:HG3	16	0.11
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG2	16	0.11
(1,849)	1:100:A:ILE:HD13	1:164:A:GLU:HG3	16	0.11
(1,846)	1:100:A:ILE:HD11	1:143:A:ARG:HB2	6	0.11
(1,846)	1:100:A:ILE:HD11	1:143:A:ARG:HB3	6	0.11
(1,846)	1:100:A:ILE:HD12	1:143:A:ARG:HB2	6	0.11
(1,846)	1:100:A:ILE:HD12	1:143:A:ARG:HB3	6	0.11
(1,846)	1:100:A:ILE:HD13	1:143:A:ARG:HB2	6	0.11
(1,846)	1:100:A:ILE:HD13	1:143:A:ARG:HB3	6	0.11
(1,838)	1:98:A:ARG:HB2	1:142:A:ALA:HA	5	0.11
(1,838)	1:98:A:ARG:HB3	1:142:A:ALA:HA	5	0.11
(1,838)	1:98:A:ARG:HB2	1:142:A:ALA:HA	6	0.11
(1,838)	1:98:A:ARG:HB3	1:142:A:ALA:HA	6	0.11
(1,832)	1:97:A:LEU:HG	1:142:A:ALA:HA	6	0.11
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	7	0.11
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	7	0.11
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	7	0.11
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	7	0.11
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	7	0.11
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	7	0.11
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB2	12	0.11
(1,829)	1:97:A:LEU:HG	1:143:A:ARG:HB3	12	0.11
(1,822)	1:76:A:ILE:HG22	1:90:A:LEU:HD12	7	0.11
(1,817)	1:76:A:ILE:HD11	1:87:A:TRP:HE1	9	0.11
(1,817)	1:76:A:ILE:HD12	1:87:A:TRP:HE1	9	0.11
(1,817)	1:76:A:ILE:HD13	1:87:A:TRP:HE1	9	0.11
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	4	0.11
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	4	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	4	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	6	0.11
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	6	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	6	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	6	0.11
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	9	0.11
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	9	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	9	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	9	0.11
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	12	0.11
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	12	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	12	0.11
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	12	0.11
(1,801)	1:73:A:LEU:HD11	1:91:A:ASN:HB2	10	0.11
(1,801)	1:73:A:LEU:HD11	1:91:A:ASN:HB3	10	0.11
(1,801)	1:73:A:LEU:HD12	1:91:A:ASN:HB2	10	0.11
(1,801)	1:73:A:LEU:HD12	1:91:A:ASN:HB3	10	0.11
(1,801)	1:73:A:LEU:HD13	1:91:A:ASN:HB2	10	0.11
(1,801)	1:73:A:LEU:HD13	1:91:A:ASN:HB3	10	0.11
(1,801)	1:73:A:LEU:HD21	1:91:A:ASN:HB2	10	0.11
(1,801)	1:73:A:LEU:HD21	1:91:A:ASN:HB3	10	0.11
(1,801)	1:73:A:LEU:HD22	1:91:A:ASN:HB2	10	0.11
(1,801)	1:73:A:LEU:HD22	1:91:A:ASN:HB3	10	0.11
(1,801)	1:73:A:LEU:HD23	1:91:A:ASN:HB2	10	0.11
(1,801)	1:73:A:LEU:HD23	1:91:A:ASN:HB3	10	0.11
(1,801)	1:73:A:LEU:HD11	1:91:A:ASN:HB2	14	0.11
(1,801)	1:73:A:LEU:HD11	1:91:A:ASN:HB3	14	0.11
(1,801)	1:73:A:LEU:HD12	1:91:A:ASN:HB2	14	0.11
(1,801)	1:73:A:LEU:HD12	1:91:A:ASN:HB3	14	0.11
(1,801)	1:73:A:LEU:HD13	1:91:A:ASN:HB2	14	0.11
(1,801)	1:73:A:LEU:HD13	1:91:A:ASN:HB3	14	0.11
(1,801)	1:73:A:LEU:HD21	1:91:A:ASN:HB2	14	0.11
(1,801)	1:73:A:LEU:HD21	1:91:A:ASN:HB3	14	0.11
(1,801)	1:73:A:LEU:HD22	1:91:A:ASN:HB2	14	0.11
(1,801)	1:73:A:LEU:HD22	1:91:A:ASN:HB3	14	0.11
(1,801)	1:73:A:LEU:HD23	1:91:A:ASN:HB2	14	0.11
(1,801)	1:73:A:LEU:HD23	1:91:A:ASN:HB3	14	0.11
(1,799)	1:73:A:LEU:HD11	1:87:A:TRP:HB2	16	0.11
(1,799)	1:73:A:LEU:HD11	1:87:A:TRP:HB3	16	0.11
(1,799)	1:73:A:LEU:HD12	1:87:A:TRP:HB2	16	0.11
(1,799)	1:73:A:LEU:HD12	1:87:A:TRP:HB3	16	0.11
(1,799)	1:73:A:LEU:HD13	1:87:A:TRP:HB2	16	0.11
(1,799)	1:73:A:LEU:HD13	1:87:A:TRP:HB3	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	1:73:A:LEU:HD21	1:87:A:TRP:HB2	16	0.11
(1,799)	1:73:A:LEU:HD21	1:87:A:TRP:HB3	16	0.11
(1,799)	1:73:A:LEU:HD22	1:87:A:TRP:HB2	16	0.11
(1,799)	1:73:A:LEU:HD22	1:87:A:TRP:HB3	16	0.11
(1,799)	1:73:A:LEU:HD23	1:87:A:TRP:HB2	16	0.11
(1,799)	1:73:A:LEU:HD23	1:87:A:TRP:HB3	16	0.11
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	7	0.11
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	11	0.11
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB2	4	0.11
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB3	4	0.11
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB2	4	0.11
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB3	4	0.11
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB2	6	0.11
(1,766)	1:67:A:ASP:HB2	1:97:A:LEU:HB3	6	0.11
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB2	6	0.11
(1,766)	1:67:A:ASP:HB3	1:97:A:LEU:HB3	6	0.11
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	4	0.11
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	4	0.11
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	4	0.11
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	4	0.11
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	14	0.11
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	14	0.11
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	14	0.11
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	14	0.11
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	20	0.11
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	20	0.11
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	20	0.11
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	20	0.11
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	2	0.11
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	2	0.11
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	2	0.11
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	2	0.11
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	2	0.11
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	2	0.11
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	2	0.11
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	2	0.11
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	2	0.11
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	2	0.11
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	2	0.11
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	2	0.11
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	2	0.11
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	2	0.11
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	2	0.11
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	2	0.11
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	2	0.11
(1,750)	1:58:A:ASP:HB2	1:68:A:ARG:HG2	19	0.11
(1,750)	1:58:A:ASP:HB2	1:68:A:ARG:HG3	19	0.11
(1,750)	1:58:A:ASP:HB3	1:68:A:ARG:HG2	19	0.11
(1,750)	1:58:A:ASP:HB3	1:68:A:ARG:HG3	19	0.11
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	3	0.11
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	3	0.11
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	3	0.11
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	5	0.11
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	5	0.11
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	5	0.11
(1,744)	1:158:A:ALA:HB1	1:190:A:TYR:H	12	0.11
(1,744)	1:158:A:ALA:HB2	1:190:A:TYR:H	12	0.11
(1,744)	1:158:A:ALA:HB3	1:190:A:TYR:H	12	0.11
(1,740)	1:156:A:PHE:H	1:167:A:LEU:HG	14	0.11
(1,717)	1:150:A:ALA:H	1:161:A:GLU:HG2	9	0.11
(1,717)	1:150:A:ALA:H	1:161:A:GLU:HG3	9	0.11
(1,715)	1:146:A:LEU:HD11	1:163:A:SER:H	14	0.11
(1,715)	1:146:A:LEU:HD12	1:163:A:SER:H	14	0.11
(1,715)	1:146:A:LEU:HD13	1:163:A:SER:H	14	0.11
(1,715)	1:146:A:LEU:HD21	1:163:A:SER:H	14	0.11
(1,715)	1:146:A:LEU:HD22	1:163:A:SER:H	14	0.11
(1,715)	1:146:A:LEU:HD23	1:163:A:SER:H	14	0.11
(1,708)	1:125:A:LEU:H	1:146:A:LEU:HA	1	0.11
(1,708)	1:125:A:LEU:H	1:146:A:LEU:HA	7	0.11
(1,708)	1:125:A:LEU:H	1:146:A:LEU:HA	10	0.11
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD11	13	0.11
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD12	13	0.11
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD13	13	0.11
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD21	13	0.11
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD22	13	0.11
(1,707)	1:125:A:LEU:H	1:146:A:LEU:HD23	13	0.11
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB2	2	0.11
(1,695)	1:121:A:ALA:H	1:182:A:PHE:HB3	2	0.11
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	9	0.11
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	9	0.11
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	13	0.11
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	13	0.11
(1,679)	1:105:A:ARG:HD2	1:125:A:LEU:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:105:A:ARG:HD3	1:125:A:LEU:H	18	0.11
(1,678)	1:105:A:ARG:HG2	1:125:A:LEU:H	4	0.11
(1,678)	1:105:A:ARG:HG3	1:125:A:LEU:H	4	0.11
(1,660)	1:95:A:TYR:HB2	1:139:A:THR:H	16	0.11
(1,660)	1:95:A:TYR:HB3	1:139:A:THR:H	16	0.11
(1,658)	1:77:A:ARG:HB2	1:87:A:TRP:H	1	0.11
(1,658)	1:77:A:ARG:HB3	1:87:A:TRP:H	1	0.11
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	4	0.11
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	4	0.11
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	4	0.11
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	13	0.11
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	13	0.11
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	13	0.11
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	16	0.11
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	16	0.11
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	16	0.11
(1,656)	1:76:A:ILE:HD11	1:87:A:TRP:H	18	0.11
(1,656)	1:76:A:ILE:HD12	1:87:A:TRP:H	18	0.11
(1,656)	1:76:A:ILE:HD13	1:87:A:TRP:H	18	0.11
(1,647)	1:73:A:LEU:HD11	1:90:A:LEU:H	15	0.11
(1,647)	1:73:A:LEU:HD12	1:90:A:LEU:H	15	0.11
(1,647)	1:73:A:LEU:HD13	1:90:A:LEU:H	15	0.11
(1,647)	1:73:A:LEU:HD21	1:90:A:LEU:H	15	0.11
(1,647)	1:73:A:LEU:HD22	1:90:A:LEU:H	15	0.11
(1,647)	1:73:A:LEU:HD23	1:90:A:LEU:H	15	0.11
(1,637)	1:58:A:ASP:HB2	1:69:A:ILE:H	16	0.11
(1,637)	1:58:A:ASP:HB3	1:69:A:ILE:H	16	0.11
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB1	20	0.11
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB2	20	0.11
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB3	20	0.11
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB1	20	0.11
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB2	20	0.11
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB3	20	0.11
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB1	20	0.11
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB2	20	0.11
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB3	20	0.11
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB1	20	0.11
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB2	20	0.11
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB3	20	0.11
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB1	20	0.11
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB2	20	0.11
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB3	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB1	20	0.11
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB2	20	0.11
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB3	20	0.11
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	5	0.11
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	5	0.11
(1,626)	1:162:A:LEU:HB2	1:167:A:LEU:HG	16	0.11
(1,626)	1:162:A:LEU:HB3	1:167:A:LEU:HG	16	0.11
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	4	0.11
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	4	0.11
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB2	9	0.11
(1,624)	1:162:A:LEU:HG	1:167:A:LEU:HB3	9	0.11
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD11	3	0.11
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD12	3	0.11
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD13	3	0.11
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD21	3	0.11
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD22	3	0.11
(1,619)	1:160:A:TRP:HD1	1:162:A:LEU:HD23	3	0.11
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG11	18	0.11
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG12	18	0.11
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG13	18	0.11
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG21	18	0.11
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG22	18	0.11
(1,598)	1:122:A:ASP:HB2	1:127:A:VAL:HG23	18	0.11
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG11	18	0.11
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG12	18	0.11
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG13	18	0.11
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG21	18	0.11
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG22	18	0.11
(1,598)	1:122:A:ASP:HB3	1:127:A:VAL:HG23	18	0.11
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE1	13	0.11
(1,592)	1:112:A:LEU:HD11	1:117:A:PHE:HE2	13	0.11
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE1	13	0.11
(1,592)	1:112:A:LEU:HD12	1:117:A:PHE:HE2	13	0.11
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE1	13	0.11
(1,592)	1:112:A:LEU:HD13	1:117:A:PHE:HE2	13	0.11
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE1	13	0.11
(1,592)	1:112:A:LEU:HD21	1:117:A:PHE:HE2	13	0.11
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE1	13	0.11
(1,592)	1:112:A:LEU:HD22	1:117:A:PHE:HE2	13	0.11
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE1	13	0.11
(1,592)	1:112:A:LEU:HD23	1:117:A:PHE:HE2	13	0.11
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	11	0.11
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE1	13	0.11
(1,591)	1:112:A:LEU:HG	1:117:A:PHE:HE2	13	0.11
(1,589)	1:112:A:LEU:HD11	1:117:A:PHE:HD1	13	0.11
(1,589)	1:112:A:LEU:HD11	1:117:A:PHE:HD2	13	0.11
(1,589)	1:112:A:LEU:HD12	1:117:A:PHE:HD1	13	0.11
(1,589)	1:112:A:LEU:HD12	1:117:A:PHE:HD2	13	0.11
(1,589)	1:112:A:LEU:HD13	1:117:A:PHE:HD1	13	0.11
(1,589)	1:112:A:LEU:HD13	1:117:A:PHE:HD2	13	0.11
(1,589)	1:112:A:LEU:HD21	1:117:A:PHE:HD1	13	0.11
(1,589)	1:112:A:LEU:HD21	1:117:A:PHE:HD2	13	0.11
(1,589)	1:112:A:LEU:HD22	1:117:A:PHE:HD1	13	0.11
(1,589)	1:112:A:LEU:HD22	1:117:A:PHE:HD2	13	0.11
(1,589)	1:112:A:LEU:HD23	1:117:A:PHE:HD1	13	0.11
(1,589)	1:112:A:LEU:HD23	1:117:A:PHE:HD2	13	0.11
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB2	11	0.11
(1,582)	1:62:A:THR:HG21	1:65:A:ASP:HB3	11	0.11
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB2	11	0.11
(1,582)	1:62:A:THR:HG22	1:65:A:ASP:HB3	11	0.11
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB2	11	0.11
(1,582)	1:62:A:THR:HG23	1:65:A:ASP:HB3	11	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB2	8	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB3	8	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB2	9	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB3	9	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB2	10	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB3	10	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB2	18	0.11
(1,580)	1:62:A:THR:HB	1:65:A:ASP:HB3	18	0.11
(1,575)	1:162:A:LEU:HG	1:167:A:LEU:H	3	0.11
(1,574)	1:162:A:LEU:HD11	1:167:A:LEU:H	3	0.11
(1,574)	1:162:A:LEU:HD12	1:167:A:LEU:H	3	0.11
(1,574)	1:162:A:LEU:HD13	1:167:A:LEU:H	3	0.11
(1,574)	1:162:A:LEU:HD21	1:167:A:LEU:H	3	0.11
(1,574)	1:162:A:LEU:HD22	1:167:A:LEU:H	3	0.11
(1,574)	1:162:A:LEU:HD23	1:167:A:LEU:H	3	0.11
(1,564)	1:155:A:ILE:H	1:160:A:TRP:HE1	6	0.11
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	7	0.11
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	7	0.11
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	7	0.11
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	14	0.11
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	14	0.11
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	12	0.11
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	16	0.11
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	3	0.11
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	3	0.11
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	3	0.11
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	6	0.11
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	6	0.11
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	6	0.11
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	7	0.11
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	7	0.11
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	7	0.11
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	10	0.11
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	10	0.11
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	10	0.11
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	18	0.11
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	18	0.11
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	18	0.11
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	5	0.11
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	8	0.11
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	16	0.11
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	17	0.11
(1,536)	1:82:A:LYS:HG2	1:84:A:SER:H	14	0.11
(1,536)	1:82:A:LYS:HG3	1:84:A:SER:H	14	0.11
(1,534)	1:80:A:GLN:HG2	1:82:A:LYS:H	20	0.11
(1,534)	1:80:A:GLN:HG3	1:82:A:LYS:H	20	0.11
(1,485)	1:106:A:ASN:HA	1:109:A:ARG:HB2	17	0.11
(1,485)	1:106:A:ASN:HA	1:109:A:ARG:HB3	17	0.11
(1,406)	1:118:A:GLN:HA	1:121:A:ALA:H	5	0.11
(1,406)	1:118:A:GLN:HA	1:121:A:ALA:H	14	0.11
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	11	0.11
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	6	0.11
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	6	0.11
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	6	0.11
(1,346)	1:153:A:THR:HG21	1:154:A:SER:H	14	0.11
(1,346)	1:153:A:THR:HG22	1:154:A:SER:H	14	0.11
(1,346)	1:153:A:THR:HG23	1:154:A:SER:H	14	0.11
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	2	0.11
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	3	0.11
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	17	0.11
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	1	0.11
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	7	0.11
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	7	0.11
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	10	0.11
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	10	0.11
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	16	0.11
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	16	0.11
(1,336)	1:149:A:LEU:HG	1:150:A:ALA:H	12	0.11
(1,333)	1:147:A:LEU:HB2	1:148:A:LYS:H	8	0.11
(1,333)	1:147:A:LEU:HB3	1:148:A:LYS:H	8	0.11
(1,330)	1:145:A:MET:HB2	1:146:A:LEU:H	10	0.11
(1,330)	1:145:A:MET:HB3	1:146:A:LEU:H	10	0.11
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	4	0.11
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	4	0.11
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	6	0.11
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	6	0.11
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	13	0.11
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	13	0.11
(1,309)	1:118:A:GLN:HG2	1:119:A:ARG:H	16	0.11
(1,309)	1:118:A:GLN:HG3	1:119:A:ARG:H	16	0.11
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB2	1	0.11
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB3	1	0.11
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB2	1	0.11
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB3	1	0.11
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB2	10	0.11
(1,308)	1:117:A:PHE:HD1	1:118:A:GLN:HB3	10	0.11
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB2	10	0.11
(1,308)	1:117:A:PHE:HD2	1:118:A:GLN:HB3	10	0.11
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	1	0.11
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	1	0.11
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	3	0.11
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	3	0.11
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	5	0.11
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	5	0.11
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	10	0.11
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	10	0.11
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	19	0.11
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	19	0.11
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	1	0.11
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	1	0.11
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	3	0.11
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	3	0.11
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	4	0.11
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	7	0.11
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	7	0.11
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	12	0.11
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	12	0.11
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	14	0.11
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	14	0.11
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	19	0.11
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	19	0.11
(1,266)	1:87:A:TRP:HB2	1:88:A:GLN:H	4	0.11
(1,266)	1:87:A:TRP:HB3	1:88:A:GLN:H	4	0.11
(1,266)	1:87:A:TRP:HB2	1:88:A:GLN:H	16	0.11
(1,266)	1:87:A:TRP:HB3	1:88:A:GLN:H	16	0.11
(1,266)	1:87:A:TRP:HB2	1:88:A:GLN:H	19	0.11
(1,266)	1:87:A:TRP:HB3	1:88:A:GLN:H	19	0.11
(1,259)	1:82:A:LYS:HG2	1:83:A:ASP:H	20	0.11
(1,259)	1:82:A:LYS:HG3	1:83:A:ASP:H	20	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	1	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	1	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	2	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	2	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	3	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	3	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	5	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	5	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	7	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	7	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	8	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	8	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	10	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	10	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	12	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	12	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	13	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	13	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	17	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	17	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	19	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	19	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG2	20	0.11
(1,233)	1:62:A:THR:H	1:63:A:GLU:HG3	20	0.11
(1,193)	1:160:A:TRP:HA	1:161:A:GLU:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	15	0.11
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	17	0.11
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	19	0.11
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	3	0.11
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	4	0.11
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	19	0.11
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	3	0.11
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	7	0.11
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	10	0.11
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	13	0.11
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	15	0.11
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	7	0.11
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	9	0.11
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	10	0.11
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	12	0.11
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	17	0.11
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	18	0.11
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	19	0.11
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	6	0.11
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	11	0.11
(1,4)	1:61:A:HIS:H	1:62:A:THR:H	12	0.11
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	1	0.1
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	8	0.1
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	16	0.1
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	18	0.1
(2,107)	1:168:A:LEU:O	1:172:A:ARG:H	19	0.1
(2,82)	1:121:A:ALA:O	1:125:A:LEU:N	20	0.1
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	2	0.1
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	11	0.1
(2,74)	1:110:A:ARG:O	1:114:A:ASP:N	19	0.1
(2,66)	1:106:A:ASN:O	1:110:A:ARG:N	14	0.1
(2,65)	1:106:A:ASN:O	1:110:A:ARG:H	2	0.1
(2,59)	1:103:A:GLU:O	1:107:A:ARG:H	1	0.1
(2,59)	1:103:A:GLU:O	1:107:A:ARG:H	14	0.1
(2,57)	1:102:A:ARG:O	1:106:A:ASN:H	9	0.1
(2,27)	1:87:A:TRP:O	1:91:A:ASN:H	2	0.1
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	6	0.1
(2,22)	1:75:A:VAL:O	1:79:A:GLN:N	12	0.1
(2,20)	1:74:A:ILE:O	1:78:A:ASN:N	10	0.1
(2,15)	1:72:A:ASN:O	1:76:A:ILE:H	13	0.1
(2,9)	1:69:A:ILE:O	1:73:A:LEU:H	4	0.1
(2,9)	1:69:A:ILE:O	1:73:A:LEU:H	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	7	0.1
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	8	0.1
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	19	0.1
(2,7)	1:68:A:ARG:O	1:72:A:ASN:H	20	0.1
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE1	11	0.1
(1,1101)	1:176:A:LEU:HD11	1:182:A:PHE:HE2	11	0.1
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE1	11	0.1
(1,1101)	1:176:A:LEU:HD12	1:182:A:PHE:HE2	11	0.1
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE1	11	0.1
(1,1101)	1:176:A:LEU:HD13	1:182:A:PHE:HE2	11	0.1
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE1	11	0.1
(1,1101)	1:176:A:LEU:HD21	1:182:A:PHE:HE2	11	0.1
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE1	11	0.1
(1,1101)	1:176:A:LEU:HD22	1:182:A:PHE:HE2	11	0.1
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE1	11	0.1
(1,1101)	1:176:A:LEU:HD23	1:182:A:PHE:HE2	11	0.1
(1,1098)	1:173:A:LEU:HD11	1:182:A:PHE:HE1	5	0.1
(1,1098)	1:173:A:LEU:HD11	1:182:A:PHE:HE2	5	0.1
(1,1098)	1:173:A:LEU:HD12	1:182:A:PHE:HE1	5	0.1
(1,1098)	1:173:A:LEU:HD12	1:182:A:PHE:HE2	5	0.1
(1,1098)	1:173:A:LEU:HD13	1:182:A:PHE:HE1	5	0.1
(1,1098)	1:173:A:LEU:HD13	1:182:A:PHE:HE2	5	0.1
(1,1098)	1:173:A:LEU:HD21	1:182:A:PHE:HE1	5	0.1
(1,1098)	1:173:A:LEU:HD21	1:182:A:PHE:HE2	5	0.1
(1,1098)	1:173:A:LEU:HD22	1:182:A:PHE:HE1	5	0.1
(1,1098)	1:173:A:LEU:HD22	1:182:A:PHE:HE2	5	0.1
(1,1098)	1:173:A:LEU:HD23	1:182:A:PHE:HE1	5	0.1
(1,1098)	1:173:A:LEU:HD23	1:182:A:PHE:HE2	5	0.1
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB2	14	0.1
(1,1075)	1:158:A:ALA:HB1	1:190:A:TYR:HB3	14	0.1
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB2	14	0.1
(1,1075)	1:158:A:ALA:HB2	1:190:A:TYR:HB3	14	0.1
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB2	14	0.1
(1,1075)	1:158:A:ALA:HB3	1:190:A:TYR:HB3	14	0.1
(1,1074)	1:158:A:ALA:HB1	1:189:A:MET:HG2	19	0.1
(1,1074)	1:158:A:ALA:HB1	1:189:A:MET:HG3	19	0.1
(1,1074)	1:158:A:ALA:HB2	1:189:A:MET:HG2	19	0.1
(1,1074)	1:158:A:ALA:HB2	1:189:A:MET:HG3	19	0.1
(1,1074)	1:158:A:ALA:HB3	1:189:A:MET:HG2	19	0.1
(1,1074)	1:158:A:ALA:HB3	1:189:A:MET:HG3	19	0.1
(1,1073)	1:158:A:ALA:HB1	1:189:A:MET:HB2	17	0.1
(1,1073)	1:158:A:ALA:HB1	1:189:A:MET:HB3	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1073)	1:158:A:ALA:HB2	1:189:A:MET:HB2	17	0.1
(1,1073)	1:158:A:ALA:HB2	1:189:A:MET:HB3	17	0.1
(1,1073)	1:158:A:ALA:HB3	1:189:A:MET:HB2	17	0.1
(1,1073)	1:158:A:ALA:HB3	1:189:A:MET:HB3	17	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	8	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	8	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	8	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	8	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	8	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	8	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	10	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	10	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	10	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	10	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	10	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	10	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	13	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	13	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	13	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	13	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	13	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	13	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB1	15	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB2	15	0.1
(1,1065)	1:157:A:PRO:HG2	1:186:A:ALA:HB3	15	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB1	15	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB2	15	0.1
(1,1065)	1:157:A:PRO:HG3	1:186:A:ALA:HB3	15	0.1
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD11	19	0.1
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD12	19	0.1
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD13	19	0.1
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD21	19	0.1
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD22	19	0.1
(1,1059)	1:156:A:PHE:HE1	1:167:A:LEU:HD23	19	0.1
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD11	19	0.1
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD12	19	0.1
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD13	19	0.1
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD21	19	0.1
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD22	19	0.1
(1,1059)	1:156:A:PHE:HE2	1:167:A:LEU:HD23	19	0.1
(1,1056)	1:156:A:PHE:HA	1:185:A:ILE:HB	3	0.1
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB2	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB3	13	0.1
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB2	13	0.1
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB3	13	0.1
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB2	17	0.1
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB3	17	0.1
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB2	17	0.1
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB3	17	0.1
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB2	20	0.1
(1,1030)	1:154:A:SER:HB2	1:189:A:MET:HB3	20	0.1
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB2	20	0.1
(1,1030)	1:154:A:SER:HB3	1:189:A:MET:HB3	20	0.1
(1,1020)	1:152:A:GLU:HG2	1:190:A:TYR:HD1	11	0.1
(1,1020)	1:152:A:GLU:HG2	1:190:A:TYR:HD2	11	0.1
(1,1020)	1:152:A:GLU:HG3	1:190:A:TYR:HD1	11	0.1
(1,1020)	1:152:A:GLU:HG3	1:190:A:TYR:HD2	11	0.1
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE1	14	0.1
(1,1013)	1:151:A:GLU:HA	1:190:A:TYR:HE2	14	0.1
(1,1012)	1:150:A:ALA:HB1	1:159:A:SER:HA	19	0.1
(1,1012)	1:150:A:ALA:HB2	1:159:A:SER:HA	19	0.1
(1,1012)	1:150:A:ALA:HB3	1:159:A:SER:HA	19	0.1
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG2	10	0.1
(1,1007)	1:149:A:LEU:HG	1:161:A:GLU:HG3	10	0.1
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG2	3	0.1
(1,1001)	1:146:A:LEU:HG	1:164:A:GLU:HG3	3	0.1
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	3	0.1
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	3	0.1
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB2	12	0.1
(1,977)	1:124:A:LEU:HG	1:152:A:GLU:HB3	12	0.1
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD1	10	0.1
(1,963)	1:124:A:LEU:HD11	1:190:A:TYR:HD2	10	0.1
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD1	10	0.1
(1,963)	1:124:A:LEU:HD12	1:190:A:TYR:HD2	10	0.1
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD1	10	0.1
(1,963)	1:124:A:LEU:HD13	1:190:A:TYR:HD2	10	0.1
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD1	10	0.1
(1,963)	1:124:A:LEU:HD21	1:190:A:TYR:HD2	10	0.1
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD1	10	0.1
(1,963)	1:124:A:LEU:HD22	1:190:A:TYR:HD2	10	0.1
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD1	10	0.1
(1,963)	1:124:A:LEU:HD23	1:190:A:TYR:HD2	10	0.1
(1,959)	1:124:A:LEU:HG	1:155:A:ILE:HB	1	0.1
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD11	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD12	8	0.1
(1,949)	1:121:A:ALA:HB1	1:185:A:ILE:HD13	8	0.1
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD11	8	0.1
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD12	8	0.1
(1,949)	1:121:A:ALA:HB2	1:185:A:ILE:HD13	8	0.1
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD11	8	0.1
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD12	8	0.1
(1,949)	1:121:A:ALA:HB3	1:185:A:ILE:HD13	8	0.1
(1,936)	1:117:A:PHE:HB2	1:180:A:GLU:HA	3	0.1
(1,936)	1:117:A:PHE:HB3	1:180:A:GLU:HA	3	0.1
(1,934)	1:117:A:PHE:HE1	1:182:A:PHE:HE1	13	0.1
(1,934)	1:117:A:PHE:HE1	1:182:A:PHE:HE2	13	0.1
(1,934)	1:117:A:PHE:HE2	1:182:A:PHE:HE1	13	0.1
(1,934)	1:117:A:PHE:HE2	1:182:A:PHE:HE2	13	0.1
(1,927)	1:112:A:LEU:HD11	1:155:A:ILE:HD11	5	0.1
(1,927)	1:112:A:LEU:HD11	1:155:A:ILE:HD12	5	0.1
(1,927)	1:112:A:LEU:HD11	1:155:A:ILE:HD13	5	0.1
(1,927)	1:112:A:LEU:HD12	1:155:A:ILE:HD11	5	0.1
(1,927)	1:112:A:LEU:HD12	1:155:A:ILE:HD12	5	0.1
(1,927)	1:112:A:LEU:HD12	1:155:A:ILE:HD13	5	0.1
(1,927)	1:112:A:LEU:HD13	1:155:A:ILE:HD11	5	0.1
(1,927)	1:112:A:LEU:HD13	1:155:A:ILE:HD12	5	0.1
(1,927)	1:112:A:LEU:HD13	1:155:A:ILE:HD13	5	0.1
(1,927)	1:112:A:LEU:HD21	1:155:A:ILE:HD11	5	0.1
(1,927)	1:112:A:LEU:HD21	1:155:A:ILE:HD12	5	0.1
(1,927)	1:112:A:LEU:HD21	1:155:A:ILE:HD13	5	0.1
(1,927)	1:112:A:LEU:HD22	1:155:A:ILE:HD11	5	0.1
(1,927)	1:112:A:LEU:HD22	1:155:A:ILE:HD12	5	0.1
(1,927)	1:112:A:LEU:HD22	1:155:A:ILE:HD13	5	0.1
(1,927)	1:112:A:LEU:HD23	1:155:A:ILE:HD11	5	0.1
(1,927)	1:112:A:LEU:HD23	1:155:A:ILE:HD12	5	0.1
(1,927)	1:112:A:LEU:HD23	1:155:A:ILE:HD13	5	0.1
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD1	7	0.1
(1,909)	1:111:A:ILE:HD11	1:183:A:PHE:HD2	7	0.1
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD1	7	0.1
(1,909)	1:111:A:ILE:HD12	1:183:A:PHE:HD2	7	0.1
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD1	7	0.1
(1,909)	1:111:A:ILE:HD13	1:183:A:PHE:HD2	7	0.1
(1,891)	1:108:A:TRP:HD1	1:170:A:VAL:HB	5	0.1
(1,882)	1:108:A:TRP:HD1	1:155:A:ILE:HG13	18	0.1
(1,880)	1:108:A:TRP:HB2	1:125:A:LEU:HG	11	0.1
(1,880)	1:108:A:TRP:HB3	1:125:A:LEU:HG	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB1	3	0.1
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB2	3	0.1
(1,878)	1:108:A:TRP:HE1	1:121:A:ALA:HB3	3	0.1
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD11	1	0.1
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD12	1	0.1
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD13	1	0.1
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD21	1	0.1
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD22	1	0.1
(1,871)	1:105:A:ARG:HG2	1:125:A:LEU:HD23	1	0.1
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD11	1	0.1
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD12	1	0.1
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD13	1	0.1
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD21	1	0.1
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD22	1	0.1
(1,871)	1:105:A:ARG:HG3	1:125:A:LEU:HD23	1	0.1
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE1	10	0.1
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE2	10	0.1
(1,861)	1:101:A:ARG:HG2	1:145:A:MET:HE3	10	0.1
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE1	10	0.1
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE2	10	0.1
(1,861)	1:101:A:ARG:HG3	1:145:A:MET:HE3	10	0.1
(1,847)	1:100:A:ILE:HG12	1:143:A:ARG:HA	11	0.1
(1,838)	1:98:A:ARG:HB2	1:142:A:ALA:HA	9	0.1
(1,838)	1:98:A:ARG:HB3	1:142:A:ALA:HA	9	0.1
(1,838)	1:98:A:ARG:HB2	1:142:A:ALA:HA	19	0.1
(1,838)	1:98:A:ARG:HB3	1:142:A:ALA:HA	19	0.1
(1,831)	1:97:A:LEU:HD11	1:143:A:ARG:HA	6	0.1
(1,831)	1:97:A:LEU:HD12	1:143:A:ARG:HA	6	0.1
(1,831)	1:97:A:LEU:HD13	1:143:A:ARG:HA	6	0.1
(1,831)	1:97:A:LEU:HD21	1:143:A:ARG:HA	6	0.1
(1,831)	1:97:A:LEU:HD22	1:143:A:ARG:HA	6	0.1
(1,831)	1:97:A:LEU:HD23	1:143:A:ARG:HA	6	0.1
(1,826)	1:77:A:ARG:HB2	1:87:A:TRP:HB2	18	0.1
(1,826)	1:77:A:ARG:HB2	1:87:A:TRP:HB3	18	0.1
(1,826)	1:77:A:ARG:HB3	1:87:A:TRP:HB2	18	0.1
(1,826)	1:77:A:ARG:HB3	1:87:A:TRP:HB3	18	0.1
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB2	20	0.1
(1,802)	1:73:A:LEU:HB2	1:91:A:ASN:HB3	20	0.1
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB2	20	0.1
(1,802)	1:73:A:LEU:HB3	1:91:A:ASN:HB3	20	0.1
(1,801)	1:73:A:LEU:HD11	1:91:A:ASN:HB2	13	0.1
(1,801)	1:73:A:LEU:HD11	1:91:A:ASN:HB3	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:73:A:LEU:HD12	1:91:A:ASN:HB2	13	0.1
(1,801)	1:73:A:LEU:HD12	1:91:A:ASN:HB3	13	0.1
(1,801)	1:73:A:LEU:HD13	1:91:A:ASN:HB2	13	0.1
(1,801)	1:73:A:LEU:HD13	1:91:A:ASN:HB3	13	0.1
(1,801)	1:73:A:LEU:HD21	1:91:A:ASN:HB2	13	0.1
(1,801)	1:73:A:LEU:HD21	1:91:A:ASN:HB3	13	0.1
(1,801)	1:73:A:LEU:HD22	1:91:A:ASN:HB2	13	0.1
(1,801)	1:73:A:LEU:HD22	1:91:A:ASN:HB3	13	0.1
(1,801)	1:73:A:LEU:HD23	1:91:A:ASN:HB2	13	0.1
(1,801)	1:73:A:LEU:HD23	1:91:A:ASN:HB3	13	0.1
(1,796)	1:73:A:LEU:HG	1:90:A:LEU:HG	12	0.1
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB2	17	0.1
(1,758)	1:61:A:HIS:HB2	1:68:A:ARG:HB3	17	0.1
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB2	17	0.1
(1,758)	1:61:A:HIS:HB3	1:68:A:ARG:HB3	17	0.1
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD11	18	0.1
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD12	18	0.1
(1,755)	1:59:A:VAL:HG11	1:69:A:ILE:HD13	18	0.1
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD11	18	0.1
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD12	18	0.1
(1,755)	1:59:A:VAL:HG12	1:69:A:ILE:HD13	18	0.1
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD11	18	0.1
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD12	18	0.1
(1,755)	1:59:A:VAL:HG13	1:69:A:ILE:HD13	18	0.1
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD11	18	0.1
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD12	18	0.1
(1,755)	1:59:A:VAL:HG21	1:69:A:ILE:HD13	18	0.1
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD11	18	0.1
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD12	18	0.1
(1,755)	1:59:A:VAL:HG22	1:69:A:ILE:HD13	18	0.1
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD11	18	0.1
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD12	18	0.1
(1,755)	1:59:A:VAL:HG23	1:69:A:ILE:HD13	18	0.1
(1,742)	1:157:A:PRO:HG2	1:186:A:ALA:H	14	0.1
(1,742)	1:157:A:PRO:HG3	1:186:A:ALA:H	14	0.1
(1,742)	1:157:A:PRO:HG2	1:186:A:ALA:H	15	0.1
(1,742)	1:157:A:PRO:HG3	1:186:A:ALA:H	15	0.1
(1,740)	1:156:A:PHE:H	1:167:A:LEU:HG	3	0.1
(1,708)	1:125:A:LEU:H	1:146:A:LEU:HA	19	0.1
(1,685)	1:111:A:ILE:HD11	1:186:A:ALA:H	1	0.1
(1,685)	1:111:A:ILE:HD12	1:186:A:ALA:H	1	0.1
(1,685)	1:111:A:ILE:HD13	1:186:A:ALA:H	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG11	8	0.1
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG12	8	0.1
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG13	8	0.1
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG21	8	0.1
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG22	8	0.1
(1,684)	1:109:A:ARG:H	1:127:A:VAL:HG23	8	0.1
(1,670)	1:100:A:ILE:HD11	1:143:A:ARG:H	11	0.1
(1,670)	1:100:A:ILE:HD12	1:143:A:ARG:H	11	0.1
(1,670)	1:100:A:ILE:HD13	1:143:A:ARG:H	11	0.1
(1,658)	1:77:A:ARG:HB2	1:87:A:TRP:H	11	0.1
(1,658)	1:77:A:ARG:HB3	1:87:A:TRP:H	11	0.1
(1,658)	1:77:A:ARG:HB2	1:87:A:TRP:H	12	0.1
(1,658)	1:77:A:ARG:HB3	1:87:A:TRP:H	12	0.1
(1,658)	1:77:A:ARG:HB2	1:87:A:TRP:H	13	0.1
(1,658)	1:77:A:ARG:HB3	1:87:A:TRP:H	13	0.1
(1,637)	1:58:A:ASP:HB2	1:69:A:ILE:H	10	0.1
(1,637)	1:58:A:ASP:HB3	1:69:A:ILE:H	10	0.1
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB1	9	0.1
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB2	9	0.1
(1,632)	1:173:A:LEU:HD11	1:178:A:ALA:HB3	9	0.1
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB1	9	0.1
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB2	9	0.1
(1,632)	1:173:A:LEU:HD12	1:178:A:ALA:HB3	9	0.1
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB1	9	0.1
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB2	9	0.1
(1,632)	1:173:A:LEU:HD13	1:178:A:ALA:HB3	9	0.1
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB1	9	0.1
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB2	9	0.1
(1,632)	1:173:A:LEU:HD21	1:178:A:ALA:HB3	9	0.1
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB1	9	0.1
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB2	9	0.1
(1,632)	1:173:A:LEU:HD22	1:178:A:ALA:HB3	9	0.1
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB1	9	0.1
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB2	9	0.1
(1,632)	1:173:A:LEU:HD23	1:178:A:ALA:HB3	9	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	5	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	5	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	5	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	5	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	5	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	5	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	5	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	5	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	5	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	5	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	5	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	5	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	5	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	5	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	5	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	5	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	5	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	5	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	5	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	5	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	5	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	5	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	5	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	5	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	5	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	5	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	5	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	5	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	5	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	5	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	5	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	5	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	5	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	5	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	5	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD11	20	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD12	20	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD13	20	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD21	20	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD22	20	0.1
(1,599)	1:125:A:LEU:HD11	1:130:A:LEU:HD23	20	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD11	20	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD12	20	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD13	20	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD21	20	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD22	20	0.1
(1,599)	1:125:A:LEU:HD12	1:130:A:LEU:HD23	20	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD11	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD12	20	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD13	20	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD21	20	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD22	20	0.1
(1,599)	1:125:A:LEU:HD13	1:130:A:LEU:HD23	20	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD11	20	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD12	20	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD13	20	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD21	20	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD22	20	0.1
(1,599)	1:125:A:LEU:HD21	1:130:A:LEU:HD23	20	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD11	20	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD12	20	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD13	20	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD21	20	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD22	20	0.1
(1,599)	1:125:A:LEU:HD22	1:130:A:LEU:HD23	20	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD11	20	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD12	20	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD13	20	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD21	20	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD22	20	0.1
(1,599)	1:125:A:LEU:HD23	1:130:A:LEU:HD23	20	0.1
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB1	12	0.1
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB2	12	0.1
(1,559)	1:153:A:THR:H	1:158:A:ALA:HB3	12	0.1
(1,557)	1:153:A:THR:HA	1:155:A:ILE:H	18	0.1
(1,555)	1:153:A:THR:HG1	1:155:A:ILE:H	10	0.1
(1,554)	1:151:A:GLU:H	1:153:A:THR:HA	7	0.1
(1,546)	1:132:A:THR:HG21	1:135:A:ASP:H	2	0.1
(1,546)	1:132:A:THR:HG22	1:135:A:ASP:H	2	0.1
(1,546)	1:132:A:THR:HG23	1:135:A:ASP:H	2	0.1
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	3	0.1
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	15	0.1
(1,544)	1:130:A:LEU:H	1:132:A:THR:HB	18	0.1
(1,536)	1:82:A:LYS:HG2	1:84:A:SER:H	17	0.1
(1,536)	1:82:A:LYS:HG3	1:84:A:SER:H	17	0.1
(1,526)	1:61:A:HIS:HB2	1:63:A:GLU:H	11	0.1
(1,526)	1:61:A:HIS:HB3	1:63:A:GLU:H	11	0.1
(1,454)	1:67:A:ASP:HA	1:70:A:LEU:HB2	12	0.1
(1,454)	1:67:A:ASP:HA	1:70:A:LEU:HB3	12	0.1
(1,449)	1:185:A:ILE:HA	1:189:A:MET:H	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:170:A:VAL:HB	1:171:A:ASP:H	18	0.1
(1,344)	1:153:A:THR:HB	1:154:A:SER:H	13	0.1
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	15	0.1
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	15	0.1
(1,340)	1:152:A:GLU:HB2	1:153:A:THR:H	19	0.1
(1,340)	1:152:A:GLU:HB3	1:153:A:THR:H	19	0.1
(1,330)	1:145:A:MET:HB2	1:146:A:LEU:H	6	0.1
(1,330)	1:145:A:MET:HB3	1:146:A:LEU:H	6	0.1
(1,330)	1:145:A:MET:HB2	1:146:A:LEU:H	7	0.1
(1,330)	1:145:A:MET:HB3	1:146:A:LEU:H	7	0.1
(1,312)	1:119:A:ARG:HB2	1:120:A:GLU:H	8	0.1
(1,312)	1:119:A:ARG:HB3	1:120:A:GLU:H	8	0.1
(1,299)	1:113:A:GLU:HB2	1:114:A:ASP:H	6	0.1
(1,299)	1:113:A:GLU:HB3	1:114:A:ASP:H	6	0.1
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	4	0.1
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	4	0.1
(1,297)	1:112:A:LEU:HB2	1:113:A:GLU:H	12	0.1
(1,297)	1:112:A:LEU:HB3	1:113:A:GLU:H	12	0.1
(1,291)	1:107:A:ARG:HB2	1:108:A:TRP:H	14	0.1
(1,291)	1:107:A:ARG:HB3	1:108:A:TRP:H	14	0.1
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	8	0.1
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	8	0.1
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	11	0.1
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	11	0.1
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	16	0.1
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	16	0.1
(1,284)	1:102:A:ARG:HB2	1:103:A:GLU:H	18	0.1
(1,284)	1:102:A:ARG:HB3	1:103:A:GLU:H	18	0.1
(1,280)	1:98:A:ARG:HB2	1:99:A:GLN:H	17	0.1
(1,280)	1:98:A:ARG:HB3	1:99:A:GLN:H	17	0.1
(1,266)	1:87:A:TRP:HB2	1:88:A:GLN:H	8	0.1
(1,266)	1:87:A:TRP:HB3	1:88:A:GLN:H	8	0.1
(1,241)	1:72:A:ASN:HB2	1:73:A:LEU:H	2	0.1
(1,241)	1:72:A:ASN:HB3	1:73:A:LEU:H	2	0.1
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	2	0.1
(1,177)	1:137:A:LYS:HA	1:138:A:ASN:H	8	0.1
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	7	0.1
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	9	0.1
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	10	0.1
(1,111)	1:61:A:HIS:HA	1:62:A:THR:H	18	0.1
(1,54)	1:120:A:GLU:H	1:121:A:ALA:H	11	0.1
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	4	0.1
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	8	0.1
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	11	0.1
(1,5)	1:62:A:THR:H	1:63:A:GLU:H	20	0.1

10 Dihedral-angle violation analysis

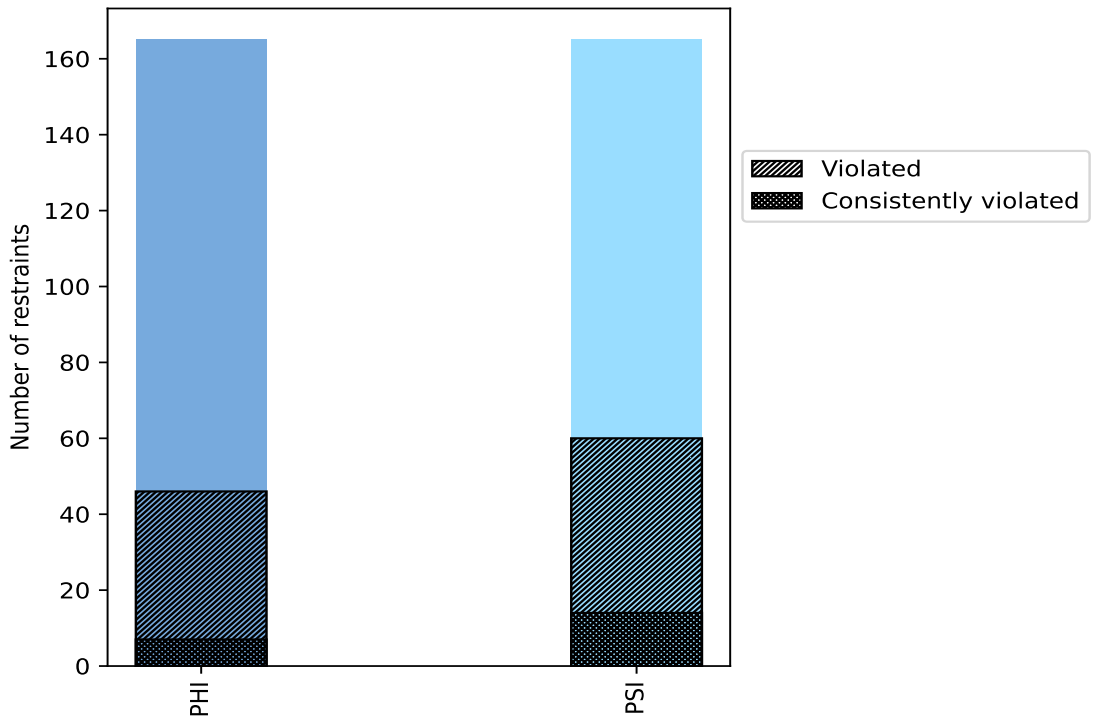
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	165	50.0	46	27.9	13.9	7	4.2	2.1
PSI	165	50.0	60	36.4	18.2	14	8.5	4.2
Total	330	100.0	106	32.1	32.1	21	6.4	6.4

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



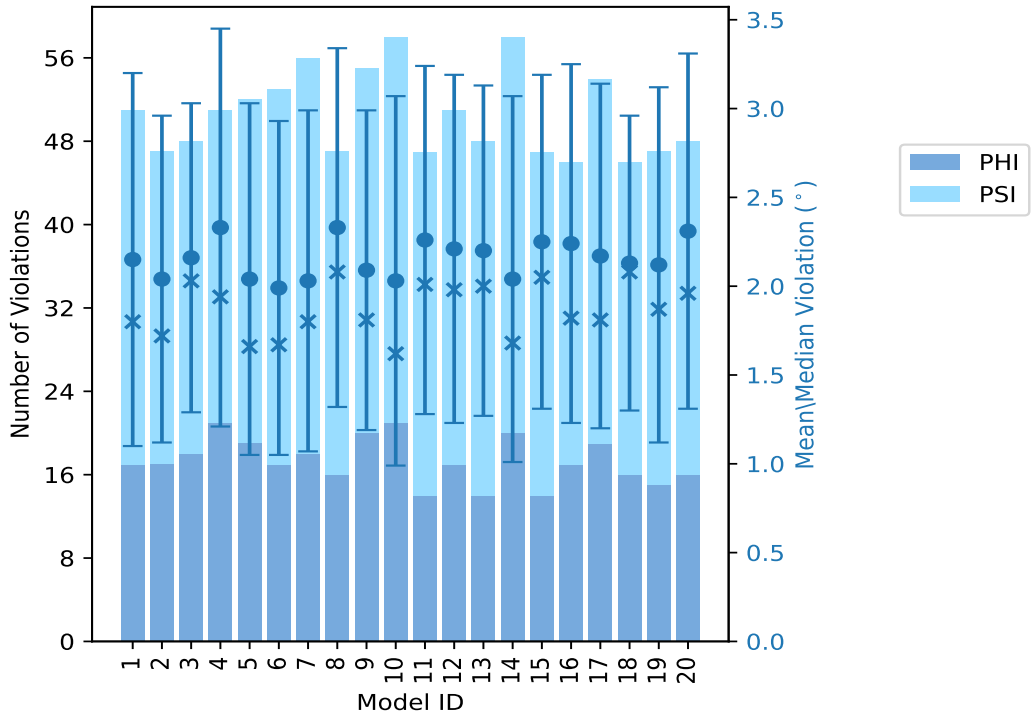
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	17	34	51	2.15	4.63	1.05	1.8
2	17	30	47	2.04	4.96	0.92	1.72
3	18	30	48	2.16	5.05	0.87	2.03
4	21	30	51	2.33	4.86	1.12	1.94
5	19	33	52	2.04	4.89	0.99	1.66
6	17	36	53	1.99	4.74	0.94	1.67
7	18	38	56	2.03	5.22	0.96	1.8
8	16	31	47	2.33	4.77	1.01	2.08
9	20	35	55	2.09	4.71	0.9	1.81
10	21	37	58	2.03	4.52	1.04	1.62
11	14	33	47	2.26	4.38	0.98	2.01
12	17	34	51	2.21	4.44	0.98	1.98
13	14	34	48	2.2	4.16	0.93	2.0
14	20	38	58	2.04	5.19	1.03	1.68
15	14	33	47	2.25	5.01	0.94	2.05
16	17	29	46	2.24	5.02	1.01	1.82
17	19	35	54	2.17	4.88	0.97	1.81
18	16	30	46	2.13	4.33	0.83	2.08
19	15	32	47	2.12	4.85	1.0	1.87
20	16	32	48	2.31	4.76	1.0	1.96

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
10	6	16	1	5.0
6	5	11	2	10.0
2	5	7	3	15.0
2	2	4	4	20.0
5	3	8	5	25.0
3	3	6	6	30.0
2	1	3	7	35.0
1	3	4	8	40.0
1	2	3	9	45.0
0	1	1	10	50.0
1	1	2	11	55.0

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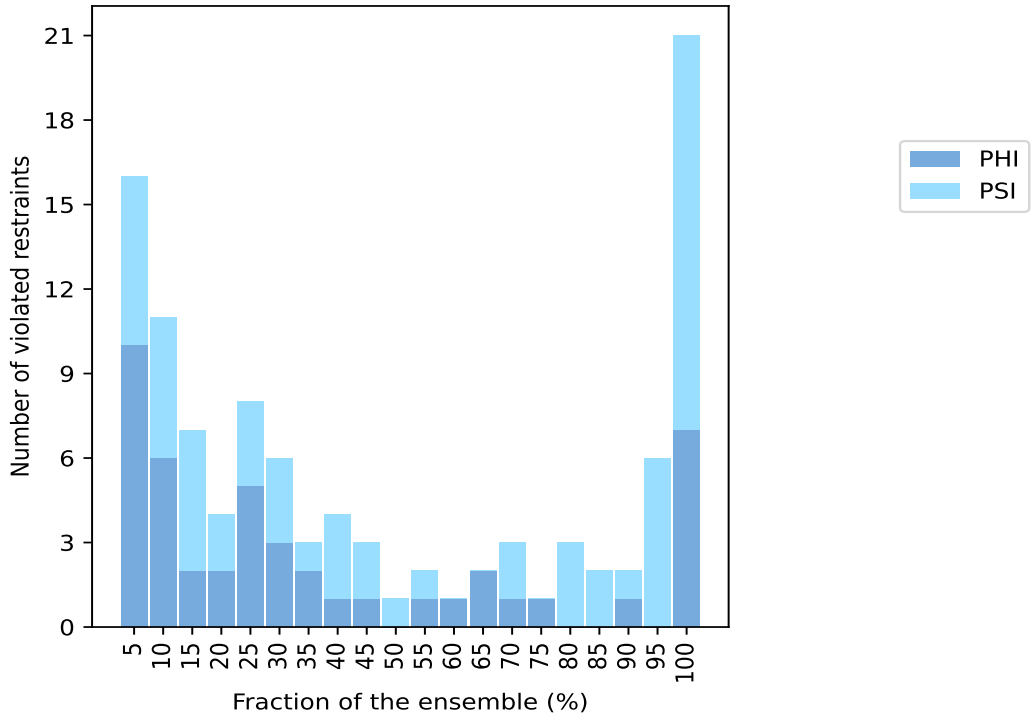
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	0	1	12	60.0
2	0	2	13	65.0
1	2	3	14	70.0
1	0	1	15	75.0
0	3	3	16	80.0
0	2	2	17	85.0
1	1	2	18	90.0
0	6	6	19	95.0
7	14	21	20	100.0

[1] Number of models with violations

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

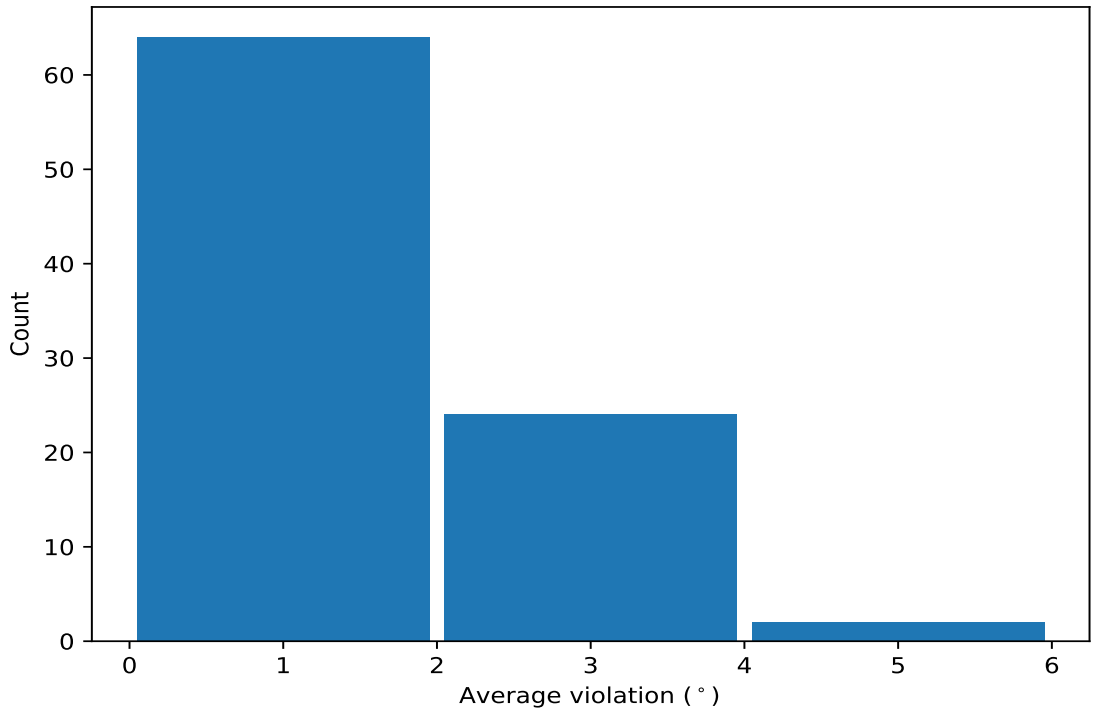


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	20	4.77	0.28	4.81
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	20	4.05	0.25	3.97
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	20	3.69	0.62	3.58
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	20	3.66	0.38	3.58
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	20	3.49	0.57	3.57
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	20	3.27	0.34	3.32
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	20	3.1	0.75	3.11
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	20	2.85	0.2	2.9
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	20	2.85	0.4	2.85
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	20	2.79	0.63	2.7
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	20	2.68	0.33	2.72
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	20	2.64	0.27	2.65
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	20	2.54	0.28	2.5
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	20	2.2	0.2	2.14
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	20	2.15	0.31	2.24
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	20	2.1	0.3	2.05
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	20	2.03	0.2	2.02
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	20	1.95	0.34	2.08
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	20	1.64	0.27	1.7
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	20	1.64	0.28	1.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	20	1.58	0.28	1.6
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	19	3.61	0.5	3.53
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	19	3.56	0.69	3.84
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	19	2.34	0.67	2.09
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	19	2.11	0.55	2.02
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	19	2.02	0.48	2.13
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	19	1.56	0.25	1.54
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	18	1.86	0.43	1.88
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	18	1.67	0.5	1.63
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	17	1.72	0.45	1.75
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	17	1.55	0.39	1.46
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	16	1.76	0.3	1.76
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	16	1.48	0.32	1.43
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	16	1.37	0.27	1.34
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	15	1.41	0.21	1.37
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	14	2.73	0.74	2.85
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	14	1.42	0.33	1.29
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	14	1.28	0.11	1.28
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	13	1.74	0.27	1.8
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	13	1.48	0.17	1.47
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	12	1.27	0.13	1.33
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	11	1.48	0.17	1.44
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	11	1.23	0.17	1.17
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	10	1.71	0.23	1.69
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	9	3.61	0.59	3.62
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	9	3.3	0.55	3.28
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	9	1.22	0.17	1.16
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	8	1.3	0.25	1.23
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	8	1.29	0.19	1.21
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	8	1.2	0.15	1.2
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	8	1.19	0.15	1.17
(1,192)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:TYR:N	7	1.26	0.12	1.26
(1,89)	1:135:A:ASP:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	7	1.19	0.12	1.17
(1,35)	1:77:A:ARG:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	7	1.14	0.1	1.12
(1,68)	1:111:A:ILE:C	1:112:A:LEU:N	1:112:A:LEU:CA	1:112:A:LEU:C	6	1.78	0.46	1.78
(1,300)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:LYS:N	6	1.44	0.21	1.4
(1,65)	1:108:A:TRP:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	6	1.31	0.15	1.36
(1,145)	1:192:A:LYS:C	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	6	1.26	0.14	1.27
(1,311)	1:194:A:PRO:N	1:194:A:PRO:CA	1:194:A:PRO:C	1:195:A:GLY:N	6	1.2	0.22	1.14
(1,310)	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	1:194:A:PRO:N	6	1.11	0.08	1.09
(1,17)	1:59:A:VAL:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	5	1.36	0.2	1.28
(1,74)	1:117:A:PHE:C	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	5	1.35	0.36	1.23
(1,71)	1:114:A:ASP:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	5	1.33	0.13	1.38
(1,20)	1:62:A:THR:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	5	1.23	0.18	1.13
(1,296)	1:179:A:ALA:N	1:179:A:ALA:CA	1:179:A:ALA:C	1:180:A:GLU:N	5	1.22	0.14	1.29
(1,188)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:ASP:N	5	1.22	0.1	1.26
(1,181)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:SER:N	5	1.13	0.07	1.12
(1,126)	1:173:A:LEU:C	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	5	1.07	0.04	1.09
(1,113)	1:160:A:TRP:C	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	4	2.58	0.24	2.53
(1,228)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:TRP:N	4	1.32	0.2	1.25
(1,285)	1:168:A:LEU:N	1:168:A:LEU:CA	1:168:A:LEU:C	1:169:A:VAL:N	4	1.3	0.12	1.35

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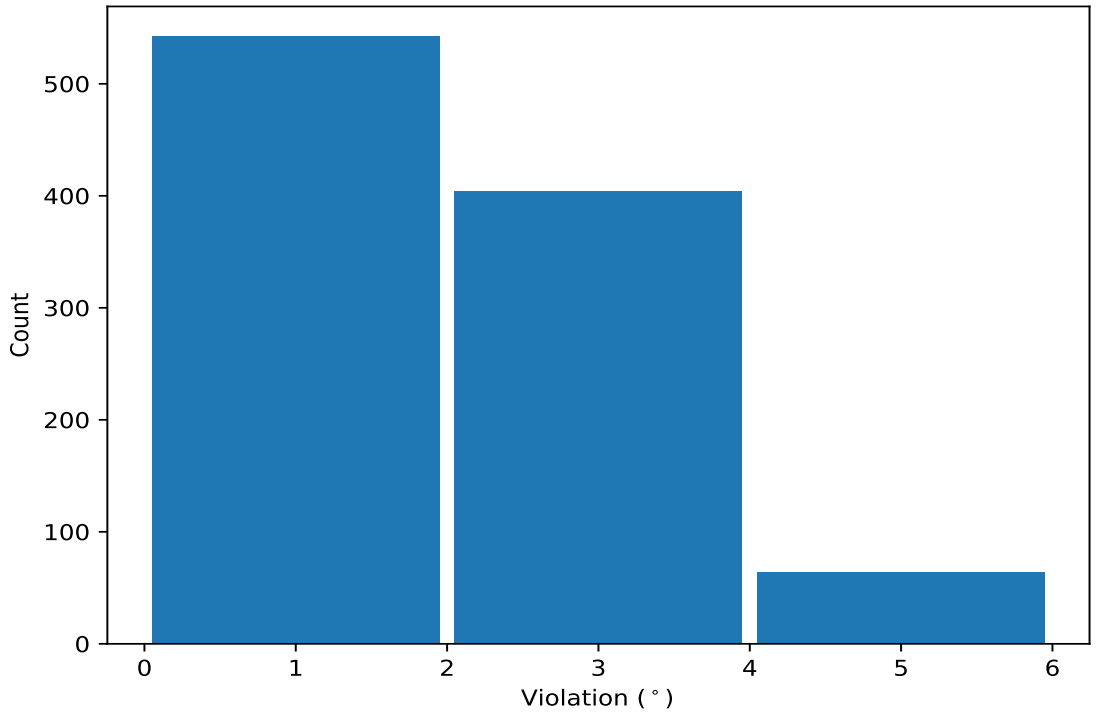
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,109)	1:156:A:PHE:C	1:157:A:PRO:N	1:157:A:PRO:CA	1:157:A:PRO:C	4	1.1	0.06	1.12
(1,315)	1:198:A:CYS:N	1:198:A:CYS:CA	1:198:A:CYS:C	1:199:A:LEU:N	3	1.88	1.16	1.1
(1,312)	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	1:196:A:VAL:N	3	1.42	0.03	1.42
(1,114)	1:161:A:GLU:C	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	3	1.25	0.28	1.06
(1,234)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASP:N	3	1.2	0.25	1.03
(1,318)	1:201:A:ASP:N	1:201:A:ASP:CA	1:201:A:ASP:C	1:202:A:GLY:N	3	1.13	0.09	1.11
(1,22)	1:64:A:ALA:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	3	1.11	0.07	1.14
(1,248)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:SER:N	3	1.09	0.07	1.07
(1,143)	1:190:A:TYR:C	1:191:A:PRO:N	1:191:A:PRO:CA	1:191:A:PRO:C	2	1.46	0.08	1.46
(1,232)	1:111:A:ILE:N	1:111:A:ILE:CA	1:111:A:ILE:C	1:112:A:LEU:N	2	1.41	0.17	1.41
(1,104)	1:151:A:GLU:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	2	1.33	0.1	1.33
(1,18)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	2	1.14	0.02	1.14
(1,231)	1:110:A:ARG:N	1:110:A:ARG:CA	1:110:A:ARG:C	1:111:A:ILE:N	2	1.14	0.07	1.14
(1,281)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:ARG:N	2	1.14	0.04	1.14
(1,227)	1:106:A:ASN:N	1:106:A:ASN:CA	1:106:A:ASN:C	1:107:A:ARG:N	2	1.1	0.04	1.1
(1,130)	1:177:A:ASP:C	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	2	1.1	0.04	1.1
(1,27)	1:69:A:ILE:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	2	1.1	0.06	1.1
(1,325)	1:208:A:CYS:N	1:208:A:CYS:CA	1:208:A:CYS:C	1:209:A:LEU:N	2	1.06	0.0	1.06
(1,33)	1:75:A:VAL:C	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	2	1.02	0.02	1.02

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	7	5.22
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	14	5.19
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	3	5.05
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	16	5.02
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	15	5.01
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	2	4.96
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	5	4.89
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	17	4.88
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	4	4.86
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	19	4.85
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	8	4.77
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	4	4.76
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	20	4.76
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	6	4.74
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	9	4.71
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	1	4.63
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	1	4.58
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	2	4.58
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	1	4.52
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	10	4.52
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	5	4.52

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	20	4.5
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	10	4.49
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	16	4.48
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	12	4.44
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	4	4.41
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	14	4.38
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	6	4.38
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	11	4.38
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	4	4.38
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	11	4.36
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	9	4.35
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	14	4.33
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	18	4.33
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	7	4.32
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	12	4.28
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	8	4.27
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	11	4.25
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	4	4.24
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	1	4.23
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	16	4.23
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	15	4.22
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	16	4.22
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	5	4.18
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	8	4.18
(1,106)	1:153:A:THR:C	1:154:A:SER:N	1:154:A:SER:CA	1:154:A:SER:C	13	4.16
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	11	4.15
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	20	4.15
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	14	4.14
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	10	4.12
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	19	4.12
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	7	4.11
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	12	4.11
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	8	4.1
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	11	4.1
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	13	4.07
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	14	4.07
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	10	4.05
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	19	4.04
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	6	4.04
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	20	4.03
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	20	4.0
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	10	4.0
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	13	4.0
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	3	3.99
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	19	3.99
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	4	3.98
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	14	3.95
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	9	3.95
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	17	3.94
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	4	3.93
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	5	3.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	19	3.93
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	11	3.92
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	1	3.92
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	2	3.92
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	10	3.9
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	2	3.9
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	20	3.9
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	17	3.89
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	15	3.88
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	8	3.86
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	17	3.86
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	12	3.85
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	1	3.85
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	4	3.84
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	6	3.84
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	5	3.81
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	17	3.8
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	1	3.78
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	13	3.77
(1,151)	1:198:A:CYS:C	1:199:A:LEU:N	1:199:A:LEU:CA	1:199:A:LEU:C	12	3.77
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	10	3.76
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	17	3.76
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	18	3.75
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	15	3.74
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	8	3.73
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	5	3.72
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	13	3.72
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	12	3.72
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	11	3.71
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	10	3.71
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	4	3.7
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	15	3.68
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	5	3.67
(1,249)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:THR:N	7	3.66
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	19	3.65
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	10	3.64
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	12	3.63
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	7	3.63
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	18	3.63
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	6	3.62
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	15	3.62
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	9	3.62
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	9	3.61
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	18	3.59
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	8	3.59
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	10	3.59
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	16	3.57
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	19	3.54
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	7	3.53
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	6	3.53
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	19	3.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	8	3.52
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	14	3.52
(1,315)	1:198:A:CYS:N	1:198:A:CYS:CA	1:198:A:CYS:C	1:199:A:LEU:N	12	3.51
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	8	3.51
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	12	3.5
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	16	3.49
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	7	3.49
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	17	3.48
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	12	3.47
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	4	3.47
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	3	3.46
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	16	3.45
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	13	3.44
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	15	3.43
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	18	3.42
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	9	3.42
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	17	3.41
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	11	3.4
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	6	3.39
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	4	3.38
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	20	3.38
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	3	3.37
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	20	3.36
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	13	3.35
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	20	3.34
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	14	3.34
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	15	3.33
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	20	3.32
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	2	3.29
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	3	3.28
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	12	3.28
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	7	3.28
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	1	3.28
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	3	3.27
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	3	3.27
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	4	3.27
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	2	3.26
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	11	3.26
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	16	3.26
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	8	3.26
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	17	3.25
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	2	3.24
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	19	3.23
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	4	3.23
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	13	3.23
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	17	3.2
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	18	3.18
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	8	3.18
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	9	3.17
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	13	3.17
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	1	3.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	4	3.15
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	14	3.15
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	13	3.14
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	15	3.14
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	1	3.12
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	20	3.12
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	12	3.11
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	3	3.11
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	14	3.1
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	13	3.1
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	16	3.09
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	20	3.08
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	10	3.08
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	16	3.07
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	15	3.07
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	10	3.07
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	4	3.06
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	20	3.06
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	6	3.06
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	6	3.06
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	12	3.06
(1,268)	1:151:A:GLU:N	1:151:A:GLU:CA	1:151:A:GLU:C	1:152:A:GLU:N	7	3.05
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	17	3.05
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	17	3.03
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	20	3.03
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	17	3.02
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	13	3.02
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	16	3.02
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	1	3.02
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	3	3.02
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	11	3.01
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	5	3.0
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	9	2.97
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	8	2.97
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	16	2.97
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	8	2.97
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	11	2.97
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	2	2.95
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	6	2.95
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	17	2.95
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	5	2.94
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	13	2.94
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	7	2.94
(1,113)	1:160:A:TRP:C	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	18	2.94
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	5	2.94
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	14	2.93
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1	2.93
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	1	2.93
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	4	2.92
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	16	2.91
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	16	2.91

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	8	2.9
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	3	2.9
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	9	2.9
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	20	2.9
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	15	2.9
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	9	2.9
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	2	2.89
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	9	2.89
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	13	2.88
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	17	2.88
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	1	2.87
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	5	2.86
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	15	2.86
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	10	2.83
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	8	2.83
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	15	2.81
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	15	2.81
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	18	2.8
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	11	2.8
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	16	2.8
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	13	2.8
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	9	2.79
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	9	2.78
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	18	2.78
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	20	2.78
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	5	2.77
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	8	2.77
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	12	2.76
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	14	2.76
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	9	2.75
(1,242)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ASP:N	18	2.75
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	3	2.75
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	20	2.75
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	18	2.75
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	3	2.74
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	11	2.74
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	8	2.74
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	11	2.73
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	7	2.72
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	6	2.71
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	6	2.7
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	13	2.7
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	3	2.69
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	8	2.69
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	15	2.67
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	10	2.67
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	18	2.67
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	17	2.67
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	4	2.66
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	10	2.66
(1,113)	1:160:A:TRP:C	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	17	2.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	19	2.66
(1,279)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:SER:N	14	2.65
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	6	2.65
(1,105)	1:152:A:GLU:C	1:153:A:THR:N	1:153:A:THR:CA	1:153:A:THR:C	9	2.65
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	7	2.64
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	15	2.64
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	5	2.64
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	12	2.64
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	3	2.63
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	12	2.63
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	9	2.61
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	2	2.6
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	9	2.59
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	1	2.58
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	18	2.57
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	13	2.56
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	16	2.55
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	19	2.55
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	9	2.54
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	14	2.54
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	8	2.53
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	15	2.53
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	11	2.53
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	6	2.53
(1,68)	1:111:A:ILE:C	1:112:A:LEU:N	1:112:A:LEU:CA	1:112:A:LEU:C	14	2.53
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	3	2.52
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	14	2.52
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	18	2.52
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	3	2.51
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	19	2.5
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	4	2.5
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	2	2.5
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	1	2.49
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	11	2.49
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	19	2.49
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	7	2.49
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	18	2.49
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	14	2.48
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	8	2.48
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	14	2.48
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	20	2.48
(1,110)	1:157:A:PRO:C	1:158:A:ALA:N	1:158:A:ALA:CA	1:158:A:ALA:C	7	2.48
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	3	2.47
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	8	2.47
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	19	2.47
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	12	2.47
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	18	2.47
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	5	2.47
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	17	2.46
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	12	2.46
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	7	2.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	4	2.45
(1,19)	1:61:A:HIS:C	1:62:A:THR:N	1:62:A:THR:CA	1:62:A:THR:C	16	2.45
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	16	2.44
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	13	2.44
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	4	2.44
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	17	2.43
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	4	2.43
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	18	2.43
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	19	2.43
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	19	2.42
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	17	2.41
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	10	2.4
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	13	2.4
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	13	2.39
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	20	2.39
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	12	2.39
(1,113)	1:160:A:TRP:C	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	19	2.39
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	9	2.38
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	12	2.38
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	18	2.37
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	1	2.37
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	17	2.37
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	4	2.37
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	2	2.36
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	7	2.35
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	3	2.35
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	20	2.35
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	17	2.35
(1,113)	1:160:A:TRP:C	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	2	2.35
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	15	2.35
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	13	2.34
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	3	2.34
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	18	2.34
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	10	2.34
(1,115)	1:162:A:LEU:C	1:163:A:SER:N	1:163:A:SER:CA	1:163:A:SER:C	14	2.34
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	18	2.33
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	11	2.33
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	7	2.33
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	15	2.31
(1,269)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:THR:N	18	2.31
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	19	2.31
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	3	2.31
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	9	2.3
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	6	2.29
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	1	2.29
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	17	2.28
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	4	2.28
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	7	2.28
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	10	2.28
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	11	2.27
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	11	2.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	2	2.25
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	5	2.25
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	19	2.25
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	5	2.25
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	9	2.25
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	8	2.24
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	20	2.24
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	10	2.23
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	13	2.23
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	15	2.23
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	7	2.22
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	7	2.21
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	8	2.21
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	6	2.21
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	15	2.21
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	7	2.2
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	3	2.2
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	11	2.2
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	18	2.2
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	5	2.19
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	20	2.18
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	20	2.18
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	10	2.17
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	3	2.17
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	2	2.16
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	9	2.16
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	14	2.16
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	11	2.15
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	11	2.15
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	12	2.15
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	18	2.15
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	16	2.14
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	10	2.14
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	5	2.13
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	14	2.13
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	14	2.13
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	10	2.13
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	19	2.13
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	11	2.12
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	1	2.11
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	3	2.11
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	7	2.11
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	13	2.11
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	7	2.1
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	1	2.1
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	19	2.09
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	15	2.09
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	14	2.09
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	7	2.09
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	8	2.08
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	16	2.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	2	2.07
(1,292)	1:175:A:ALA:N	1:175:A:ALA:CA	1:175:A:ALA:C	1:176:A:LEU:N	15	2.07
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	9	2.07
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	3	2.07
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	6	2.07
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	5	2.06
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	10	2.06
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	12	2.06
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	17	2.06
(1,68)	1:111:A:ILE:C	1:112:A:LEU:N	1:112:A:LEU:CA	1:112:A:LEU:C	7	2.06
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	15	2.05
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	17	2.05
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	13	2.05
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	1	2.05
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	12	2.04
(1,295)	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	1:179:A:ALA:N	15	2.04
(1,266)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ALA:N	2	2.04
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	1	2.04
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	1	2.04
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	16	2.04
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	5	2.04
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	12	2.04
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	7	2.03
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	8	2.03
(1,140)	1:187:A:SER:C	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	15	2.03
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	17	2.02
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	1	2.02
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	7	2.02
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	18	2.02
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	12	2.02
(1,74)	1:117:A:PHE:C	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	6	2.02
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	6	2.01
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	11	2.01
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	8	2.01
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	2	2.0
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	16	2.0
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	9	2.0
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	18	2.0
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	10	2.0
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	9	1.99
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	6	1.99
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	3	1.99
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	11	1.99
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	8	1.98
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	5	1.98
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	14	1.98
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	11	1.98
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	12	1.98
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	15	1.98
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	4	1.97
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	20	1.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	18	1.97
(1,185)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:ALA:N	6	1.97
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	4	1.96
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	13	1.96
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	15	1.96
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	20	1.95
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	3	1.95
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	4	1.94
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	14	1.93
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	4	1.93
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	13	1.93
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	1	1.92
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	2	1.92
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	20	1.92
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	9	1.91
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	3	1.91
(1,306)	1:189:A:MET:N	1:189:A:MET:CA	1:189:A:MET:C	1:190:A:TYR:N	19	1.9
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	2	1.9
(1,68)	1:111:A:ILE:C	1:112:A:LEU:N	1:112:A:LEU:CA	1:112:A:LEU:C	19	1.9
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	13	1.89
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	20	1.89
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	11	1.89
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	19	1.87
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	9	1.87
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	20	1.87
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	16	1.87
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	6	1.87
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	15	1.86
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	18	1.86
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	4	1.86
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	12	1.85
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	14	1.85
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	14	1.85
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	5	1.85
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	7	1.85
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	2	1.85
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	10	1.85
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	12	1.85
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	12	1.84
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	11	1.84
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	6	1.83
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	6	1.83
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	17	1.83
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	5	1.82
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	3	1.81
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	4	1.81
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	2	1.81
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	4	1.81
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	9	1.81
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	8	1.8
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	9	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	12	1.8
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	19	1.8
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	4	1.8
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	9	1.8
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1	1.8
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	8	1.8
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	18	1.79
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	8	1.79
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	3	1.79
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	17	1.79
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	18	1.78
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	6	1.78
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1	1.78
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	4	1.77
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	17	1.77
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	16	1.77
(1,300)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:LYS:N	17	1.76
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	17	1.76
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	4	1.76
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	19	1.76
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	10	1.76
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	5	1.76
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	10	1.75
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	13	1.75
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	3	1.75
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	8	1.75
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	9	1.75
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	10	1.74
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	18	1.74
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	6	1.74
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	7	1.74
(1,17)	1:59:A:VAL:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	16	1.73
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	12	1.72
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	17	1.72
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	11	1.72
(1,205)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:SER:N	14	1.72
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	12	1.72
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	2	1.72
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	2	1.72
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	20	1.71
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	2	1.71
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	19	1.71
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	16	1.71
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	5	1.7
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	7	1.7
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	2	1.69
(1,245)	1:124:A:LEU:N	1:124:A:LEU:CA	1:124:A:LEU:C	1:125:A:LEU:N	3	1.69
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	15	1.69
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	5	1.69
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	14	1.69
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	9	1.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	14	1.68
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	17	1.68
(1,241)	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	1:121:A:ALA:N	2	1.68
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	1	1.68
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	20	1.68
(1,311)	1:194:A:PRO:N	1:194:A:PRO:CA	1:194:A:PRO:C	1:195:A:GLY:N	20	1.67
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	8	1.67
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	13	1.67
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	1	1.67
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	6	1.67
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1	1.67
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	13	1.66
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	16	1.66
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	11	1.66
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	3	1.66
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	8	1.66
(1,300)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:LYS:N	9	1.65
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	15	1.65
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	17	1.65
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	7	1.65
(1,228)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:TRP:N	2	1.65
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	16	1.65
(1,68)	1:111:A:ILE:C	1:112:A:LEU:N	1:112:A:LEU:CA	1:112:A:LEU:C	10	1.65
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	7	1.64
(1,114)	1:161:A:GLU:C	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	9	1.64
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	3	1.64
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	18	1.63
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	5	1.63
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	16	1.63
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	5	1.63
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	16	1.62
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	11	1.62
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	3	1.61
(1,258)	1:141:A:LYS:N	1:141:A:LYS:CA	1:141:A:LYS:C	1:142:A:ALA:N	2	1.61
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	4	1.61
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	17	1.61
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	20	1.61
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	11	1.61
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	4	1.61
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	9	1.6
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	16	1.6
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	15	1.6
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	13	1.6
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	7	1.59
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	10	1.59
(1,272)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:PHE:N	17	1.58
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	4	1.58
(1,232)	1:111:A:ILE:N	1:111:A:ILE:CA	1:111:A:ILE:C	1:112:A:LEU:N	14	1.58
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	15	1.58
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	10	1.57
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	5	1.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	12	1.57
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	15	1.56
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	5	1.56
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	2	1.56
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	9	1.56
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	13	1.56
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	6	1.56
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	6	1.56
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	6	1.56
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	11	1.55
(1,234)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASP:N	2	1.55
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	14	1.55
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	11	1.55
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	1	1.54
(1,143)	1:190:A:TYR:C	1:191:A:PRO:N	1:191:A:PRO:CA	1:191:A:PRO:C	10	1.54
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	8	1.54
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	19	1.53
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	20	1.53
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	6	1.53
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	13	1.53
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	12	1.53
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	18	1.52
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	7	1.52
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	15	1.52
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	14	1.52
(1,20)	1:62:A:THR:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	6	1.52
(1,300)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:LYS:N	20	1.5
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	9	1.5
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	16	1.5
(1,71)	1:114:A:ASP:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	3	1.5
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	7	1.49
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	5	1.49
(1,111)	1:158:A:ALA:C	1:159:A:SER:N	1:159:A:SER:CA	1:159:A:SER:C	5	1.49
(1,68)	1:111:A:ILE:C	1:112:A:LEU:N	1:112:A:LEU:CA	1:112:A:LEU:C	5	1.49
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	15	1.49
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	4	1.49
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	3	1.48
(1,192)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:TYR:N	19	1.48
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	12	1.47
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	17	1.47
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	19	1.47
(1,145)	1:192:A:LYS:C	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	16	1.47
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	1	1.47
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	10	1.47
(1,312)	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	1:196:A:VAL:N	14	1.46
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	14	1.46
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	6	1.46
(1,65)	1:108:A:TRP:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	17	1.46
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	1	1.45
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	19	1.45
(1,65)	1:108:A:TRP:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	9	1.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	17	1.45
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	8	1.44
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	16	1.44
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	16	1.44
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	1	1.43
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	19	1.43
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	11	1.43
(1,183)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:THR:N	12	1.43
(1,104)	1:151:A:GLU:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	2	1.43
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	13	1.43
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	6	1.43
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	7	1.43
(1,312)	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	1:196:A:VAL:N	10	1.42
(1,239)	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	1:119:A:ARG:N	7	1.42
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	20	1.42
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	17	1.42
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	20	1.42
(1,65)	1:108:A:TRP:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	20	1.42
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	17	1.42
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	16	1.41
(1,285)	1:168:A:LEU:N	1:168:A:LEU:CA	1:168:A:LEU:C	1:169:A:VAL:N	7	1.41
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	15	1.41
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	20	1.41
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	20	1.41
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	2	1.41
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	8	1.41
(1,71)	1:114:A:ASP:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	12	1.41
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	9	1.41
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	6	1.4
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	5	1.4
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	6	1.4
(1,74)	1:117:A:PHE:C	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	9	1.4
(1,143)	1:190:A:TYR:C	1:191:A:PRO:N	1:191:A:PRO:CA	1:191:A:PRO:C	14	1.39
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	20	1.39
(1,312)	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	1:196:A:VAL:N	3	1.38
(1,296)	1:179:A:ALA:N	1:179:A:ALA:CA	1:179:A:ALA:C	1:180:A:GLU:N	14	1.38
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	12	1.38
(1,89)	1:135:A:ASP:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	4	1.38
(1,71)	1:114:A:ASP:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	18	1.38
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	19	1.38
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	15	1.38
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	3	1.37
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	10	1.37
(1,149)	1:196:A:VAL:C	1:197:A:PRO:N	1:197:A:PRO:CA	1:197:A:PRO:C	2	1.37
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	1	1.37
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	14	1.37
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	7	1.37
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	16	1.37
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	18	1.37
(1,17)	1:59:A:VAL:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	19	1.37
(1,285)	1:168:A:LEU:N	1:168:A:LEU:CA	1:168:A:LEU:C	1:169:A:VAL:N	2	1.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	11	1.36
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	18	1.36
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	2	1.36
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	18	1.36
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	2	1.36
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	14	1.36
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	1	1.35
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	5	1.35
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	19	1.35
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	20	1.35
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	6	1.35
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	9	1.35
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	5	1.35
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	9	1.34
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	16	1.34
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	1	1.34
(1,35)	1:77:A:ARG:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	11	1.34
(1,20)	1:62:A:THR:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	11	1.34
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	12	1.33
(1,285)	1:168:A:LEU:N	1:168:A:LEU:CA	1:168:A:LEU:C	1:169:A:VAL:N	9	1.33
(1,145)	1:192:A:LYS:C	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	3	1.33
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	8	1.33
(1,296)	1:179:A:ALA:N	1:179:A:ALA:CA	1:179:A:ALA:C	1:180:A:GLU:N	5	1.32
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	8	1.32
(1,192)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:TYR:N	15	1.32
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	13	1.32
(1,182)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:HIS:N	13	1.32
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	14	1.32
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	15	1.32
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	9	1.32
(1,300)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:LYS:N	6	1.31
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	19	1.31
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	4	1.31
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	5	1.31
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	5	1.31
(1,192)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:TYR:N	14	1.31
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	13	1.3
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	16	1.3
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	15	1.3
(1,188)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:ASP:N	16	1.3
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	11	1.3
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	10	1.3
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	20	1.3
(1,89)	1:135:A:ASP:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1	1.3
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	2	1.3
(1,78)	1:121:A:ALA:C	1:122:A:ASP:N	1:122:A:ASP:CA	1:122:A:ASP:C	2	1.3
(1,65)	1:108:A:TRP:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	13	1.3
(1,296)	1:179:A:ALA:N	1:179:A:ALA:CA	1:179:A:ALA:C	1:180:A:GLU:N	19	1.29
(1,91)	1:137:A:LYS:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	3	1.29
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	17	1.29
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	12	1.28

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	13	1.28
(1,89)	1:135:A:ASP:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	11	1.28
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	5	1.28
(1,56)	1:99:A:GLN:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	13	1.28
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	5	1.28
(1,17)	1:59:A:VAL:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	9	1.28
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	11	1.27
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	13	1.27
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	20	1.27
(1,228)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:TRP:N	19	1.27
(1,145)	1:192:A:LYS:C	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	14	1.27
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1	1.27
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	3	1.27
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	12	1.27
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	12	1.26
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	1	1.26
(1,192)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:TYR:N	1	1.26
(1,188)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:ASP:N	9	1.26
(1,188)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:ASP:N	10	1.26
(1,145)	1:192:A:LYS:C	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	10	1.26
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	4	1.26
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	13	1.26
(1,318)	1:201:A:ASP:N	1:201:A:ASP:CA	1:201:A:ASP:C	1:202:A:GLY:N	2	1.25
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	8	1.25
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	5	1.24
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	6	1.24
(1,232)	1:111:A:ILE:N	1:111:A:ILE:CA	1:111:A:ILE:C	1:112:A:LEU:N	19	1.24
(1,228)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:TRP:N	17	1.24
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	7	1.24
(1,188)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:ASP:N	18	1.24
(1,150)	1:197:A:PRO:C	1:198:A:CYS:N	1:198:A:CYS:CA	1:198:A:CYS:C	16	1.24
(1,311)	1:194:A:PRO:N	1:194:A:PRO:CA	1:194:A:PRO:C	1:195:A:GLY:N	2	1.23
(1,310)	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	1:194:A:PRO:N	5	1.23
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	7	1.23
(1,300)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:LYS:N	7	1.23
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	6	1.23
(1,181)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:SER:N	16	1.23
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	5	1.23
(1,104)	1:151:A:GLU:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	7	1.23
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	18	1.23
(1,74)	1:117:A:PHE:C	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	20	1.23
(1,71)	1:114:A:ASP:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	17	1.23
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	14	1.23
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	12	1.22
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	10	1.22
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	11	1.22
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	3	1.22
(1,85)	1:131:A:SER:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	4	1.22
(1,67)	1:110:A:ARG:C	1:111:A:ILE:N	1:111:A:ILE:CA	1:111:A:ILE:C	12	1.22
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	8	1.21
(1,231)	1:110:A:ARG:N	1:110:A:ARG:CA	1:110:A:ARG:C	1:111:A:ILE:N	9	1.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,210)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LEU:N	6	1.21
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	14	1.21
(1,192)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:TYR:N	11	1.21
(1,17)	1:59:A:VAL:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	10	1.21
(1,310)	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	1:194:A:PRO:N	10	1.2
(1,300)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:LYS:N	2	1.2
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	12	1.2
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	10	1.2
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	2	1.2
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	6	1.2
(1,146)	1:193:A:LYS:C	1:194:A:PRO:N	1:194:A:PRO:CA	1:194:A:PRO:C	10	1.2
(1,248)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:SER:N	7	1.19
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	15	1.19
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	11	1.19
(1,35)	1:77:A:ARG:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	12	1.19
(1,17)	1:59:A:VAL:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	18	1.19
(1,281)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:ARG:N	2	1.18
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	6	1.18
(1,192)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:TYR:N	10	1.18
(1,35)	1:77:A:ARG:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	14	1.18
(1,22)	1:64:A:ALA:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	10	1.18
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	20	1.17
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	5	1.17
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	9	1.17
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	14	1.17
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	19	1.17
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	1	1.17
(1,145)	1:192:A:LYS:C	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	8	1.17
(1,89)	1:135:A:ASP:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	5	1.17
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	8	1.17
(1,28)	1:70:A:LEU:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	17	1.17
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	1	1.16
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	11	1.16
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	14	1.16
(1,261)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:MET:N	16	1.16
(1,181)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:SER:N	10	1.16
(1,27)	1:69:A:ILE:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	8	1.16
(1,18)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	6	1.16
(1,311)	1:194:A:PRO:N	1:194:A:PRO:CA	1:194:A:PRO:C	1:195:A:GLY:N	1	1.15
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	1	1.15
(1,227)	1:106:A:ASN:N	1:106:A:ASN:CA	1:106:A:ASN:C	1:107:A:ARG:N	12	1.15
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	5	1.15
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	19	1.15
(1,109)	1:156:A:PHE:C	1:157:A:PRO:N	1:157:A:PRO:CA	1:157:A:PRO:C	4	1.15
(1,89)	1:135:A:ASP:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	17	1.15
(1,71)	1:114:A:ASP:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	4	1.15
(1,311)	1:194:A:PRO:N	1:194:A:PRO:CA	1:194:A:PRO:C	1:195:A:GLY:N	6	1.14
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	15	1.14
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	16	1.14
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	10	1.14
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	7	1.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	14	1.14
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	4	1.14
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	11	1.14
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	10	1.14
(1,236)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:GLY:N	5	1.14
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	18	1.14
(1,206)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:GLU:N	19	1.14
(1,130)	1:177:A:ASP:C	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	10	1.14
(1,109)	1:156:A:PHE:C	1:157:A:PRO:N	1:157:A:PRO:CA	1:157:A:PRO:C	8	1.14
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	2	1.14
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	10	1.14
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	7	1.14
(1,22)	1:64:A:ALA:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	18	1.14
(1,16)	1:58:A:ASP:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	13	1.14
(1,310)	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	1:194:A:PRO:N	19	1.13
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	6	1.13
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	11	1.13
(1,20)	1:62:A:THR:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	12	1.13
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	6	1.12
(1,259)	1:142:A:ALA:N	1:142:A:ALA:CA	1:142:A:ALA:C	1:143:A:ARG:N	6	1.12
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	15	1.12
(1,181)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:SER:N	9	1.12
(1,35)	1:77:A:ARG:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	9	1.12
(1,20)	1:62:A:THR:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	7	1.12
(1,318)	1:201:A:ASP:N	1:201:A:ASP:CA	1:201:A:ASP:C	1:202:A:GLY:N	6	1.11
(1,257)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:LYS:N	10	1.11
(1,181)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:SER:N	18	1.11
(1,126)	1:173:A:LEU:C	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	16	1.11
(1,126)	1:173:A:LEU:C	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	20	1.11
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	4	1.11
(1,65)	1:108:A:TRP:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	7	1.11
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	3	1.11
(1,18)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	2	1.11
(1,315)	1:198:A:CYS:N	1:198:A:CYS:CA	1:198:A:CYS:C	1:199:A:LEU:N	14	1.1
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	14	1.1
(1,285)	1:168:A:LEU:N	1:168:A:LEU:CA	1:168:A:LEU:C	1:169:A:VAL:N	5	1.1
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	2	1.1
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	20	1.1
(1,228)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:TRP:N	5	1.1
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	6	1.1
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	15	1.1
(1,84)	1:130:A:LEU:C	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	14	1.1
(1,65)	1:108:A:TRP:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	4	1.1
(1,45)	1:88:A:GLN:C	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	6	1.1
(1,281)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:ARG:N	10	1.09
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	4	1.09
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	13	1.09
(1,126)	1:173:A:LEU:C	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	4	1.09
(1,109)	1:156:A:PHE:C	1:157:A:PRO:N	1:157:A:PRO:CA	1:157:A:PRO:C	16	1.09
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	4	1.09
(1,274)	1:157:A:PRO:N	1:157:A:PRO:CA	1:157:A:PRO:C	1:158:A:ALA:N	8	1.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	14	1.08
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	20	1.08
(1,251)	1:133:A:MET:N	1:133:A:MET:CA	1:133:A:MET:C	1:134:A:SER:N	10	1.08
(1,209)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	18	1.08
(1,192)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:TYR:N	18	1.08
(1,172)	1:46:A:ARG:N	1:46:A:ARG:CA	1:46:A:ARG:C	1:47:A:ASP:N	7	1.08
(1,35)	1:77:A:ARG:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	4	1.08
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	14	1.07
(1,296)	1:179:A:ALA:N	1:179:A:ALA:CA	1:179:A:ALA:C	1:180:A:GLU:N	1	1.07
(1,248)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:SER:N	17	1.07
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	7	1.07
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	1	1.07
(1,89)	1:135:A:ASP:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	18	1.07
(1,74)	1:117:A:PHE:C	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	10	1.07
(1,68)	1:111:A:ILE:C	1:112:A:LEU:N	1:112:A:LEU:CA	1:112:A:LEU:C	1	1.07
(1,37)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1	1.07
(1,35)	1:77:A:ARG:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	3	1.07
(1,325)	1:208:A:CYS:N	1:208:A:CYS:CA	1:208:A:CYS:C	1:209:A:LEU:N	9	1.06
(1,325)	1:208:A:CYS:N	1:208:A:CYS:CA	1:208:A:CYS:C	1:209:A:LEU:N	13	1.06
(1,231)	1:110:A:ARG:N	1:110:A:ARG:CA	1:110:A:ARG:C	1:111:A:ILE:N	17	1.06
(1,227)	1:106:A:ASN:N	1:106:A:ASN:CA	1:106:A:ASN:C	1:107:A:ARG:N	4	1.06
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	13	1.06
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	1	1.06
(1,130)	1:177:A:ASP:C	1:178:A:ALA:N	1:178:A:ALA:CA	1:178:A:ALA:C	14	1.06
(1,114)	1:161:A:GLU:C	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	13	1.06
(1,63)	1:106:A:ASN:C	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	17	1.06
(1,310)	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	1:194:A:PRO:N	7	1.05
(1,310)	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	1:194:A:PRO:N	12	1.05
(1,296)	1:179:A:ALA:N	1:179:A:ALA:CA	1:179:A:ALA:C	1:180:A:GLU:N	10	1.05
(1,278)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:LEU:N	17	1.05
(1,253)	1:135:A:ASP:N	1:135:A:ASP:CA	1:135:A:ASP:C	1:136:A:SER:N	3	1.05
(1,213)	1:92:A:TYR:N	1:92:A:TYR:CA	1:92:A:TYR:C	1:93:A:ASP:N	9	1.05
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	15	1.05
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	8	1.05
(1,186)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:ASP:N	12	1.05
(1,147)	1:194:A:PRO:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	6	1.05
(1,126)	1:173:A:LEU:C	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	5	1.04
(1,114)	1:161:A:GLU:C	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	12	1.04
(1,33)	1:75:A:VAL:C	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	15	1.04
(1,234)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASP:N	14	1.03
(1,188)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:ASP:N	19	1.03
(1,181)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:SER:N	19	1.03
(1,145)	1:192:A:LYS:C	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	9	1.03
(1,124)	1:171:A:ASP:C	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	14	1.03
(1,27)	1:69:A:ILE:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	5	1.03
(1,20)	1:62:A:THR:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	17	1.03
(1,318)	1:201:A:ASP:N	1:201:A:ASP:CA	1:201:A:ASP:C	1:202:A:GLY:N	14	1.02
(1,315)	1:198:A:CYS:N	1:198:A:CYS:CA	1:198:A:CYS:C	1:199:A:LEU:N	3	1.02
(1,305)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:MET:N	3	1.02
(1,288)	1:171:A:ASP:N	1:171:A:ASP:CA	1:171:A:ASP:C	1:172:A:ARG:N	1	1.02
(1,267)	1:150:A:ALA:N	1:150:A:ALA:CA	1:150:A:ALA:C	1:151:A:GLU:N	17	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,265)	1:148:A:LYS:N	1:148:A:LYS:CA	1:148:A:LYS:C	1:149:A:LEU:N	7	1.02
(1,248)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:SER:N	10	1.02
(1,234)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASP:N	7	1.02
(1,187)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ASP:N	10	1.02
(1,180)	1:58:A:ASP:N	1:58:A:ASP:CA	1:58:A:ASP:C	1:59:A:VAL:N	10	1.02
(1,132)	1:179:A:ALA:C	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	3	1.02
(1,311)	1:194:A:PRO:N	1:194:A:PRO:CA	1:194:A:PRO:C	1:195:A:GLY:N	7	1.01
(1,311)	1:194:A:PRO:N	1:194:A:PRO:CA	1:194:A:PRO:C	1:195:A:GLY:N	17	1.01
(1,310)	1:193:A:LYS:N	1:193:A:LYS:CA	1:193:A:LYS:C	1:194:A:PRO:N	6	1.01
(1,246)	1:125:A:LEU:N	1:125:A:LEU:CA	1:125:A:LEU:C	1:126:A:SER:N	7	1.01
(1,120)	1:167:A:LEU:C	1:168:A:LEU:N	1:168:A:LEU:CA	1:168:A:LEU:C	9	1.01
(1,109)	1:156:A:PHE:C	1:157:A:PRO:N	1:157:A:PRO:CA	1:157:A:PRO:C	14	1.01
(1,74)	1:117:A:PHE:C	1:118:A:GLN:N	1:118:A:GLN:CA	1:118:A:GLN:C	17	1.01
(1,22)	1:64:A:ALA:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	9	1.01
(1,291)	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	1:175:A:ALA:N	13	1.0
(1,207)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:TRP:N	8	1.0
(1,126)	1:173:A:LEU:C	1:174:A:ILE:N	1:174:A:ILE:CA	1:174:A:ILE:C	19	1.0
(1,89)	1:135:A:ASP:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	7	1.0
(1,35)	1:77:A:ARG:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	18	1.0
(1,33)	1:75:A:VAL:C	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	19	1.0