Full wwPDB NMR Structure Validation Report (i)

Mar 9, 2026 – 01:29 PM UTC

PDB ID	:	9LLV / pdb_00009llv
BMRB ID	:	52887
Title	:	Dimer Sgt2 from S.cerevisiae
Authors	:	Huang, C.; Ji, T.
Deposited on	:	2025-01-17

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 (i) 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 (1)) were used in the production of this report:

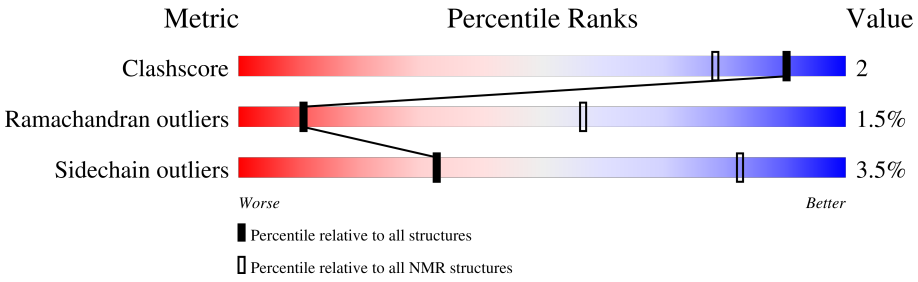
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (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 8%.

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	347	56% · 43%
1	B	347	51% · 48%

2 Ensemble composition and analysis (i)

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:70, B:2-B:70 (138)	1.36	20
2	A:102-A:216 (115)	2.17	17
3	A:310-A:322 (13)	2.41	8
4	B:105-B:215 (111)	2.45	2

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 5 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10318 atoms, of which 5088 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Small glutamine-rich tetratricopeptide repeat-containing protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	347	Total	C	H	N	O	S	0
			5159	1606	2544	446	547	16	
1	B	347	Total	C	H	N	O	S	0
			5159	1606	2544	446	547	16	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	TYR	-	expression tag	UNP Q12118
B	347	TYR	-	expression tag	UNP Q12118

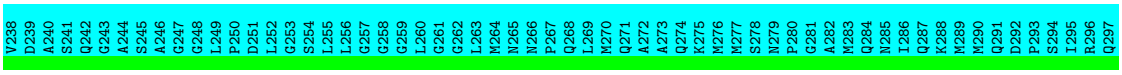
4 Residue-property plots

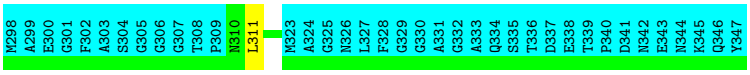
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

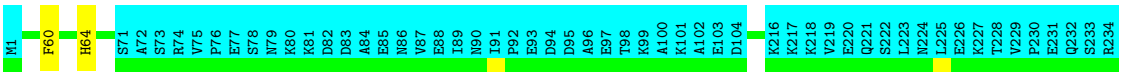
Chain A:





• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain B:



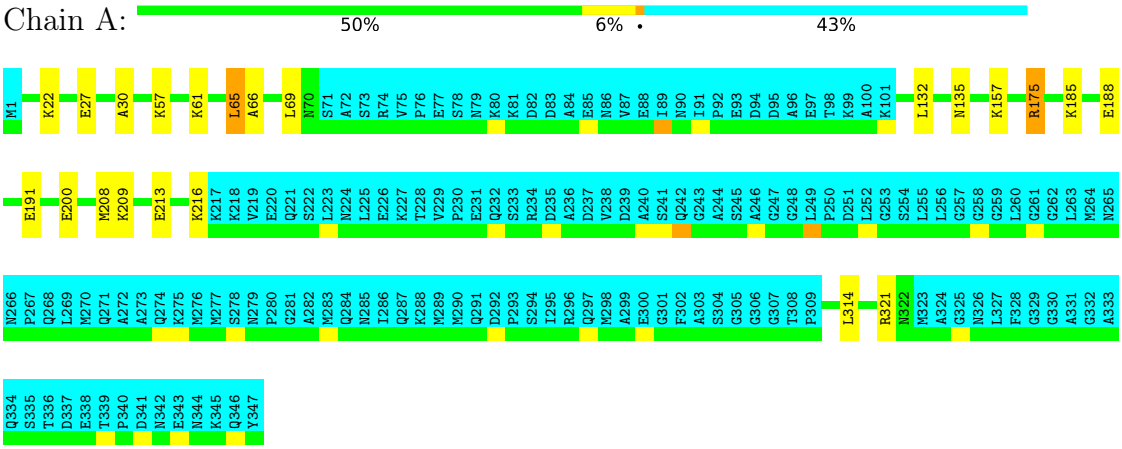
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

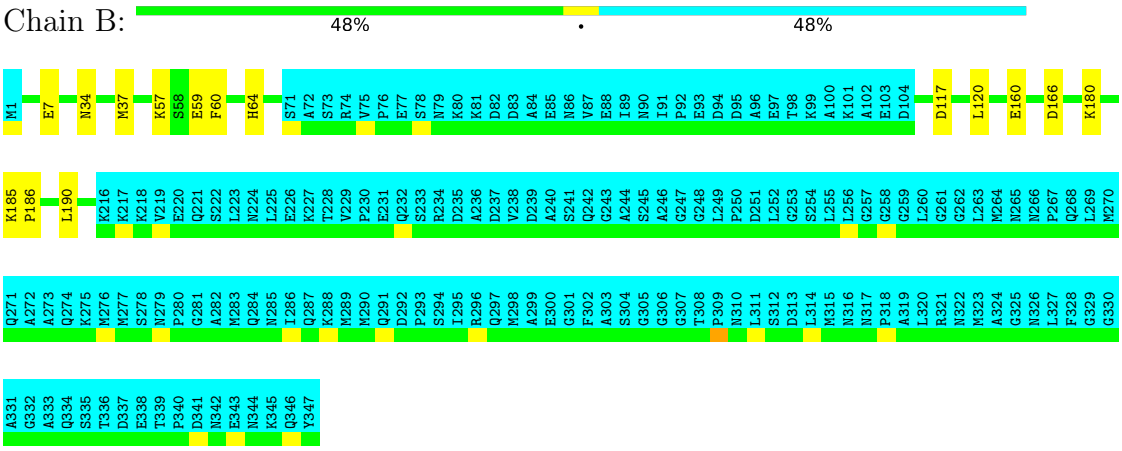
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

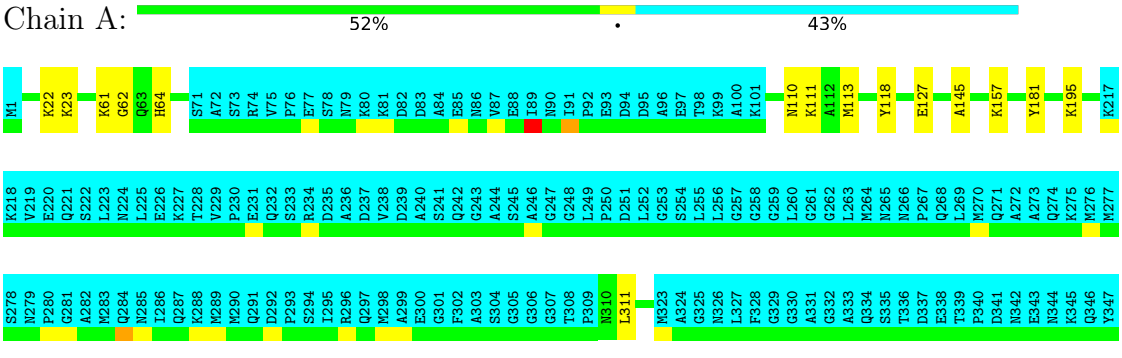
Chain B:



4.2.2 Score per residue for model 2

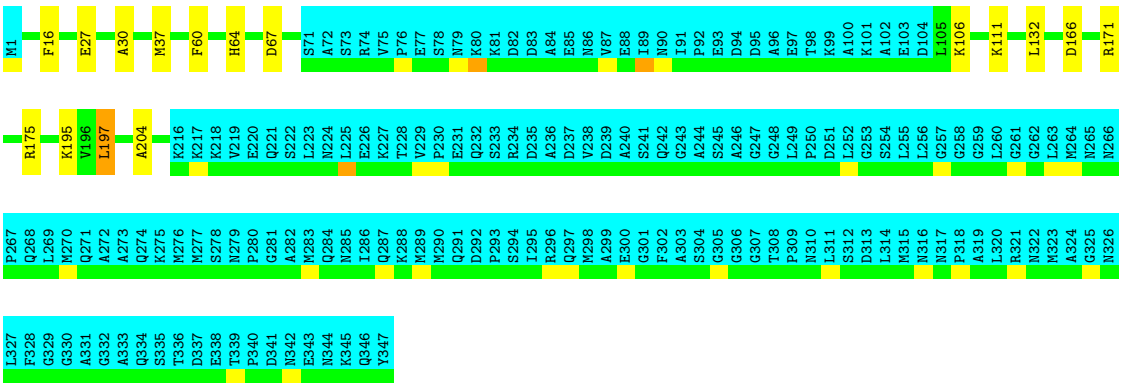
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

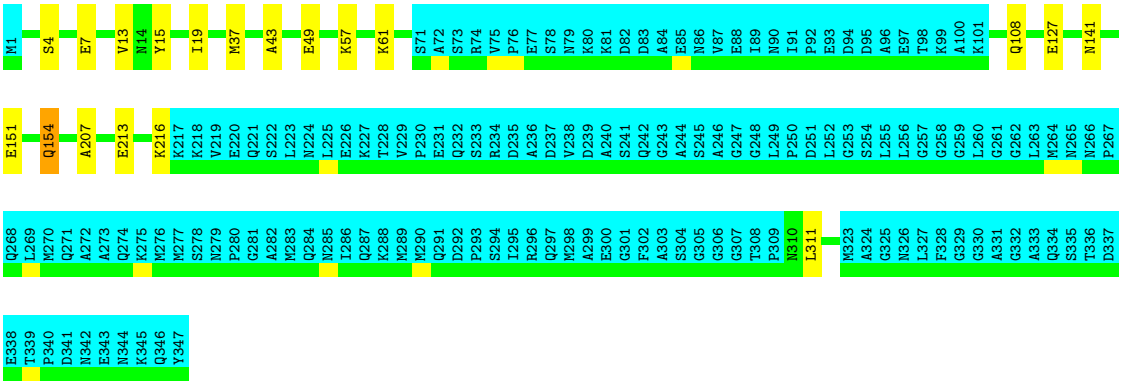
Chain B:



4.2.3 Score per residue for model 3

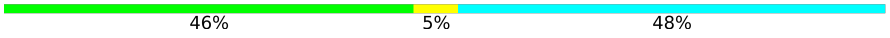
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

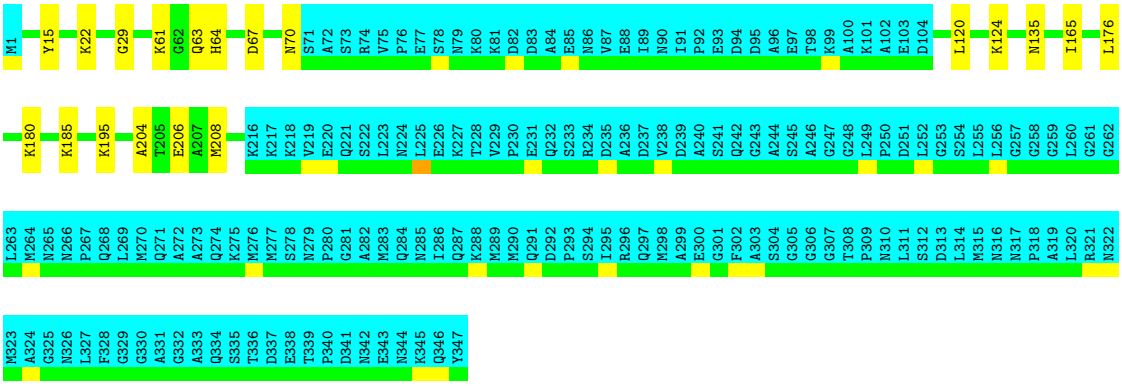
Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain B:

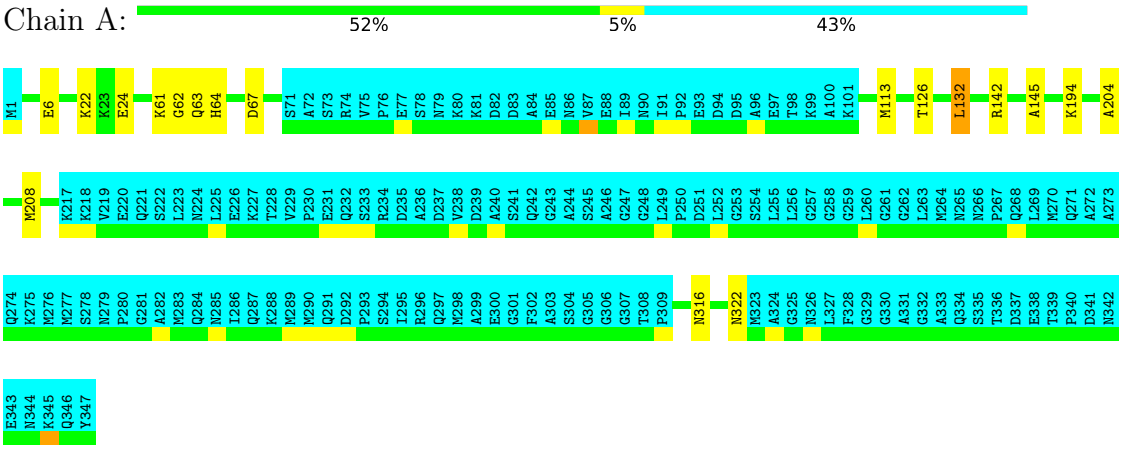




4.2.4 Score per residue for model 4

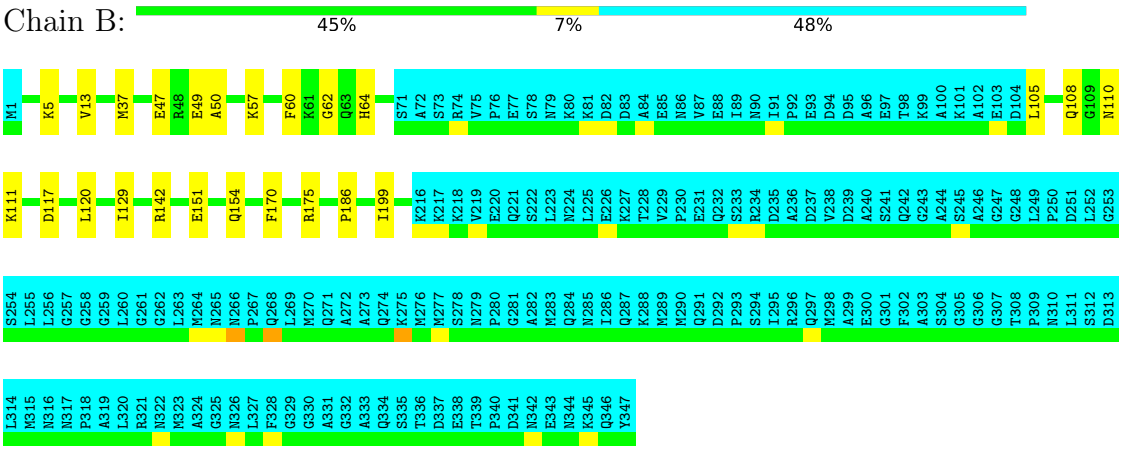
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

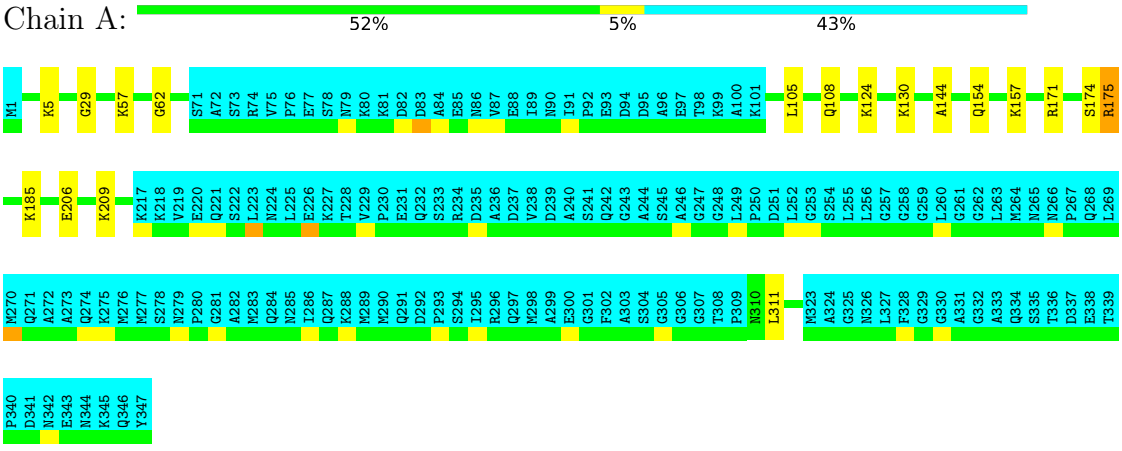
Chain B:



4.2.5 Score per residue for model 5

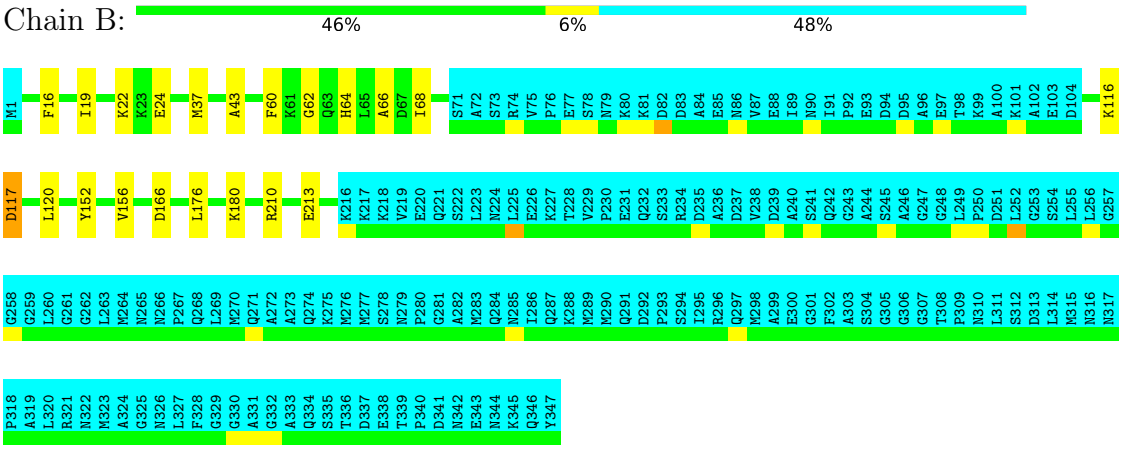
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

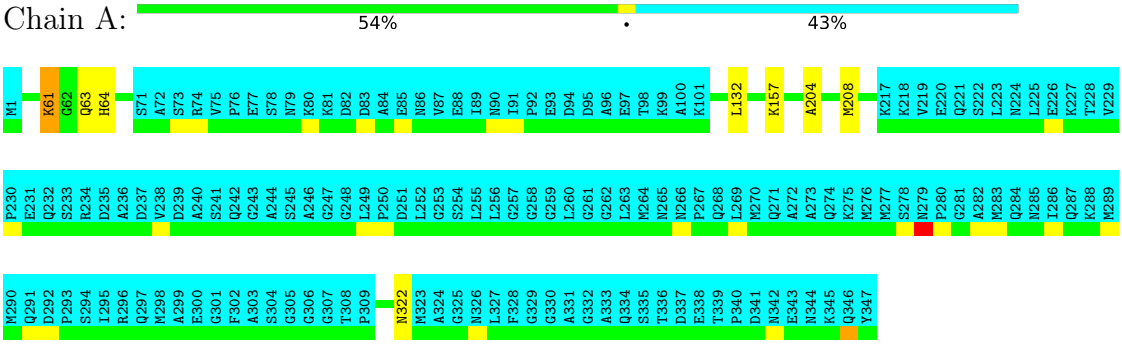
Chain B:



4.2.6 Score per residue for model 6

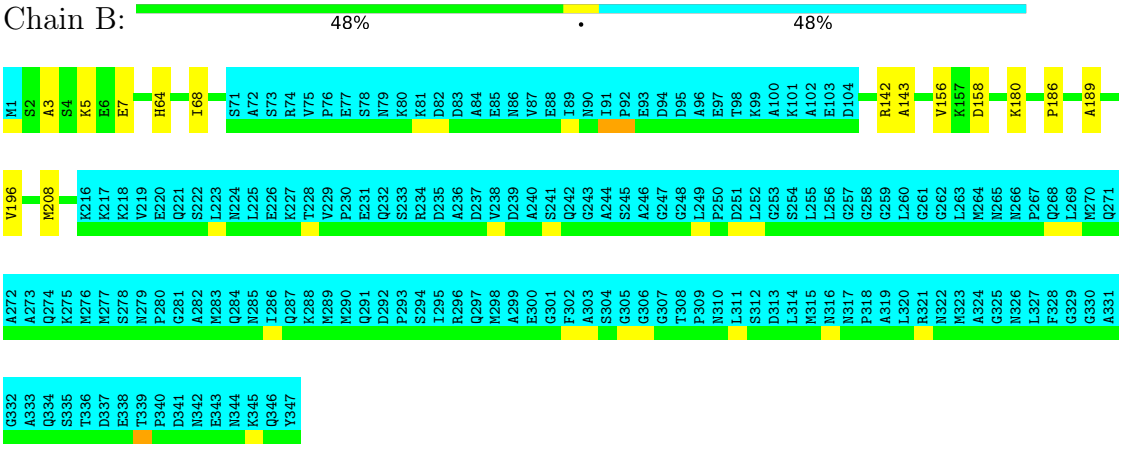
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

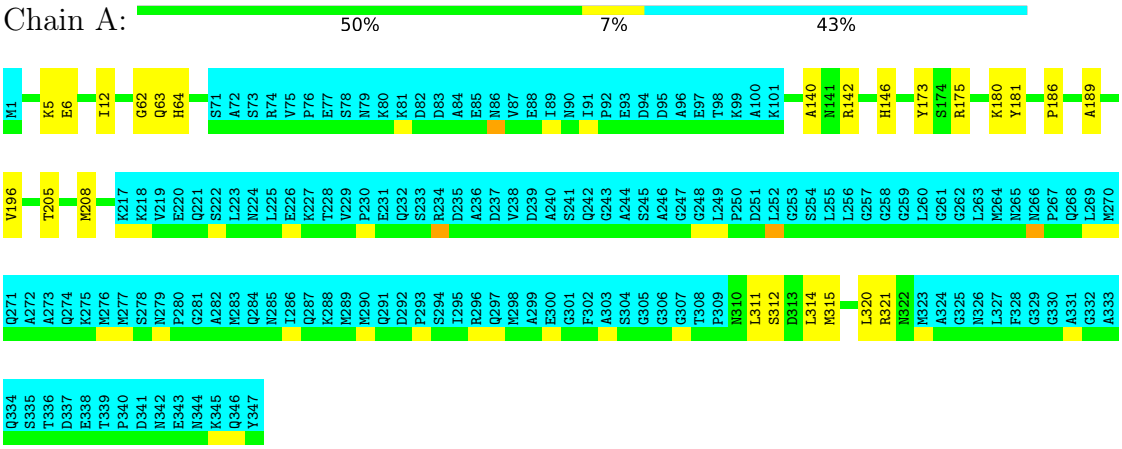
Chain B:



4.2.7 Score per residue for model 7

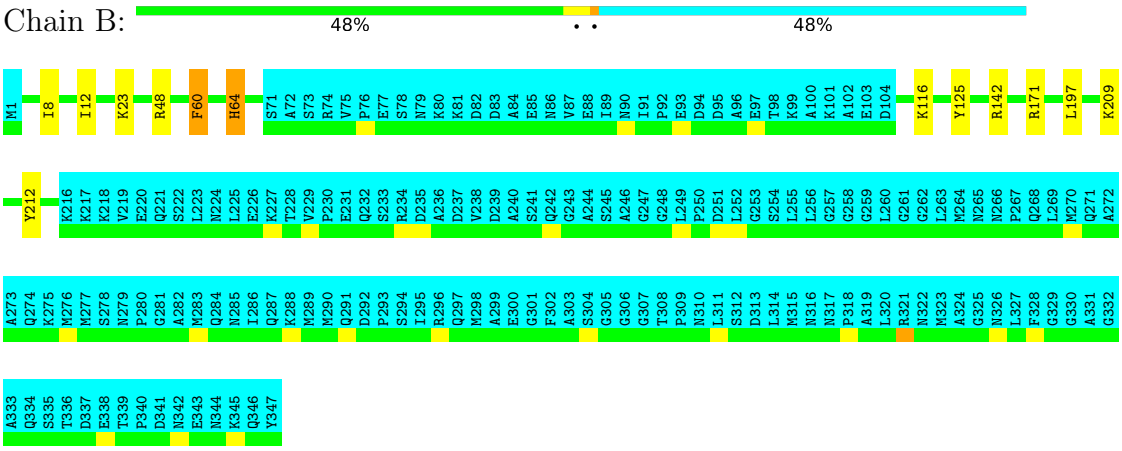
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

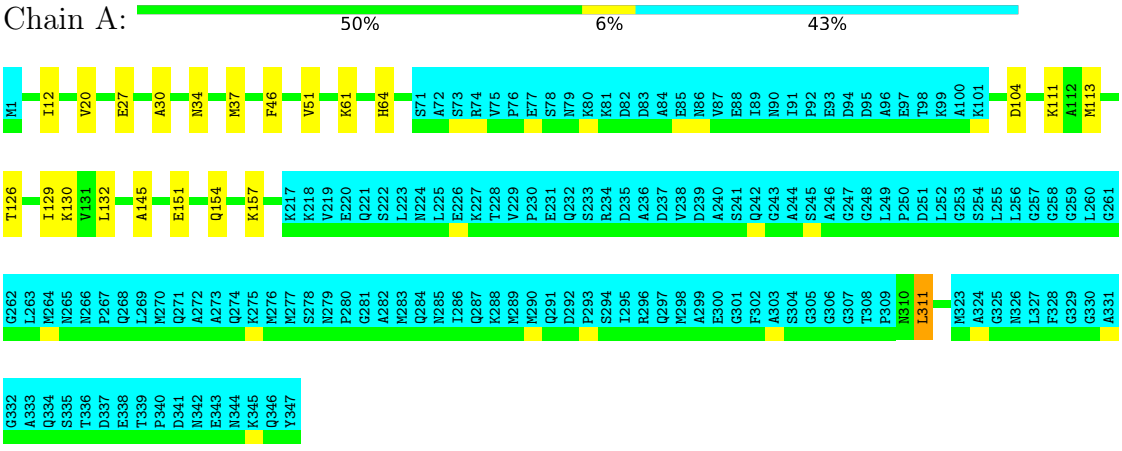
Chain B:



4.2.8 Score per residue for model 8

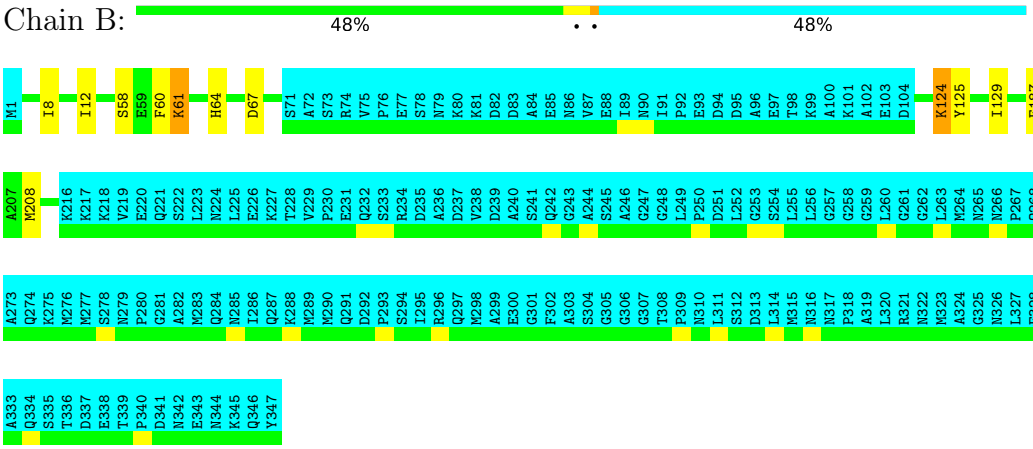
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

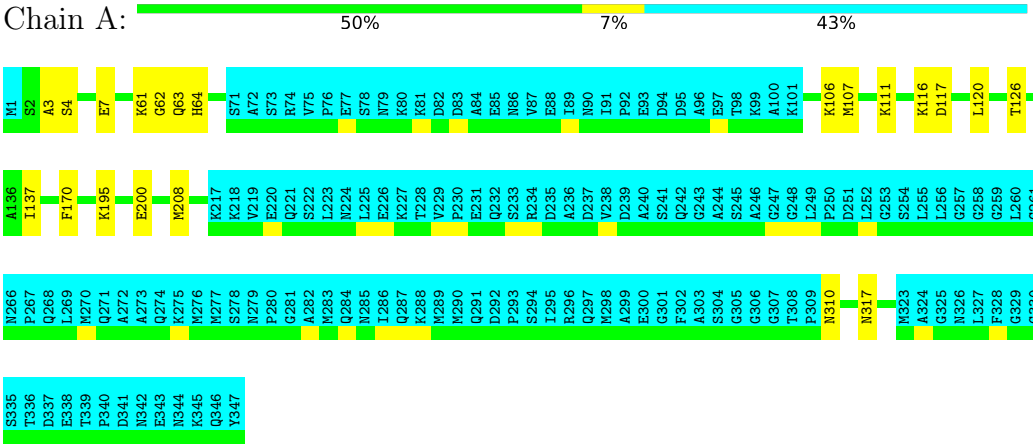
Chain B:



4.2.9 Score per residue for model 9

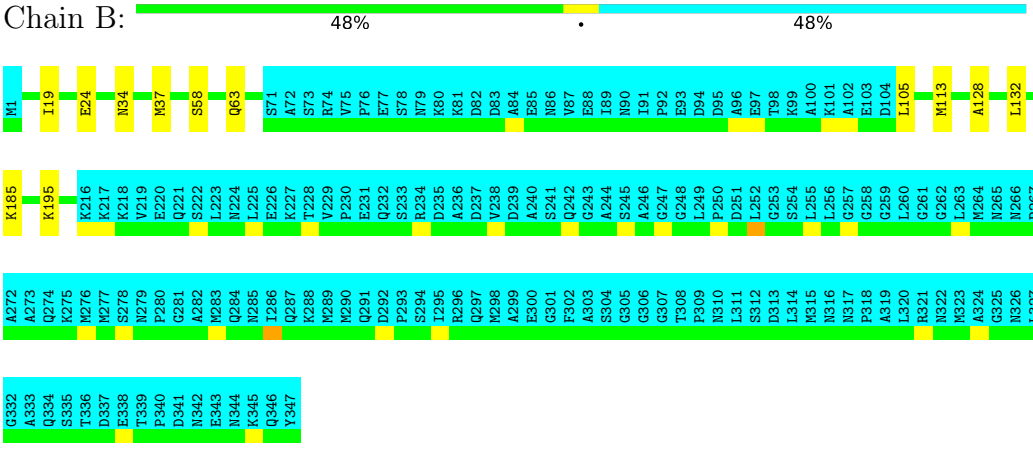
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

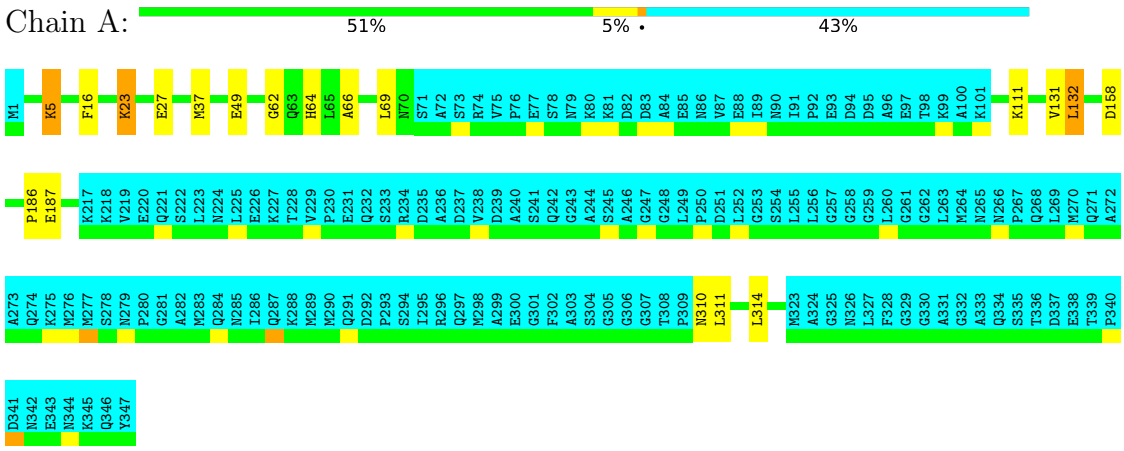
Chain B:



4.2.10 Score per residue for model 10

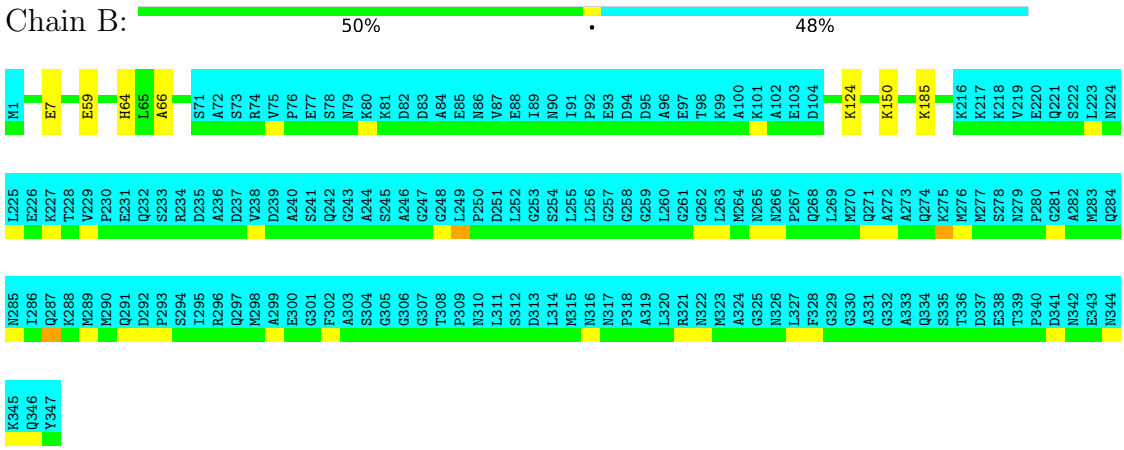
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

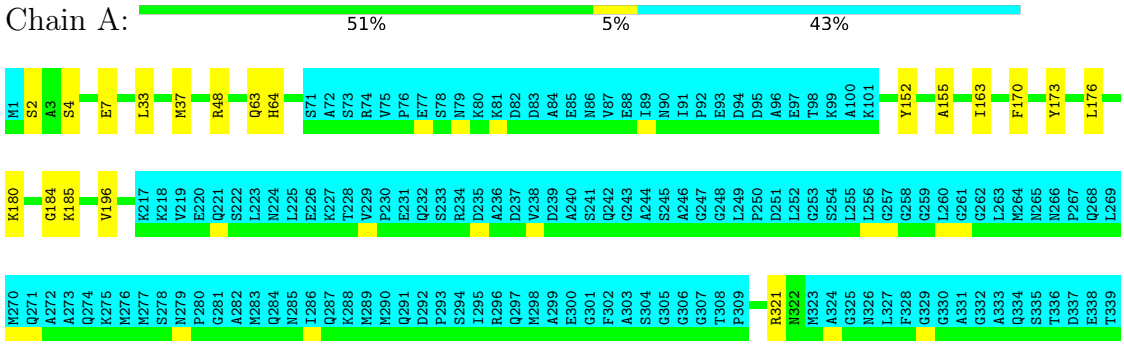
Chain B:

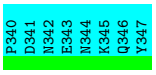


4.2.11 Score per residue for model 11

• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

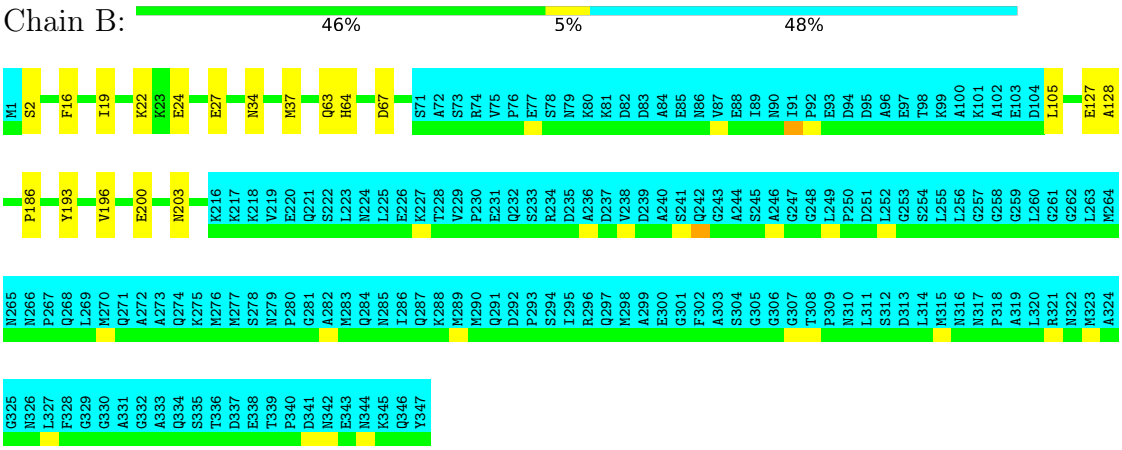
Chain A:





• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

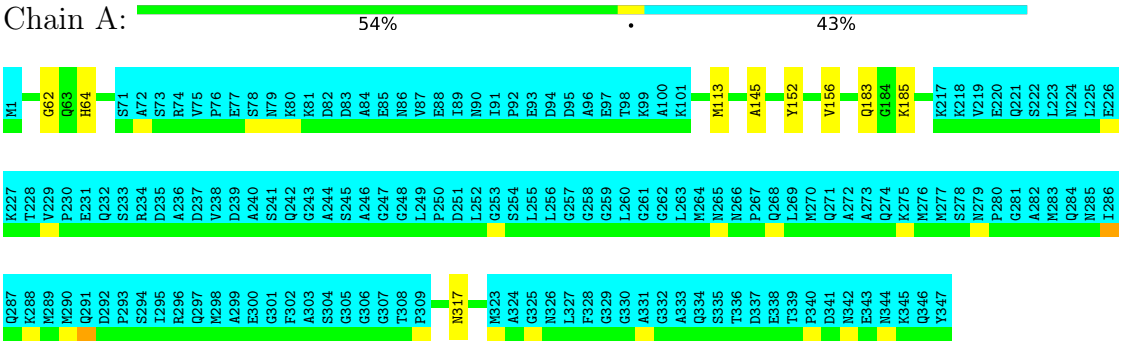
Chain B:



4.2.12 Score per residue for model 12

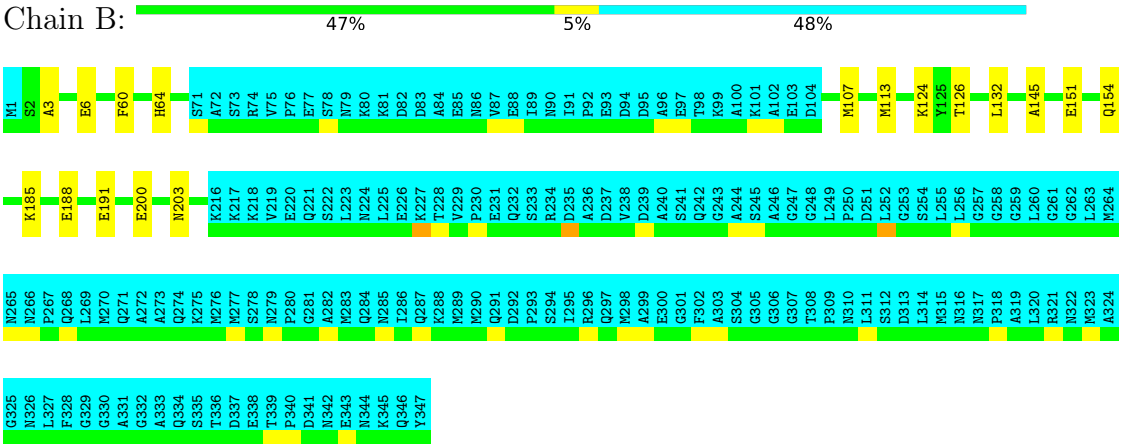
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

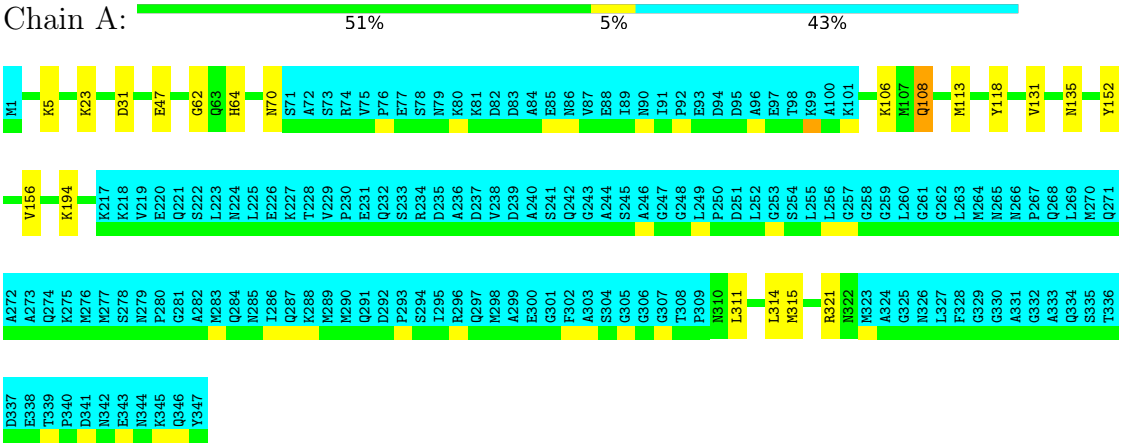
Chain B:



4.2.13 Score per residue for model 13

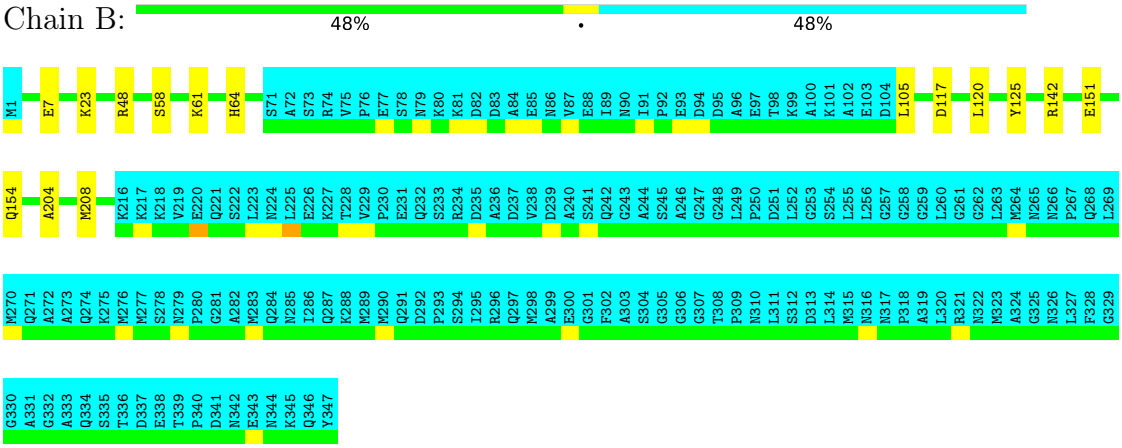
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

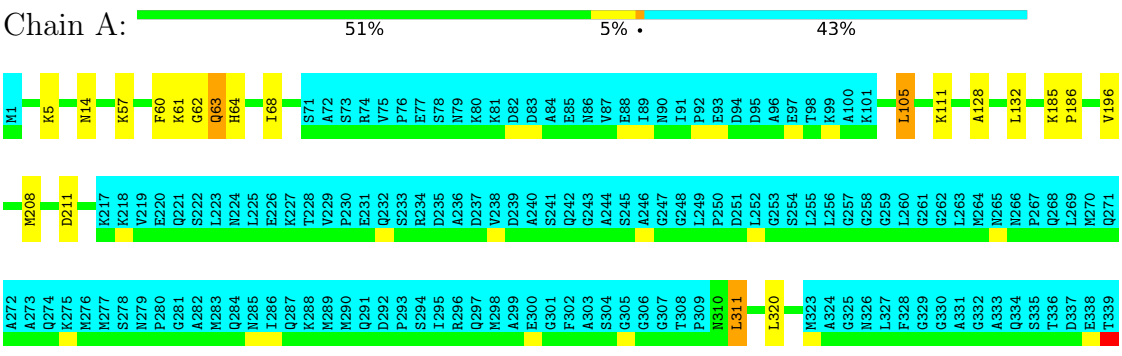
Chain B:

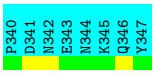


4.2.14 Score per residue for model 14

• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

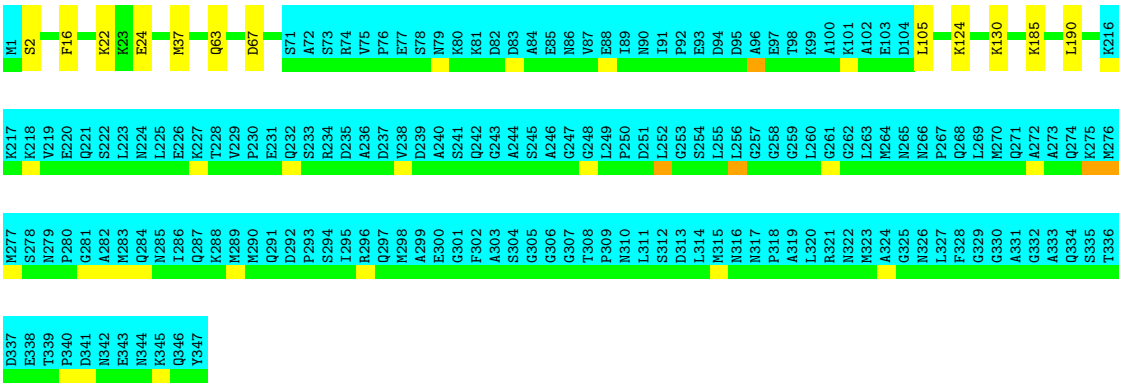
Chain A:





• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

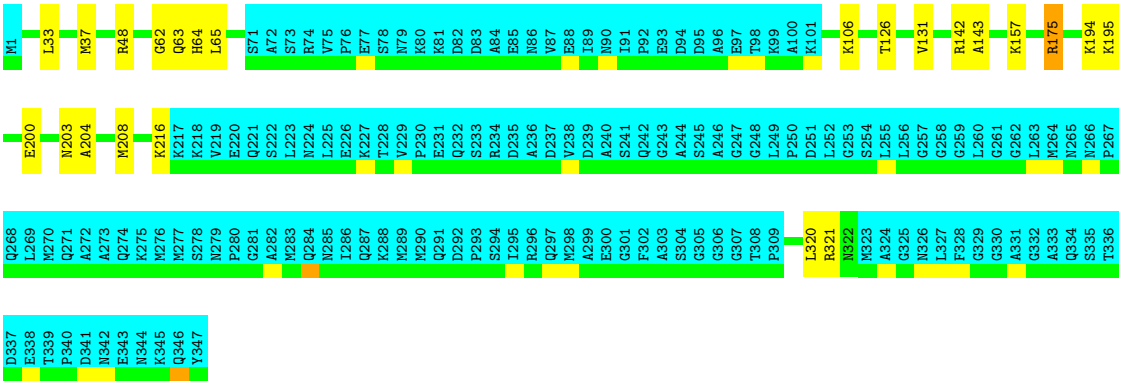
Chain B:



4.2.15 Score per residue for model 15

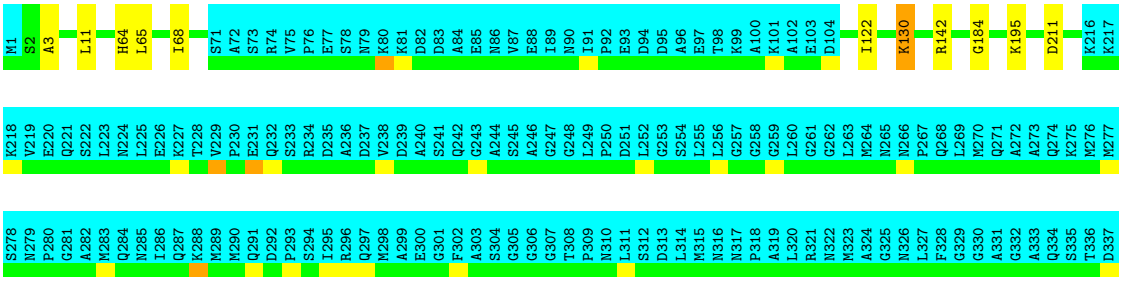
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

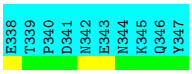
Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain B:





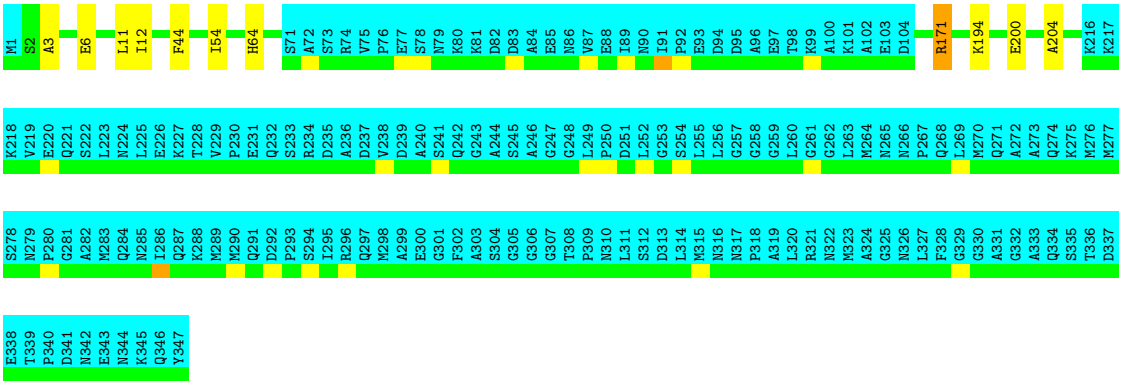
4.2.16 Score per residue for model 16

• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:

• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

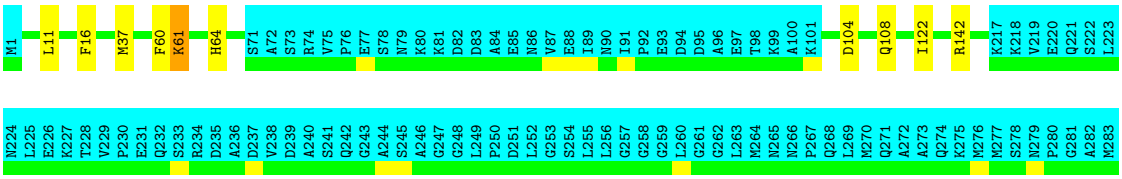
Chain B:

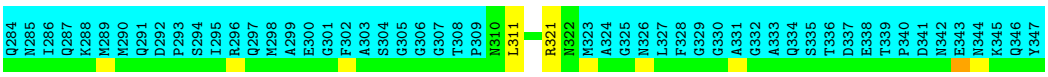


4.2.17 Score per residue for model 17

• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

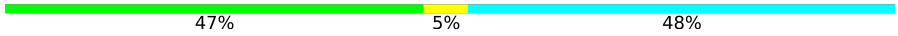
Chain A:

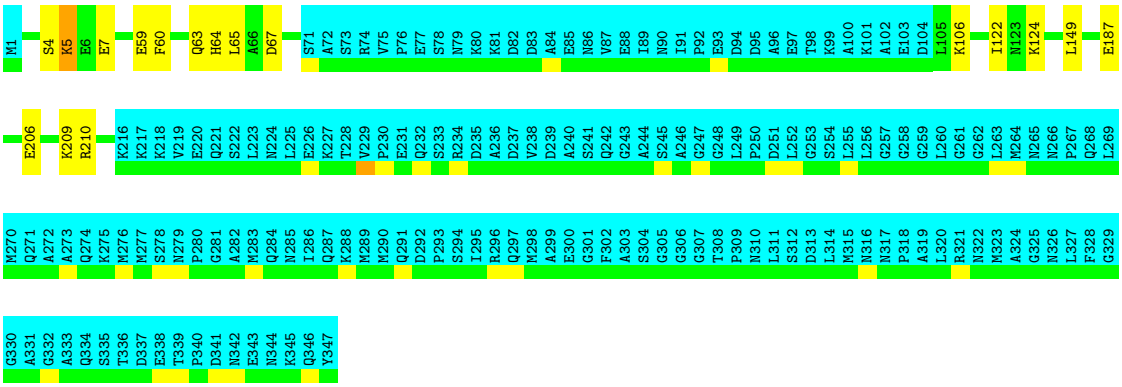




• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain B:

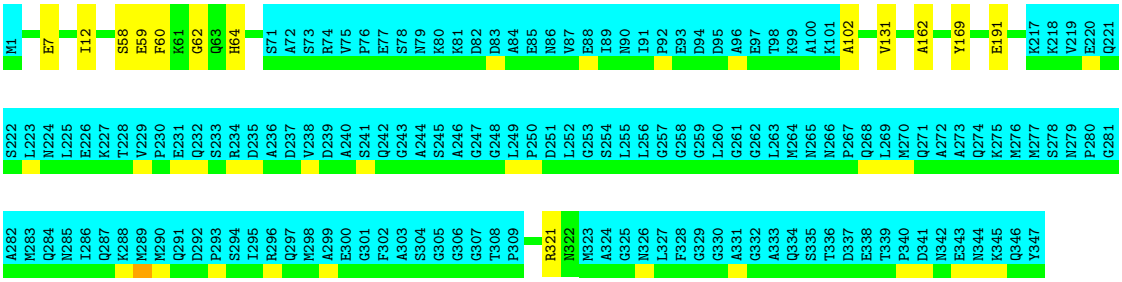




4.2.18 Score per residue for model 18

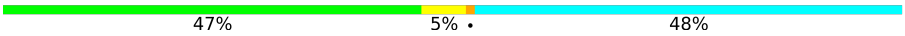
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

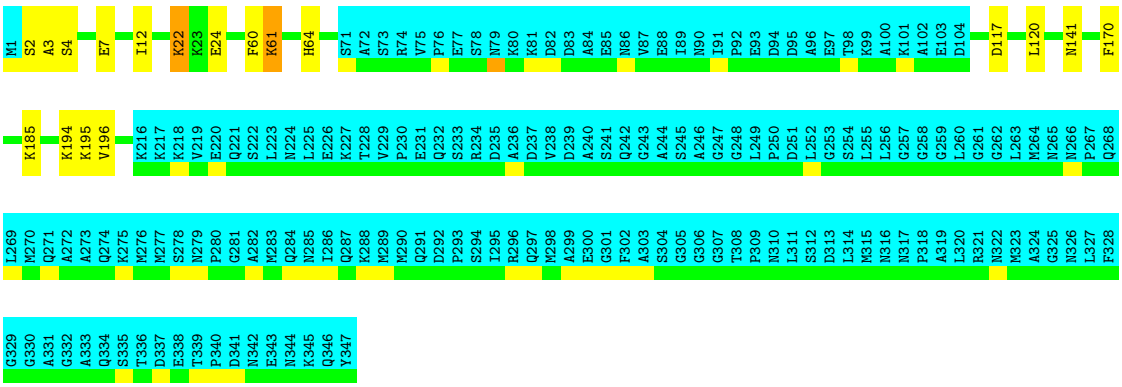
Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain B:

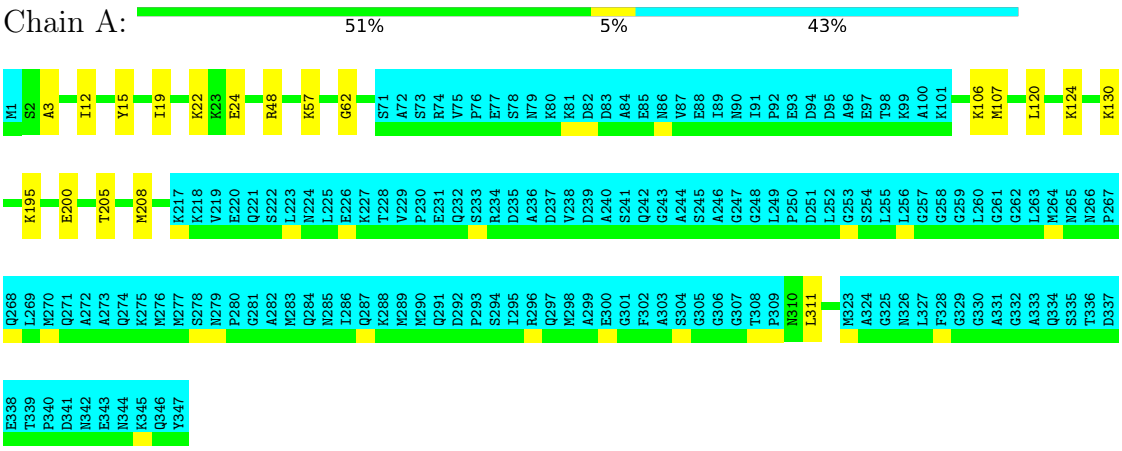




4.2.19 Score per residue for model 19

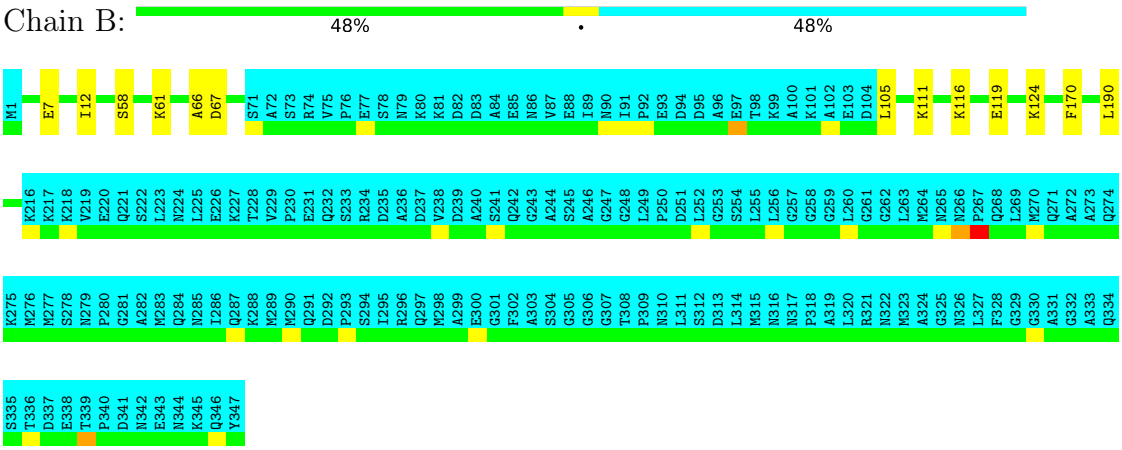
• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain A:



• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

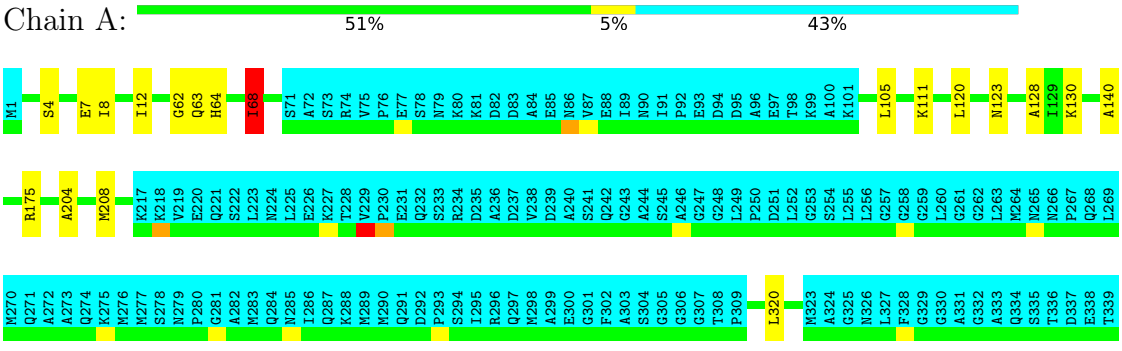
Chain B:

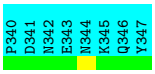


4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

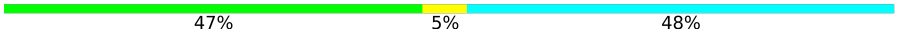
Chain A:

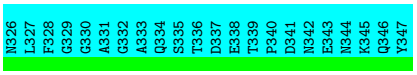




• Molecule 1: Small glutamine-rich tetratricopeptide repeat-containing protein 2

Chain B:





5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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	750
Number of shifts mapped to atoms	750
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

6 Model quality

6.1 Standard geometry

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	1.20±0.03	0±1/1548 (0.0± 0.0%)	1.10±0.02	0±0/2083 (0.0± 0.0%)
1	B	1.20±0.03	0±0/1415 (0.0± 0.0%)	1.08±0.02	0±0/1903 (0.0± 0.0%)
All	All	1.20	14/59260 (0.0%)	1.09	2/79720 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	185	LYS	C-N	6.03	1.38	1.33	12	1
1	A	166	ASP	C-N	5.78	1.38	1.33	16	1
1	B	166	ASP	C-N	5.76	1.38	1.33	2	3
1	B	68	ILE	CA-CB	5.62	1.59	1.53	6	1
1	B	132	LEU	CA-CB	5.53	1.58	1.53	12	1
1	A	132	LEU	C-N	5.43	1.37	1.33	8	3
1	A	156	VAL	CA-CB	5.26	1.60	1.54	12	1
1	B	132	LEU	C-N	5.16	1.37	1.33	9	1
1	A	68	ILE	CA-CB	5.14	1.60	1.53	20	1
1	A	132	LEU	CA-CB	5.10	1.58	1.53	10	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	185	LYS	CA-C-N	5.01	124.31	118.85	14	1
1	A	185	LYS	C-N-CA	5.01	124.31	118.85	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	1525	1493	1491	6±3
1	B	1393	1365	1363	5±2
All	All	58360	57160	57080	195

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:204:ALA:HA	1:A:208:MET:SD	0.69	2.28	15	4
1:A:151:GLU:HB3	1:A:154:GLN:HB3	0.65	1.66	3	2
1:A:43:ALA:HB1	1:B:29:GLY:HA2	0.63	1.71	3	1
1:A:105:LEU:HD21	1:A:128:ALA:HB2	0.62	1.70	14	1
1:B:204:ALA:HA	1:B:208:MET:SD	0.58	2.39	13	3
1:A:196:VAL:HG12	1:A:208:MET:HE3	0.58	1.74	14	1
1:B:7:GLU:HB3	1:B:58:SER:HB3	0.57	1.76	19	2
1:A:205:THR:HB	1:A:208:MET:SD	0.57	2.39	7	2
1:A:200:GLU:HB3	1:A:203:ASN:HB2	0.56	1.77	15	1
1:B:200:GLU:HG3	1:B:203:ASN:HB2	0.56	1.78	12	1
1:A:180:LYS:HB3	1:A:189:ALA:HB2	0.55	1.78	7	1
1:B:16:PHE:HB2	1:B:37:MET:SD	0.54	2.42	2	3
1:A:143:ALA:HB1	1:A:175:ARG:HG2	0.54	1.79	15	1
1:A:37:MET:SD	1:A:48:ARG:NE	0.53	2.81	11	1
1:A:180:LYS:HD3	1:A:188:GLU:HB2	0.53	1.78	16	1
1:B:6:GLU:HG2	1:B:54:ILE:HD11	0.53	1.80	16	1
1:A:185:LYS:HB3	1:A:188:GLU:HB2	0.53	1.80	1	1
1:A:170:PHE:CZ	1:A:208:MET:SD	0.53	3.01	9	1
1:A:208:MET:N	1:A:208:MET:SD	0.53	2.82	19	1
1:A:7:GLU:HG2	1:A:57:LYS:HE2	0.53	1.79	3	1
1:A:106:LYS:HD2	1:A:107:MET:SD	0.53	2.43	19	1
1:B:60:PHE:HB3	1:B:63:GLN:HE21	0.53	1.63	20	1
1:A:117:ASP:HB3	1:A:120:LEU:HD23	0.53	1.79	9	1
1:B:197:LEU:HD12	1:B:204:ALA:HB1	0.53	1.81	2	1
1:A:12:ILE:HG12	1:B:12:ILE:HG12	0.53	1.80	7	3
1:B:200:GLU:HB2	1:B:204:ALA:HA	0.52	1.82	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LYS:HB3	1:B:67:ASP:HB3	0.52	1.81	17	2
1:A:200:GLU:HG3	1:A:208:MET:HG2	0.52	1.81	19	1
1:B:170:PHE:HB2	1:B:196:VAL:HG13	0.52	1.81	18	2
1:A:140:ALA:HB1	1:A:175:ARG:HG3	0.52	1.81	7	1
1:A:102:ALA:HB2	1:A:131:VAL:HB	0.52	1.82	18	1
1:B:151:GLU:HB3	1:B:154:GLN:HB2	0.51	1.83	4	2
1:A:29:GLY:HA2	1:B:43:ALA:HB1	0.51	1.82	5	1
1:B:143:ALA:HB2	1:B:158:ASP:HB2	0.51	1.82	6	1
1:B:27:GLU:HA	1:B:30:ALA:HB3	0.51	1.82	2	1
1:B:135:ASN:HD21	1:B:137:ILE:HB	0.51	1.64	20	1
1:A:113:MET:HE2	1:A:145:ALA:HB2	0.50	1.84	4	2
1:B:22:LYS:HG3	1:B:24:GLU:HG2	0.50	1.82	18	1
1:A:108:GLN:HE21	1:A:108:GLN:N	0.50	2.04	13	1
1:A:5:LYS:H	1:A:5:LYS:HD2	0.50	1.67	7	1
1:A:12:ILE:HG12	1:B:12:ILE:HD12	0.50	1.83	20	1
1:A:213:GLU:HA	1:A:216:LYS:HB3	0.49	1.84	1	1
1:B:176:LEU:HD11	1:B:180:LYS:HE3	0.49	1.83	3	1
1:B:170:PHE:HB3	1:B:199:ILE:HG13	0.49	1.84	4	1
1:A:4:SER:HB2	1:A:7:GLU:HG2	0.49	1.83	11	1
1:B:105:LEU:HA	1:B:108:GLN:HB3	0.49	1.84	4	1
1:B:47:GLU:HB2	1:B:50:ALA:HB3	0.49	1.83	4	1
1:A:144:ALA:HA	1:A:175:ARG:HH21	0.48	1.66	5	1
1:B:196:VAL:HG11	1:B:208:MET:HB3	0.48	1.86	6	1
1:A:3:ALA:HA	1:A:61:LYS:HD3	0.48	1.85	9	1
1:A:126:THR:HA	1:A:129:ILE:HD12	0.48	1.85	9	2
1:B:105:LEU:HD22	1:B:128:ALA:HB2	0.48	1.85	9	1
1:B:200:GLU:HB3	1:B:203:ASN:HB2	0.47	1.84	11	1
1:B:113:MET:HE1	1:B:145:ALA:HB2	0.47	1.86	9	1
1:B:105:LEU:HG	1:B:127:GLU:HB2	0.47	1.86	11	1
1:B:34:ASN:HA	1:B:37:MET:HE2	0.47	1.85	1	3
1:B:60:PHE:HB2	1:B:64:HIS:HA	0.47	1.86	7	1
1:A:61:LYS:HB2	1:B:67:ASP:HA	0.47	1.85	2	3
1:B:22:LYS:HD2	1:B:24:GLU:HB2	0.47	1.87	11	1
1:A:105:LEU:HD22	1:A:124:LYS:HD2	0.47	1.85	5	1
1:A:16:PHE:HB2	1:A:37:MET:SD	0.47	2.49	10	2
1:B:117:ASP:HB3	1:B:120:LEU:HB3	0.46	1.87	18	5
1:A:311:LEU:H	1:A:311:LEU:HD13	0.46	1.70	14	2
1:B:13:VAL:HA	1:B:37:MET:HB2	0.46	1.88	4	1
1:B:130:LYS:HA	1:B:130:LYS:HE3	0.46	1.87	15	1
1:A:113:MET:HE1	1:A:145:ALA:HB2	0.46	1.87	2	3
1:B:122:ILE:HG23	1:B:142:ARG:HG2	0.46	1.88	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:GLU:HG3	1:B:44:PHE:HB3	0.46	1.86	16	1
1:A:2:SER:HA	1:B:67:ASP:O	0.46	2.10	11	1
1:B:135:ASN:HA	1:B:165:ILE:HG21	0.45	1.86	3	1
1:B:105:LEU:HD21	1:B:128:ALA:HB2	0.45	1.88	11	1
1:B:156:VAL:HG21	1:B:180:LYS:HG3	0.45	1.88	6	1
1:A:57:LYS:HA	1:A:57:LYS:HE2	0.45	1.88	5	1
1:A:126:THR:HA	1:A:142:ARG:NH2	0.45	2.26	4	1
1:A:180:LYS:HB3	1:A:185:LYS:HB2	0.45	1.87	11	1
1:B:185:LYS:HB3	1:B:188:GLU:HB2	0.45	1.88	12	1
1:A:122:ILE:HG12	1:A:142:ARG:HG3	0.45	1.89	17	1
1:B:4:SER:HB3	1:B:7:GLU:HG2	0.45	1.89	18	1
1:B:135:ASN:ND2	1:B:137:ILE:HB	0.45	2.27	20	1
1:A:105:LEU:HD23	1:A:128:ALA:HA	0.44	1.89	20	1
1:A:4:SER:HB3	1:A:7:GLU:HG3	0.44	1.89	9	3
1:A:154:GLN:HA	1:A:157:LYS:HD3	0.44	1.89	5	1
1:A:315:MET:SD	1:B:209:LYS:NZ	0.44	2.91	7	1
1:A:314:LEU:HD23	1:A:315:MET:N	0.44	2.27	16	1
1:A:24:GLU:HB3	1:B:5:LYS:HD3	0.44	1.90	4	1
1:A:15:TYR:O	1:A:19:ILE:HG12	0.44	2.13	19	2
1:A:12:ILE:HD13	1:B:12:ILE:HG12	0.44	1.89	8	1
1:A:176:LEU:HD11	1:A:180:LYS:HE3	0.44	1.88	11	1
1:A:67:ASP:HB2	1:B:62:GLY:H	0.44	1.72	4	1
1:A:107:MET:O	1:A:111:LYS:HG2	0.44	2.12	9	1
1:A:163:ILE:HD11	1:A:173:TYR:HA	0.44	1.89	11	1
1:B:129:ILE:HD12	1:B:142:ARG:NH2	0.44	2.28	4	1
1:B:48:ARG:HD3	1:B:48:ARG:H	0.44	1.72	7	1
1:B:125:TYR:HB2	1:B:142:ARG:HD3	0.43	1.90	7	1
1:B:124:LYS:HE3	1:B:124:LYS:HA	0.43	1.90	8	1
1:A:113:MET:SD	1:A:118:TYR:CE2	0.43	3.11	13	1
1:A:126:THR:HG22	1:A:142:ARG:HH11	0.43	1.72	15	1
1:B:206:GLU:O	1:B:210:ARG:HG3	0.43	2.13	17	1
1:A:120:LEU:HD11	1:A:124:LYS:HE2	0.43	1.89	19	1
1:B:15:TYR:HA	1:B:70:ASN:ND2	0.43	2.27	3	1
1:B:107:MET:SD	1:B:107:MET:C	0.43	3.01	12	1
1:A:63:GLN:HB3	1:A:68:ILE:HD11	0.43	1.89	20	1
1:A:312:SER:HB3	1:B:197:LEU:HB3	0.43	1.90	7	1
1:A:170:PHE:HB2	1:A:196:VAL:HG13	0.43	1.88	11	1
1:A:118:TYR:HB3	1:A:145:ALA:HB1	0.43	1.88	2	1
1:A:33:LEU:O	1:A:37:MET:HG3	0.43	2.13	11	2
1:B:193:TYR:O	1:B:196:VAL:HG22	0.43	2.13	11	1
1:B:120:LEU:HG	1:B:124:LYS:HE2	0.43	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:GLN:NE2	1:A:127:GLU:HG3	0.43	2.29	3	1
1:B:152:TYR:O	1:B:156:VAL:HG23	0.43	2.13	5	1
1:A:65:LEU:HD13	1:A:66:ALA:H	0.43	1.73	1	1
1:B:113:MET:HE3	1:B:145:ALA:HB2	0.43	1.90	12	1
1:A:200:GLU:HG2	1:A:208:MET:SD	0.42	2.54	1	1
1:A:105:LEU:HD23	1:A:108:GLN:NE2	0.42	2.29	5	1
1:A:61:LYS:HA	1:A:61:LYS:HE3	0.42	1.91	6	1
1:A:135:ASN:HD21	1:A:137:ILE:HB	0.42	1.75	9	1
1:A:19:ILE:HG23	1:A:24:GLU:HB2	0.42	1.92	19	1
1:B:151:GLU:HB3	1:B:154:GLN:HB3	0.42	1.90	13	1
1:B:19:ILE:HG23	1:B:24:GLU:HB3	0.42	1.90	5	1
1:A:46:PHE:HE2	1:A:51:VAL:HG12	0.42	1.74	8	1
1:B:186:PRO:HA	1:B:189:ALA:HB3	0.42	1.91	6	1
1:A:152:TYR:HA	1:A:155:ALA:HB3	0.42	1.91	11	1
1:A:63:GLN:HB3	1:B:63:GLN:HG3	0.42	1.91	14	1
1:A:120:LEU:HA	1:A:123:ASN:HD21	0.42	1.75	20	1
1:B:8:ILE:O	1:B:12:ILE:HG13	0.42	2.15	8	2
1:A:5:LYS:HD3	1:A:5:LYS:H	0.42	1.73	10	1
1:A:311:LEU:O	1:A:314:LEU:HG	0.42	2.15	10	1
1:A:7:GLU:HG2	1:A:58:SER:HB3	0.42	1.91	18	1
1:A:13:VAL:O	1:A:37:MET:SD	0.42	2.78	3	1
1:A:20:VAL:HG12	1:A:30:ALA:HB1	0.41	1.91	8	1
1:A:34:ASN:HA	1:A:37:MET:HE3	0.41	1.93	8	1
1:A:8:ILE:O	1:A:12:ILE:HG13	0.41	2.15	20	1
1:B:180:LYS:HD2	1:B:185:LYS:HD2	0.41	1.93	1	1
1:A:152:TYR:HB2	1:A:183:GLN:NE2	0.41	2.30	12	1
1:B:171:ARG:HE	1:B:171:ARG:HA	0.41	1.75	16	1
1:A:60:PHE:HB2	1:A:64:HIS:H	0.41	1.75	17	1
1:A:171:ARG:HA	1:A:174:SER:HB3	0.41	1.92	5	1
1:B:176:LEU:HG	1:B:180:LYS:NZ	0.41	2.30	5	1
1:A:12:ILE:HD12	1:B:12:ILE:HG12	0.41	1.91	19	1
1:A:173:TYR:HB2	1:A:196:VAL:HG22	0.41	1.92	7	1
1:A:181:TYR:HA	1:A:186:PRO:HB3	0.41	1.92	7	1
1:B:16:PHE:HD1	1:B:19:ILE:HD12	0.41	1.74	11	1
1:A:140:ALA:O	1:A:175:ARG:HG2	0.41	2.16	20	1
1:B:11:LEU:HD21	1:B:68:ILE:HG21	0.41	1.92	15	1
1:B:8:ILE:O	1:B:12:ILE:HG12	0.41	2.16	20	1
1:A:142:ARG:O	1:A:146:HIS:HB2	0.41	2.16	7	1
1:A:162:ALA:HB1	1:A:169:TYR:OH	0.41	2.16	18	1
1:B:200:GLU:HG3	1:B:208:MET:SD	0.41	2.55	20	1
1:B:122:ILE:HD12	1:B:149:LEU:HD12	0.41	1.91	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ALA:HB2	1:B:67:ASP:HB2	0.41	1.91	19	1
1:A:27:GLU:HA	1:A:30:ALA:HB3	0.40	1.91	1	2
1:B:125:TYR:CD2	1:B:142:ARG:HG2	0.40	2.51	13	1
1:B:19:ILE:HG23	1:B:24:GLU:HB2	0.40	1.93	9	1
1:A:152:TYR:O	1:A:156:VAL:HG23	0.40	2.15	13	1
1:B:204:ALA:HB1	1:B:208:MET:SD	0.40	2.56	3	1
1:A:175:ARG:HD2	1:A:175:ARG:H	0.40	1.75	1	1
1:B:125:TYR:O	1:B:129:ILE:HG13	0.40	2.16	8	1
1:A:68:ILE:HA	1:B:2:SER:HB2	0.40	1.93	14	1
1:A:208:MET:SD	1:A:208:MET:N	0.40	2.94	7	1
1:A:23:LYS:HB3	1:A:23:LYS:NZ	0.40	2.31	10	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	197/347 (57%)	165±50 (84±25%)	11±5 (6±2%)	3±1 (1±1%)	12	60
1	B	180/347 (52%)	166±4 (92±2%)	11±3 (6±2%)	3±2 (2±1%)	10	55
All	All	7177/13880 (52%)	6614 (92%)	454 (6%)	109 (2%)	11	57

All 29 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	64	HIS	16
1	A	64	HIS	15
1	A	62	GLY	14
1	B	60	PHE	10
1	A	321	ARG	7
1	A	63	GLN	7
1	B	3	ALA	5
1	B	63	GLN	3
1	B	66	ALA	3
1	B	61	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	60	PHE	3
1	B	186	PRO	2
1	A	322	ASN	2
1	B	58	SER	2
1	B	2	SER	2
1	B	27	GLU	2
1	B	57	LYS	1
1	A	316	ASN	1
1	B	62	GLY	1
1	B	206	GLU	1
1	A	310	ASN	1
1	A	66	ALA	1
1	B	150	LYS	1
1	B	184	GLY	1
1	B	5	LYS	1
1	B	59	GLU	1
1	B	65	LEU	1
1	B	170	PHE	1
1	B	25	ILE	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	158/274 (58%)	130±41 (82±26%)	6±3 (3±2%)	32 82
1	B	143/274 (52%)	132±30 (92±21%)	4±1 (3±1%)	38 86
All	All	5425/10960 (49%)	5234 (96%)	191 (4%)	32 82

All 93 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	311	LEU	10
1	B	124	LYS	7
1	A	157	LYS	6
1	A	111	LYS	5
1	B	195	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	B	22	LYS	5
1	A	130	LYS	5
1	A	22	LYS	4
1	A	132	LEU	4
1	A	314	LEU	4
1	B	7	GLU	4
1	A	195	LYS	4
1	B	171	ARG	4
1	B	61	LYS	4
1	A	5	LYS	4
1	B	185	LYS	4
1	A	57	LYS	3
1	A	61	LYS	3
1	A	175	ARG	3
1	A	23	LYS	3
1	B	111	LYS	3
1	A	194	LYS	3
1	B	116	LYS	3
1	A	106	LYS	3
1	B	130	LYS	3
1	A	65	LEU	2
1	A	135	ASN	2
1	A	191	GLU	2
1	A	209	LYS	2
1	B	59	GLU	2
1	B	106	LYS	2
1	B	175	ARG	2
1	A	49	GLU	2
1	A	206	GLU	2
1	B	23	LYS	2
1	A	104	ASP	2
1	B	187	GLU	2
1	A	317	ASN	2
1	A	108	GLN	2
1	A	320	LEU	2
1	A	48	ARG	2
1	B	194	LYS	2
1	A	69	LEU	1
1	B	160	GLU	1
1	A	110	ASN	1
1	A	127	GLU	1
1	A	181	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	B	132	LEU	1
1	B	197	LEU	1
1	A	141	ASN	1
1	A	154	GLN	1
1	B	206	GLU	1
1	A	6	GLU	1
1	B	49	GLU	1
1	B	57	LYS	1
1	B	110	ASN	1
1	A	185	LYS	1
1	B	68	ILE	1
1	B	117	ASP	1
1	B	210	ARG	1
1	B	142	ARG	1
1	B	212	TYR	1
1	A	116	LYS	1
1	A	200	GLU	1
1	B	63	GLN	1
1	B	180	LYS	1
1	A	27	GLU	1
1	A	158	ASP	1
1	A	187	GLU	1
1	B	6	GLU	1
1	B	126	THR	1
1	B	191	GLU	1
1	A	47	GLU	1
1	A	70	ASN	1
1	A	315	MET	1
1	B	48	ARG	1
1	B	105	LEU	1
1	A	14	ASN	1
1	A	105	LEU	1
1	A	211	ASP	1
1	B	24	GLU	1
1	A	216	LYS	1
1	B	65	LEU	1
1	B	211	ASP	1
1	A	21	GLU	1
1	B	11	LEU	1
1	A	11	LEU	1
1	B	5	LYS	1
1	B	209	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	59	GLU	1
1	B	141	ASN	1
1	B	119	GLU	1
1	A	68	ILE	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 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	750
Number of shifts mapped to atoms	750
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
$^{13}C_{\alpha}$	91	0.37 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	102	0.86 ± 0.07	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	230	0.44 ± 0.11	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 416 atoms were assigned a chemical shift out of a possible 4958. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	319/1891 (17%)	162/767 (21%)	12/754 (2%)	145/370 (39%)
Sidechain	97/2717 (4%)	0/1759 (0%)	97/860 (11%)	0/98 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/350 (0%)	0/164 (0%)	0/178 (0%)	0/8 (0%)
Overall	416/4958 (8%)	162/2690 (6%)	109/1792 (6%)	145/476 (30%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 750 atoms were assigned a chemical shift out of a possible 8850. 0 out of 74 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	569/3474 (16%)	248/1418 (17%)	91/1388 (7%)	230/668 (34%)
Sidechain	181/4968 (4%)	0/3206 (0%)	181/1572 (12%)	0/190 (0%)
Aromatic	0/408 (0%)	0/192 (0%)	0/208 (0%)	0/8 (0%)
Overall	750/8850 (8%)	248/4816 (5%)	272/3168 (9%)	230/866 (27%)

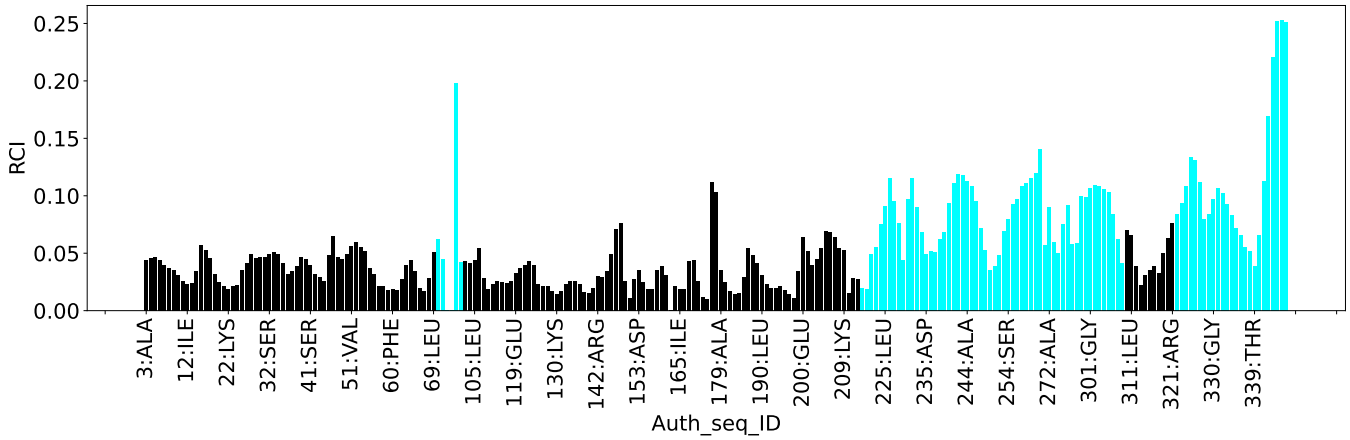
7.1.4 Statistically unusual chemical shifts (i)

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	4235
Intra-residue (|i-j|=0)	20
Sequential (|i-j|=1)	1694
Medium range (|i-j|>1 and |i-j|<5)	1556
Long range (|i-j|≥5)	756
Inter-chain	209
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	906
Number of unmapped restraints	0
Number of restraints per residue	7.4
Number of long range restraints per residue[1]	1.1

[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)	56.7	0.2
0.2-0.5 (Medium)	116.5	0.5
>0.5 (Large)	160.5	6.83

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)	31.4	10.0
10.0-20.0 (Medium)	10.8	19.98
>20.0 (Large)	24.1	147.69

9 Distance violation analysis (i)

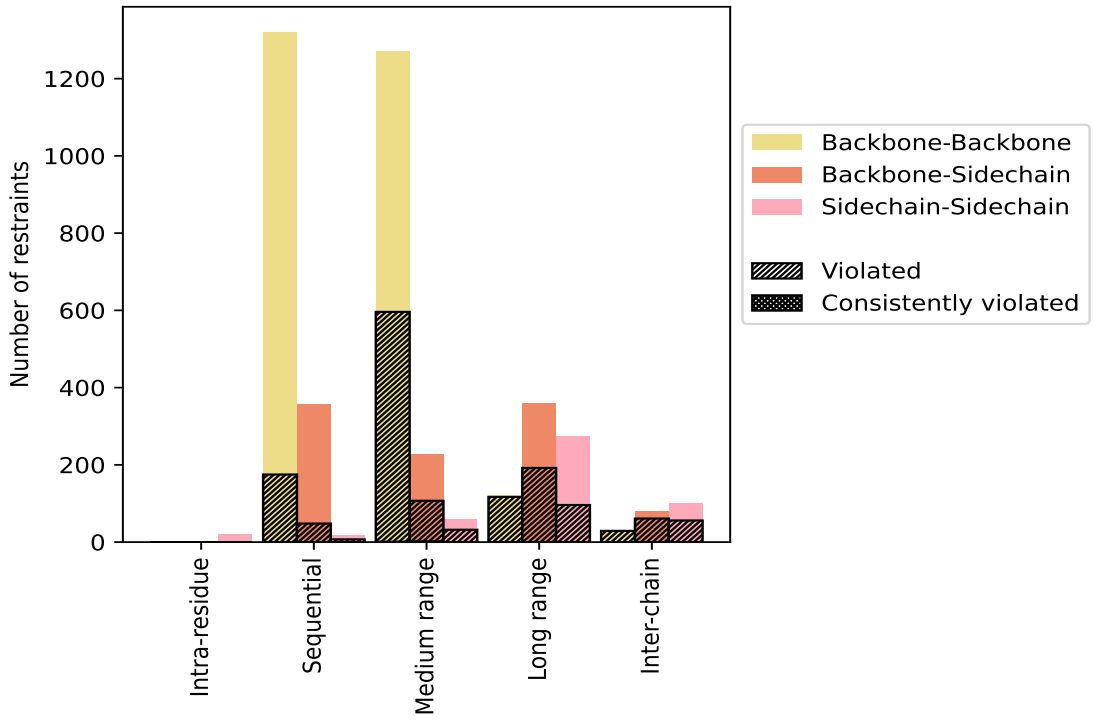
9.1 Summary of distance violations (i)

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)	20	0.5	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	20	0.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1694	40.0	230	13.6	5.4	0	0.0	0.0
Backbone-Backbone	1320	31.2	175	13.3	4.1	0	0.0	0.0
Backbone-Sidechain	356	8.4	48	13.5	1.1	0	0.0	0.0
Sidechain-Sidechain	18	0.4	7	38.9	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1556	36.7	735	47.2	17.4	3	0.2	0.1
Backbone-Backbone	1270	30.0	596	46.9	14.1	1	0.1	0.0
Backbone-Sidechain	226	5.3	107	47.3	2.5	2	0.9	0.0
Sidechain-Sidechain	60	1.4	32	53.3	0.8	0	0.0	0.0
Long range (|i-j|≥5)	756	17.9	405	53.6	9.6	0	0.0	0.0
Backbone-Backbone	122	2.9	117	95.9	2.8	0	0.0	0.0
Backbone-Sidechain	360	8.5	192	53.3	4.5	0	0.0	0.0
Sidechain-Sidechain	274	6.5	96	35.0	2.3	0	0.0	0.0
Inter-chain	209	4.9	146	69.9	3.4	0	0.0	0.0
Backbone-Backbone	29	0.7	29	100.0	0.7	0	0.0	0.0
Backbone-Sidechain	79	1.9	61	77.2	1.4	0	0.0	0.0
Sidechain-Sidechain	101	2.4	56	55.4	1.3	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4235	100.0	1516	35.8	35.8	3	0.1	0.1
Backbone-Backbone	2741	64.7	917	33.5	21.7	1	0.0	0.0
Backbone-Sidechain	1021	24.1	408	40.0	9.6	2	0.2	0.0
Sidechain-Sidechain	473	11.2	191	40.4	4.5	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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	55	150	85	34	324	0.64	3.8	0.55	0.46
2	0	49	141	107	54	351	0.77	5.93	0.8	0.48
3	0	53	186	157	63	459	0.77	4.09	0.74	0.51
4	0	40	126	85	31	282	0.62	2.94	0.52	0.46
5	0	58	155	68	39	320	0.66	4.44	0.63	0.43
6	0	48	144	73	44	309	0.59	3.24	0.52	0.44
7	0	44	172	112	44	372	0.66	4.9	0.58	0.5
8	0	56	168	124	38	386	0.71	4.15	0.64	0.49
9	0	49	140	130	52	371	0.72	5.19	0.72	0.5
10	0	57	155	103	49	364	0.72	6.65	0.7	0.5

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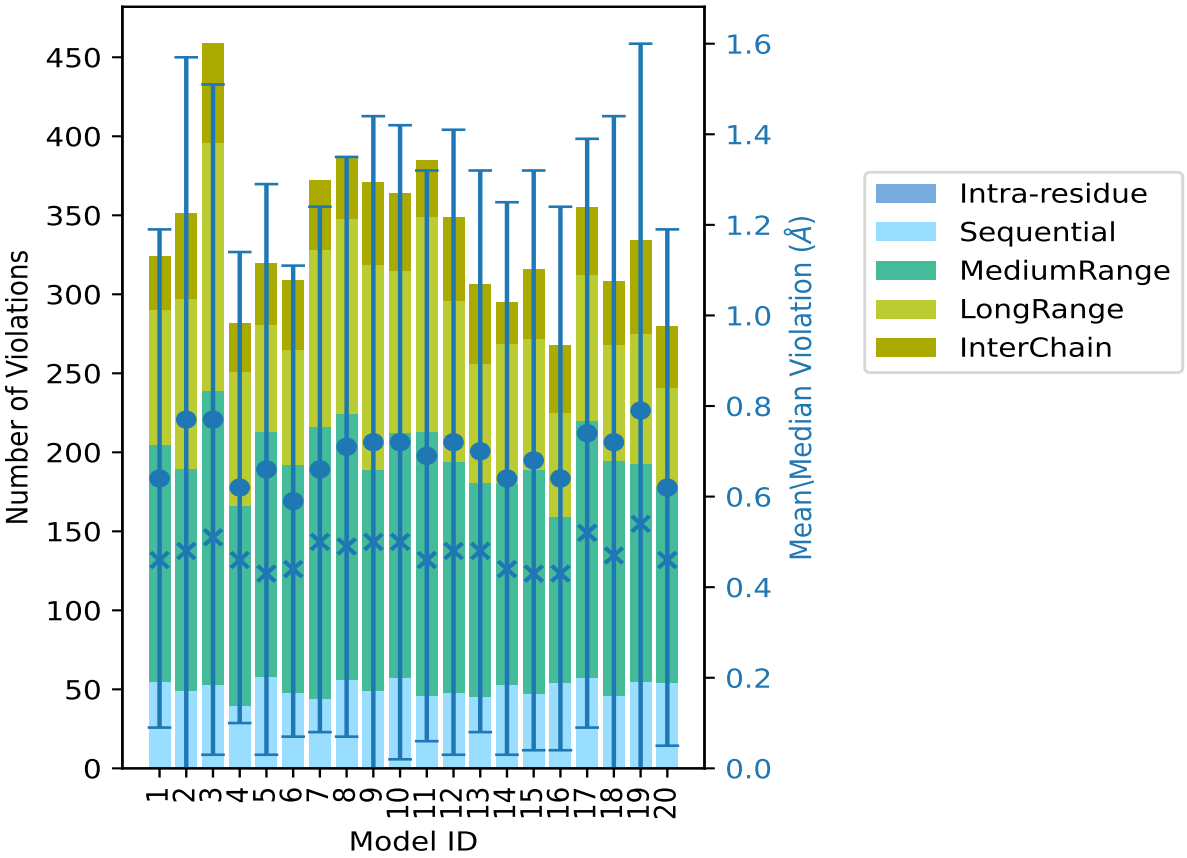
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	46	167	136	36	385	0.69	3.58	0.63	0.46
12	0	48	146	102	53	349	0.72	4.67	0.69	0.48
13	0	45	136	75	50	306	0.7	3.07	0.62	0.48
14	0	53	127	89	26	295	0.64	4.18	0.61	0.44
15	0	47	142	83	44	316	0.68	3.46	0.64	0.43
16	0	54	105	66	43	268	0.64	3.09	0.6	0.43
17	0	57	163	92	43	355	0.74	4.66	0.65	0.52
18	0	46	149	73	40	308	0.72	4.7	0.72	0.47
19	0	55	138	82	59	334	0.79	6.83	0.81	0.54
20	0	54	124	63	39	280	0.62	3.74	0.57	0.46

[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

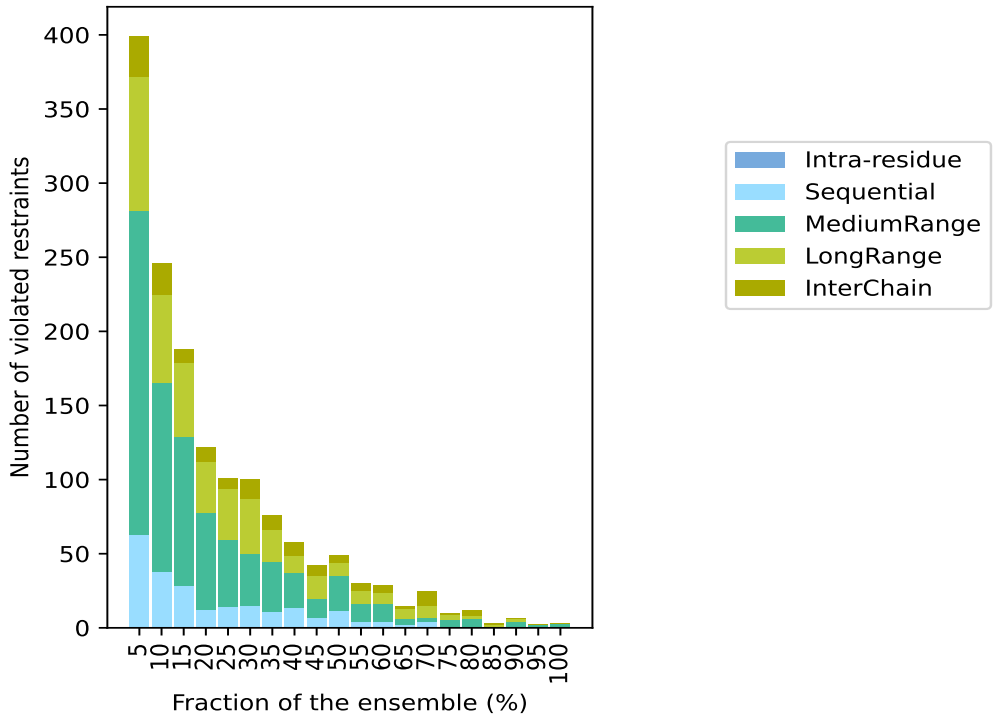
9.3 Distance violation statistics for the ensemble (i)

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, 2719(IR:20, SQ:1464, MR:821, LR:351, IC:63) 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	63	218	91	27	399	1	5.0
0	38	127	60	21	246	2	10.0
0	28	101	50	9	188	3	15.0
0	12	66	34	10	122	4	20.0
0	14	45	35	7	101	5	25.0
0	15	35	37	13	100	6	30.0
0	11	34	21	10	76	7	35.0
0	14	23	12	9	58	8	40.0
0	7	13	15	7	42	9	45.0
0	12	23	9	5	49	10	50.0
0	4	12	9	5	30	11	55.0
0	4	12	8	5	29	12	60.0
0	2	4	7	2	15	13	65.0
0	4	3	8	10	25	14	70.0
0	0	5	4	1	10	15	75.0
0	0	6	2	4	12	16	80.0
0	0	1	1	1	3	17	85.0
0	1	3	2	0	6	18	90.0
0	1	1	0	0	2	19	95.0
0	0	3	0	0	3	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

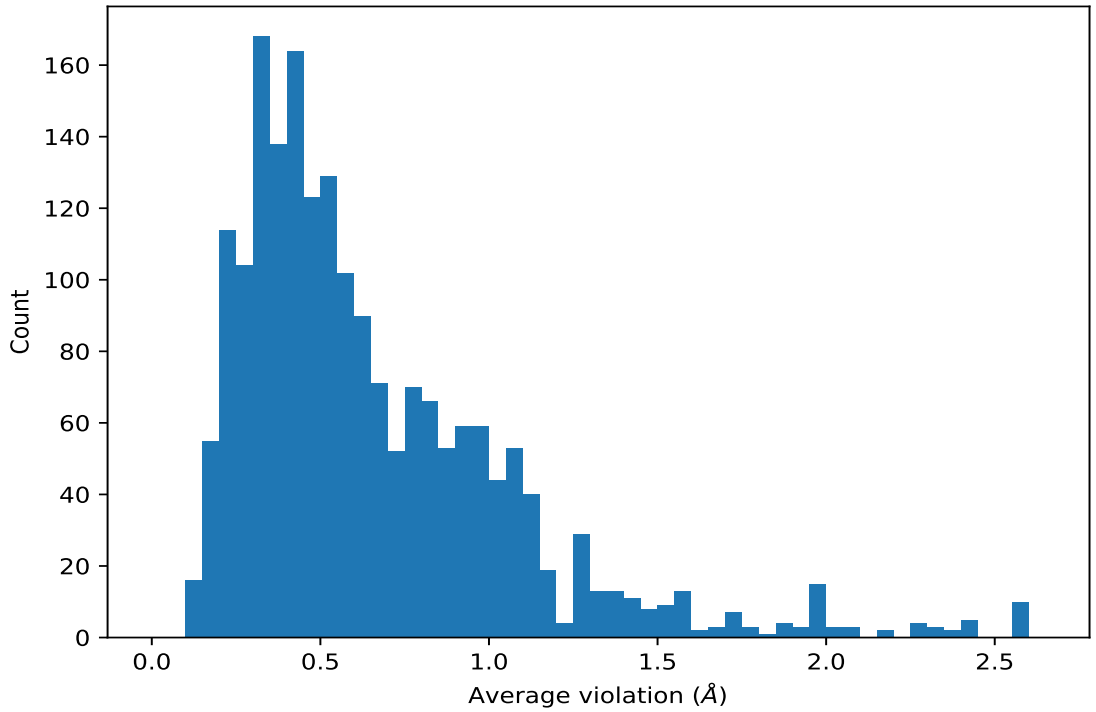
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

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)
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	20	2.44	1.52	2.42
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	20	2.44	1.52	2.42
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	20	2.36	0.91	2.32
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	20	2.36	0.91	2.32
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	20	1.53	0.93	1.55
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	19	2.25	0.94	1.89
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	19	2.25	0.94	1.89
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	19	0.86	0.29	0.88
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	19	0.86	0.29	0.88
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	18	1.62	0.66	1.51
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	18	1.62	0.66	1.51
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	18	1.58	0.8	1.52
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	18	1.47	0.82	1.48
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	18	1.32	0.92	1.08
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	18	1.32	0.92	1.08
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	18	1.32	0.92	1.08

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	18	1.32	0.74	1.36
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	18	0.88	0.37	0.9
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	18	0.88	0.37	0.9
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	17	2.31	1.54	1.86
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	17	2.31	1.54	1.86
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	17	1.7	0.86	1.58
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	17	0.83	0.44	0.74
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	16	2.59	1.78	2.96
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	16	1.86	0.98	1.8
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	16	1.86	0.98	1.8
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	16	1.51	1.18	1.38
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	16	1.15	0.96	0.68
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	16	1.15	0.96	0.68
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	16	1.11	0.55	1.12
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	16	1.11	0.55	1.12
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	16	1.11	0.55	1.12
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	16	1.11	0.55	1.12
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	16	1.03	0.58	1.28
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	16	0.96	0.76	0.82
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	16	0.96	0.76	0.82
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	16	0.96	0.76	0.82
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	16	0.9	0.63	0.89
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	16	0.83	0.49	0.98
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	16	0.83	0.49	0.98
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	16	0.83	0.49	0.98
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	16	0.83	0.49	0.98
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	16	0.58	0.26	0.6
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	16	0.58	0.3	0.52
(1,2205)	1:169:A:TYR:HD1	1:171:A:ARG:H	16	0.45	0.23	0.52
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	16	0.45	0.23	0.52
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	15	2.31	1.24	2.82
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	15	2.29	1.13	2.56
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	15	2.29	1.13	2.56
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	15	1.53	1.04	1.35
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	15	1.53	1.04	1.35
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	15	1.34	0.79	1.13
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	15	1.05	0.35	0.92
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	15	0.9	0.44	0.8
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	15	0.56	0.47	0.43
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	15	0.52	0.25	0.52
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	15	0.52	0.25	0.52
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	15	0.52	0.25	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	15	0.49	0.22	0.47
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	15	0.36	0.15	0.36
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	15	0.36	0.15	0.36
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	14	2.18	1.04	2.41
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	14	2.18	1.04	2.41
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	14	1.89	1.53	1.57
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	14	1.89	1.53	1.57
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	14	1.47	1.31	0.97
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	14	1.47	1.31	0.97
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	14	1.47	1.31	0.97
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	14	1.47	1.31	0.97
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	14	1.41	0.39	1.51
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	14	1.41	0.39	1.51
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	14	1.25	1.0	0.99
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	14	1.25	1.0	0.99
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	14	1.14	0.49	1.34
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	14	1.14	0.49	1.34
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	14	1.14	0.49	1.34
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	14	1.14	0.49	1.34
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	14	1.08	0.53	1.1
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	14	1.05	0.83	0.77
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	14	1.05	0.84	0.75
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	14	1.05	0.84	0.75
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	14	1.05	0.84	0.75
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	14	1.05	0.84	0.75
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	14	1.05	0.6	1.17
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	14	1.05	0.6	1.17
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	14	1.05	0.6	1.17
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	14	1.05	0.6	1.17
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	14	1.05	0.63	0.84
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	14	1.0	0.74	0.81
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	14	1.0	0.74	0.81
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	14	0.92	0.78	0.78
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	14	0.92	0.78	0.78
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	14	0.88	0.6	0.67
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	14	0.88	0.6	0.67
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	14	0.88	0.6	0.67
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	14	0.88	0.6	0.67
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	14	0.88	0.22	0.83
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	14	0.88	0.52	0.87
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	14	0.78	0.57	0.68
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	14	0.71	0.53	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	14	0.66	0.63	0.39
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	14	0.54	0.22	0.53
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	14	0.54	0.22	0.53
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	14	0.52	0.26	0.54
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	14	0.52	0.26	0.54
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	14	0.52	0.24	0.53
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	14	0.5	0.33	0.5
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	14	0.48	0.16	0.5
(1,3511)	1:169:B:TYR:HD2	1:171:B:ARG:H	14	0.48	0.16	0.5
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	14	0.38	0.11	0.36
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	14	0.38	0.11	0.36
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	13	1.43	0.95	1.2
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	13	1.43	0.98	1.2
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	13	1.25	0.77	1.0
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	13	1.17	0.42	1.16
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	13	1.17	0.42	1.16
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	13	1.08	1.04	0.74
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	13	1.08	1.04	0.74
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	13	1.08	1.04	0.74
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	13	1.04	0.46	1.06
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	13	0.96	0.75	0.7
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	13	0.96	0.75	0.7
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	13	0.96	0.75	0.7
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	13	0.96	0.75	0.7
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	13	0.93	0.29	0.86
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	13	0.93	0.29	0.86
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	13	0.85	0.55	0.88
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	13	0.85	0.55	0.88
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	13	0.78	0.43	0.75
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	13	0.78	0.43	0.75
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	13	0.71	0.46	0.57
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	13	0.52	0.26	0.48
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	13	0.52	0.26	0.48
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	13	0.44	0.15	0.5
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	13	0.44	0.28	0.31
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	13	0.18	0.06	0.17
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	13	0.18	0.06	0.17
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	12	1.94	1.06	2.07
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	12	1.94	1.06	2.07
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	12	1.94	1.06	2.07
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	12	1.82	1.22	2.62
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	12	1.74	0.85	1.92

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	12	1.74	0.85	1.92
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	12	1.74	0.85	1.92
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	12	1.56	1.25	1.13
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	12	1.56	1.25	1.13
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	12	1.56	1.25	1.13
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	12	1.5	0.46	1.59
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	12	1.46	0.41	1.61
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	12	1.46	0.41	1.61
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	12	1.41	0.72	1.62
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	12	1.41	0.72	1.62
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	12	1.23	0.67	1.12
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	12	1.13	0.45	1.18
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	12	1.13	0.45	1.18
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	12	1.13	0.45	1.18
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	12	1.13	0.45	1.18
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	12	1.12	0.52	1.31
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	12	1.1	0.84	0.9
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	12	1.1	1.15	0.56
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	12	1.06	0.45	1.19
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	12	0.94	0.56	0.92
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	12	0.91	0.28	0.94
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	12	0.9	0.71	0.72
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	12	0.89	0.63	0.71
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	12	0.86	0.7	0.62
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	12	0.8	0.35	0.8
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	12	0.77	0.45	0.72
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	12	0.77	0.45	0.72
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	12	0.75	0.27	0.74
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	12	0.75	0.27	0.74
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	12	0.72	0.47	0.64
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	12	0.71	0.37	0.72
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	12	0.63	0.21	0.56
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	12	0.57	0.24	0.63
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	12	0.44	0.39	0.3
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	12	0.44	0.39	0.3
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	12	0.43	0.18	0.45
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	12	0.43	0.18	0.45
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	12	0.42	0.2	0.42
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	12	0.31	0.18	0.29
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	11	1.69	0.45	1.84
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	11	1.44	0.82	1.41
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	11	1.44	0.82	1.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	11	1.29	0.67	1.01
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	11	1.17	0.65	1.23
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	11	1.08	0.46	1.08
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	11	1.08	0.46	1.08
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG3	11	0.94	0.64	0.84
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG2	11	0.94	0.64	0.84
(1,3367)	1:152:B:TYR:HD1	1:183:B:GLN:HG2	11	0.94	0.64	0.84
(1,3367)	1:152:B:TYR:HD1	1:183:B:GLN:HG3	11	0.94	0.64	0.84
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	11	0.82	0.43	0.9
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	11	0.81	0.73	0.43
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	11	0.81	0.73	0.43
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	11	0.81	0.73	0.43
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	11	0.81	0.73	0.43
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	11	0.8	0.52	0.62
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	11	0.8	0.33	0.97
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	11	0.78	0.67	0.4
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	11	0.75	0.37	0.67
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	11	0.75	0.37	0.67
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	11	0.72	0.38	0.59
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	11	0.72	0.38	0.59
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	11	0.7	0.36	0.55
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	11	0.7	0.45	0.58
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	11	0.67	0.43	0.56
(1,2464)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	11	0.67	0.5	0.37
(1,2464)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	11	0.67	0.5	0.37
(1,2464)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	11	0.67	0.5	0.37
(1,2464)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	11	0.67	0.5	0.37
(1,2464)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	11	0.67	0.5	0.37
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	11	0.66	0.54	0.54
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	11	0.65	0.41	0.57
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	11	0.64	0.31	0.57
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	11	0.64	0.31	0.57
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	11	0.64	0.31	0.57
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	11	0.64	0.31	0.57
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	11	0.59	0.38	0.61
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	11	0.59	0.38	0.61
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	11	0.58	0.3	0.51
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	11	0.52	0.27	0.5
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	11	0.51	0.25	0.42
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	11	0.51	0.25	0.38
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	11	0.37	0.35	0.21
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	11	0.34	0.12	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	11	0.34	0.2	0.31
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	11	0.28	0.11	0.25
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	11	0.27	0.13	0.25
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	10	1.53	0.69	1.96
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	10	1.42	1.25	1.06
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	10	1.42	1.25	1.06
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	10	1.42	1.25	1.06
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	10	1.17	0.62	1.23
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	10	1.16	1.27	0.75
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	10	1.01	0.58	0.86
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	10	0.91	0.52	0.78
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	10	0.89	0.53	0.8
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	10	0.89	0.56	0.75
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	10	0.88	0.54	0.8
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	10	0.79	0.57	0.65
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	10	0.79	0.57	0.65
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	10	0.78	0.37	0.74
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	10	0.77	0.63	0.54
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	10	0.76	0.38	0.84
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	10	0.76	0.38	0.84
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	10	0.76	0.42	0.58
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	10	0.76	0.42	0.58
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	10	0.76	0.42	0.58
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	10	0.76	0.42	0.58
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	10	0.74	0.48	0.62
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	10	0.72	0.47	0.61
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	10	0.71	0.24	0.82
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	10	0.71	0.24	0.82
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	10	0.71	0.33	0.74
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	10	0.71	0.19	0.68
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	10	0.71	0.19	0.68
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	10	0.65	0.18	0.73
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	10	0.61	0.2	0.6
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	10	0.61	0.21	0.6
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	10	0.6	0.25	0.69
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	10	0.6	0.5	0.49
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	10	0.6	0.58	0.39
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	10	0.6	0.3	0.48
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	10	0.57	0.41	0.4
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	10	0.56	0.34	0.46
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	10	0.56	0.23	0.48
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	10	0.56	0.29	0.49

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	10	0.56	0.29	0.49
(1,3082)	1:125:B:TYR:HD1	1:141:B:ASN:HB3	10	0.56	0.33	0.56
(1,3082)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	10	0.56	0.33	0.56
(1,3082)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	10	0.56	0.33	0.56
(1,3082)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	10	0.56	0.33	0.56
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	10	0.54	0.13	0.58
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	10	0.54	0.13	0.58
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	10	0.53	0.29	0.46
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	10	0.52	0.25	0.48
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	10	0.52	0.25	0.48
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	10	0.51	0.21	0.54
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	10	0.49	0.26	0.49
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	10	0.46	0.21	0.44
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	10	0.45	0.27	0.44
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	10	0.44	0.41	0.18
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	10	0.42	0.18	0.38
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	10	0.42	0.18	0.38
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	10	0.41	0.19	0.36
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	10	0.41	0.28	0.36
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	10	0.4	0.2	0.37
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	10	0.38	0.45	0.24
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	10	0.33	0.28	0.22
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	10	0.33	0.15	0.32
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	10	0.27	0.1	0.28
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	10	0.24	0.07	0.26
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	10	0.24	0.07	0.26
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	10	0.24	0.1	0.24
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	9	1.98	1.43	1.83
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	9	1.27	0.54	1.42
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	9	1.27	0.54	1.42
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	9	1.25	0.69	1.22
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	9	1.25	0.69	1.22
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	9	1.25	0.69	1.22
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	9	1.08	0.96	0.64
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	9	1.08	0.96	0.64
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	9	1.08	0.96	0.64
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	9	1.06	0.71	0.88
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	9	1.05	0.63	0.84
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	9	1.05	0.63	0.84
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	9	1.05	0.63	0.84
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	9	1.05	0.63	0.84
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	9	1.05	0.63	0.84

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	9	1.05	0.63	0.84
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	9	1.04	0.84	0.8
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	9	1.04	0.84	0.8
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	9	1.04	0.84	0.8
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	9	1.04	0.84	0.8
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	9	1.02	0.75	1.0
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	9	0.99	0.42	1.0
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	9	0.97	0.51	0.94
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	9	0.97	0.51	0.94
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	9	0.94	0.51	0.98
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	9	0.9	0.4	0.83
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	9	0.87	0.62	1.07
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	9	0.79	0.56	0.86
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	9	0.77	0.53	0.7
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	9	0.77	0.3	0.85
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	9	0.77	0.3	0.85
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	9	0.77	0.3	0.85
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	9	0.77	0.3	0.85
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	9	0.75	0.42	0.73
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	9	0.75	0.42	0.73
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	9	0.73	0.42	0.69
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	9	0.7	0.29	0.78
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	9	0.66	0.26	0.63
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	9	0.65	0.39	0.61
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	9	0.65	0.39	0.61
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	9	0.62	0.83	0.21
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	9	0.6	0.36	0.47
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE1	9	0.57	0.3	0.5
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE2	9	0.57	0.3	0.5
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	9	0.55	0.28	0.49
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	9	0.55	0.28	0.49
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	9	0.55	0.28	0.44
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	9	0.51	0.25	0.54
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	9	0.51	0.25	0.54
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	9	0.5	0.27	0.47
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	9	0.46	0.24	0.51
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE2	9	0.46	0.24	0.51
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	9	0.46	0.2	0.44
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	9	0.45	0.22	0.39
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	9	0.45	0.22	0.39
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	9	0.43	0.2	0.46
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	9	0.41	0.3	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	9	0.41	0.27	0.38
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	9	0.41	0.27	0.38
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	9	0.4	0.23	0.3
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	9	0.38	0.15	0.33
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	9	0.36	0.27	0.3
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	9	0.36	0.27	0.3
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	9	0.33	0.12	0.25
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	9	0.33	0.17	0.3
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	9	0.29	0.12	0.33
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	9	0.29	0.12	0.33
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	9	0.27	0.1	0.23
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	9	0.2	0.06	0.17
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	8	1.59	0.89	1.62
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	8	1.59	0.89	1.62
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	8	1.59	0.89	1.62
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	8	1.52	1.59	0.91
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	8	1.37	0.76	1.15
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	8	1.37	0.76	1.15
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	8	1.37	0.76	1.15
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	8	1.33	1.17	0.96
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	8	1.33	1.17	0.96
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	8	1.33	1.17	0.96
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	8	1.18	0.14	1.23
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	8	1.11	1.2	0.77
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	8	1.11	1.2	0.77
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	8	1.08	0.91	0.8
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	8	1.03	0.75	1.02
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	8	1.01	0.38	1.12
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	8	1.01	0.38	1.12
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	8	1.01	0.38	1.12
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	8	0.98	0.58	0.96
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	8	0.98	0.58	0.96
(1,3770)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	8	0.97	0.73	0.84
(1,3770)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	8	0.97	0.73	0.84
(1,3770)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	8	0.97	0.73	0.84
(1,3770)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	8	0.97	0.73	0.84
(1,3770)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	8	0.97	0.73	0.84
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	8	0.92	0.87	0.48
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	8	0.88	0.64	0.78
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	8	0.88	0.64	0.78
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	8	0.88	0.64	0.78
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	8	0.85	0.7	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	8	0.85	0.7	0.52
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	8	0.84	0.46	0.72
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	8	0.81	0.43	0.74
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	8	0.81	0.43	0.74
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	8	0.8	0.71	0.54
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	8	0.8	0.71	0.54
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	8	0.79	0.53	0.78
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	8	0.76	0.55	0.73
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	8	0.76	0.55	0.73
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	8	0.76	0.55	0.73
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	8	0.76	0.29	0.85
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	8	0.76	0.29	0.85
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	8	0.73	0.47	0.78
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	8	0.72	0.44	0.6
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	8	0.72	0.44	0.6
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	8	0.7	0.39	0.5
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	8	0.68	0.4	0.59
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	8	0.68	0.4	0.59
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	8	0.68	0.29	0.73
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	8	0.66	0.49	0.46
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	8	0.65	0.43	0.52
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	8	0.64	0.19	0.61
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	8	0.6	0.28	0.57
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	8	0.57	0.32	0.51
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	8	0.57	0.24	0.54
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	8	0.53	0.1	0.52
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	8	0.53	0.1	0.52
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	8	0.52	0.29	0.5
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	8	0.51	0.22	0.48
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	8	0.49	0.22	0.49
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	8	0.49	0.36	0.42
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	8	0.48	0.17	0.55
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	8	0.48	0.17	0.55
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	8	0.48	0.28	0.48
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	8	0.47	0.25	0.43
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	8	0.46	0.26	0.38
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	8	0.44	0.13	0.44
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	8	0.44	0.37	0.32
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	8	0.44	0.37	0.32
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	8	0.43	0.17	0.46
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	8	0.42	0.28	0.38
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	8	0.41	0.26	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	8	0.4	0.24	0.38
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	8	0.4	0.21	0.36
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	8	0.39	0.25	0.36
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	8	0.38	0.13	0.38
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	8	0.38	0.13	0.38
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	8	0.37	0.22	0.34
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	8	0.37	0.22	0.34
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	8	0.37	0.22	0.34
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	8	0.37	0.22	0.34
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	8	0.33	0.22	0.27
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	8	0.33	0.22	0.27
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	8	0.33	0.22	0.27
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	8	0.31	0.16	0.32
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	8	0.31	0.11	0.29
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	8	0.29	0.12	0.28
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	8	0.24	0.09	0.23
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	8	0.24	0.09	0.23
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	8	0.2	0.06	0.2
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	8	0.18	0.06	0.18
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	8	0.16	0.02	0.16
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB2	7	1.95	0.73	1.57
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB3	7	1.95	0.73	1.57
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB2	7	1.95	0.73	1.57
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB3	7	1.95	0.73	1.57
(1,1248)	1:9:A:ALA:H	1:16:B:PHE:HZ	7	1.23	1.02	1.1
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG11	7	1.13	0.83	0.96
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG12	7	1.13	0.83	0.96
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG13	7	1.13	0.83	0.96
(1,2714)	1:223:A:LEU:HA	1:226:A:GLU:H	7	1.05	0.4	0.94
(1,2746)	1:95:B:ASP:H	1:96:B:ALA:H	7	1.02	0.28	1.06
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB2	7	0.99	0.75	1.0
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB3	7	0.99	0.75	1.0
(1,3599)	1:176:B:LEU:HA	1:180:B:LYS:H	7	0.98	0.48	0.93
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG21	7	0.96	0.7	0.64
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG22	7	0.96	0.7	0.64
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG23	7	0.96	0.7	0.64
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB2	7	0.95	0.68	0.71
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB3	7	0.95	0.68	0.71
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG2	7	0.9	0.45	0.74
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG3	7	0.9	0.45	0.74
(1,1431)	1:93:A:GLU:HA	1:95:A:ASP:H	7	0.89	0.11	0.91
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB2	7	0.89	0.47	0.85

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB3	7	0.89	0.47	0.85
(1,3651)	1:180:B:LYS:HB2	1:189:B:ALA:H	7	0.88	0.5	0.94
(1,3651)	1:180:B:LYS:HB3	1:189:B:ALA:H	7	0.88	0.5	0.94
(1,3689)	1:185:B:LYS:HA	1:188:B:GLU:H	7	0.85	0.7	0.53
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG21	7	0.84	0.53	0.97
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG22	7	0.84	0.53	0.97
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG23	7	0.84	0.53	0.97
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG21	7	0.84	0.53	0.97
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG22	7	0.84	0.53	0.97
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG23	7	0.84	0.53	0.97
(1,1537)	1:105:A:LEU:HA	1:124:A:LYS:HA	7	0.82	0.72	0.67
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG21	7	0.82	0.54	0.72
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG22	7	0.82	0.54	0.72
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG23	7	0.82	0.54	0.72
(1,1338)	1:36:A:ALA:HA	1:36:B:ALA:HA	7	0.81	0.42	1.04
(1,2973)	1:116:B:LYS:HA	1:118:B:TYR:HA	7	0.79	0.39	0.8
(1,3810)	1:197:B:LEU:HA	1:204:B:ALA:HA	7	0.79	0.36	0.84
(1,3147)	1:134:B:THR:H	1:135:B:ASN:H	7	0.78	0.17	0.81
(1,623)	1:4:B:SER:H	1:7:B:GLU:H	7	0.76	0.54	0.62
(1,1114)	1:55:B:LEU:HD11	1:71:B:SER:HA	7	0.75	0.38	0.83
(1,1114)	1:55:B:LEU:HD12	1:71:B:SER:HA	7	0.75	0.38	0.83
(1,1114)	1:55:B:LEU:HD13	1:71:B:SER:HA	7	0.75	0.38	0.83
(1,3828)	1:199:B:ILE:HA	1:201:B:GLY:H	7	0.71	0.49	0.65
(1,452)	1:47:A:GLU:HB2	1:49:A:GLU:H	7	0.68	0.24	0.65
(1,452)	1:47:A:GLU:HB3	1:49:A:GLU:H	7	0.68	0.24	0.65
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB2	7	0.67	0.22	0.63
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB3	7	0.67	0.22	0.63
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB2	7	0.67	0.22	0.63
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB3	7	0.67	0.22	0.63
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB2	7	0.67	0.22	0.63
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB3	7	0.67	0.22	0.63
(1,1519)	1:103:A:GLU:HA	1:107:A:MET:H	7	0.66	0.52	0.58
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG21	7	0.64	0.33	0.61
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG22	7	0.64	0.33	0.61
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG23	7	0.64	0.33	0.61
(1,2583)	1:207:A:ALA:HA	1:211:A:ASP:H	7	0.63	0.33	0.58
(1,2261)	1:173:A:TYR:HA	1:192:A:ALA:HA	7	0.62	0.71	0.36
(1,2805)	1:102:B:ALA:HA	1:105:B:LEU:H	7	0.62	0.33	0.6
(1,3074)	1:125:B:TYR:HB2	1:142:B:ARG:H	7	0.61	0.31	0.7
(1,3074)	1:125:B:TYR:HB3	1:142:B:ARG:H	7	0.61	0.31	0.7
(1,2828)	1:104:B:ASP:H	1:107:B:MET:H	7	0.6	0.35	0.44
(1,1281)	1:16:A:PHE:HE1	1:9:B:ALA:HB1	7	0.6	0.37	0.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1281)	1:16:A:PHE:HE2	1:9:B:ALA:HB1	7	0.6	0.37	0.51
(1,3834)	1:200:B:GLU:HB2	1:204:B:ALA:H	7	0.6	0.37	0.48
(1,3834)	1:200:B:GLU:HB3	1:204:B:ALA:H	7	0.6	0.37	0.48
(1,4105)	1:338:A:GLU:H	1:339:A:THR:H	7	0.6	0.17	0.61
(1,4048)	1:238:A:VAL:H	1:239:A:ASP:H	7	0.59	0.31	0.59
(1,1424)	1:69:A:LEU:HD11	1:2:B:SER:H	7	0.59	0.64	0.26
(1,1424)	1:69:A:LEU:HD12	1:2:B:SER:H	7	0.59	0.64	0.26
(1,1424)	1:69:A:LEU:HD13	1:2:B:SER:H	7	0.59	0.64	0.26
(1,635)	1:5:B:LYS:HA	1:9:B:ALA:H	7	0.58	0.61	0.16
(1,3291)	1:146:B:HIS:H	1:155:B:ALA:HA	7	0.57	0.34	0.48
(1,3646)	1:180:B:LYS:HA	1:185:B:LYS:H	7	0.56	0.35	0.31
(1,1374)	1:43:A:ALA:HA	1:32:B:SER:H	7	0.55	0.4	0.33
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE1	7	0.53	0.34	0.41
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE2	7	0.53	0.34	0.41
(1,3913)	1:210:B:ARG:HA	1:214:B:SER:H	7	0.52	0.2	0.49
(1,2345)	1:180:A:LYS:HB2	1:189:A:ALA:H	7	0.52	0.39	0.26
(1,2345)	1:180:A:LYS:HB3	1:189:A:ALA:H	7	0.52	0.39	0.26
(1,4088)	1:321:A:ARG:H	1:322:A:ASN:H	7	0.51	0.21	0.39
(1,1439)	1:94:A:ASP:HA	1:96:A:ALA:H	7	0.51	0.07	0.51
(1,1349)	1:39:A:CYS:HA	1:32:B:SER:HA	7	0.51	0.31	0.41
(1,3382)	1:154:B:GLN:HA	1:158:B:ASP:H	7	0.5	0.21	0.53
(1,2669)	1:218:A:LYS:H	1:221:A:GLN:H	7	0.49	0.2	0.41
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG21	7	0.49	0.32	0.38
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG22	7	0.49	0.32	0.38
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG23	7	0.49	0.32	0.38
(1,1474)	1:99:A:LYS:HA	1:102:A:ALA:H	7	0.49	0.33	0.27
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG21	7	0.47	0.27	0.4
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG22	7	0.47	0.27	0.4
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG23	7	0.47	0.27	0.4
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG21	7	0.47	0.27	0.4
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG22	7	0.47	0.27	0.4
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG23	7	0.47	0.27	0.4
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG21	7	0.47	0.27	0.4
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG22	7	0.47	0.27	0.4
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG23	7	0.47	0.27	0.4
(1,892)	1:28:B:ASP:HA	1:31:B:ASP:H	7	0.47	0.23	0.46
(1,4169)	1:300:B:GLU:H	1:301:B:GLY:H	7	0.46	0.14	0.44
(1,3551)	1:171:B:ARG:HA	1:175:B:ARG:H	7	0.45	0.28	0.41
(1,3791)	1:195:B:LYS:HA	1:199:B:ILE:H	7	0.45	0.29	0.54
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB2	7	0.43	0.1	0.45
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB3	7	0.43	0.1	0.45
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB2	7	0.43	0.1	0.45

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB3	7	0.43	0.1	0.45
(1,3898)	1:208:B:MET:HA	1:211:B:ASP:H	7	0.42	0.32	0.28
(1,4072)	1:301:A:GLY:H	1:302:A:PHE:H	7	0.42	0.2	0.43
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD11	7	0.42	0.39	0.23
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD12	7	0.42	0.39	0.23
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD13	7	0.42	0.39	0.23
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD11	7	0.42	0.39	0.23
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD12	7	0.42	0.39	0.23
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD13	7	0.42	0.39	0.23
(1,3119)	1:129:B:ILE:HA	1:133:B:PRO:HA	7	0.39	0.18	0.44
(1,4138)	1:228:B:THR:H	1:229:B:VAL:H	7	0.38	0.13	0.33
(1,2463)	1:193:A:TYR:HE1	1:211:A:ASP:HA	7	0.36	0.24	0.31
(1,2463)	1:193:A:TYR:HE2	1:211:A:ASP:HA	7	0.36	0.24	0.31
(1,2463)	1:193:A:TYR:HD2	1:211:A:ASP:HA	7	0.36	0.24	0.31
(1,1645)	1:113:A:MET:HE1	1:145:A:ALA:H	7	0.36	0.2	0.28
(1,1645)	1:113:A:MET:HE2	1:145:A:ALA:H	7	0.36	0.2	0.28
(1,1645)	1:113:A:MET:HE3	1:145:A:ALA:H	7	0.36	0.2	0.28
(1,3686)	1:185:B:LYS:H	1:186:B:PRO:HA	7	0.36	0.17	0.3
(1,3452)	1:161:B:SER:HA	1:165:B:ILE:H	7	0.35	0.26	0.19
(1,1919)	1:140:A:ALA:H	1:162:A:ALA:HA	7	0.34	0.25	0.21
(1,1133)	1:58:B:SER:HB2	1:60:B:PHE:H	7	0.31	0.26	0.19
(1,1133)	1:58:B:SER:HB3	1:60:B:PHE:H	7	0.31	0.26	0.19
(1,3335)	1:150:B:LYS:HA	1:152:B:TYR:HA	7	0.31	0.24	0.22
(1,4000)	1:221:B:GLN:H	1:224:B:ASN:H	7	0.31	0.19	0.24
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD1	7	0.3	0.12	0.26
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD2	7	0.3	0.12	0.26
(1,988)	1:39:B:CYS:HA	1:42:B:GLU:H	7	0.26	0.13	0.23
(1,1127)	1:58:B:SER:H	1:59:B:GLU:HA	7	0.26	0.11	0.21
(1,474)	1:51:A:VAL:HA	1:55:A:LEU:H	7	0.25	0.08	0.24
(1,4092)	1:325:A:GLY:H	1:326:A:ASN:H	7	0.22	0.08	0.2
(1,2952)	1:113:B:MET:HE1	1:145:B:ALA:HA	6	1.75	0.94	1.38
(1,2952)	1:113:B:MET:HE2	1:145:B:ALA:HA	6	1.75	0.94	1.38
(1,2952)	1:113:B:MET:HE3	1:145:B:ALA:HA	6	1.75	0.94	1.38
(1,2850)	1:105:B:LEU:HD21	1:124:B:LYS:HA	6	1.39	1.04	1.12
(1,2850)	1:105:B:LEU:HD22	1:124:B:LYS:HA	6	1.39	1.04	1.12
(1,2850)	1:105:B:LEU:HD23	1:124:B:LYS:HA	6	1.39	1.04	1.12
(1,3655)	1:181:B:TYR:H	1:186:B:PRO:HA	6	1.28	0.57	1.29
(1,3656)	1:181:B:TYR:H	1:189:B:ALA:H	6	1.22	0.72	1.08
(1,3542)	1:170:B:PHE:HD2	1:171:B:ARG:HD2	6	1.14	0.77	1.16
(1,3542)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	6	1.14	0.77	1.16
(1,1140)	1:59:B:GLU:HB2	1:64:B:HIS:HA	6	1.13	0.57	0.99
(1,1140)	1:59:B:GLU:HB3	1:64:B:HIS:HA	6	1.13	0.57	0.99

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1288)	1:16:A:PHE:HE1	1:12:B:ILE:HD11	6	1.12	0.74	0.76
(1,1288)	1:16:A:PHE:HE2	1:12:B:ILE:HD11	6	1.12	0.74	0.76
(1,1307)	1:25:A:ILE:HG12	1:44:B:PHE:HA	6	1.1	0.41	1.31
(1,1307)	1:25:A:ILE:HG13	1:44:B:PHE:HA	6	1.1	0.41	1.31
(1,2423)	1:190:A:LEU:HD21	1:216:A:LYS:HA	6	1.07	0.82	0.77
(1,2423)	1:190:A:LEU:HD22	1:216:A:LYS:HA	6	1.07	0.82	0.77
(1,2423)	1:190:A:LEU:HD23	1:216:A:LYS:HA	6	1.07	0.82	0.77
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD2	6	1.02	0.42	0.96
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD3	6	1.02	0.42	0.96
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	6	1.02	0.42	0.96
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD3	6	1.02	0.42	0.96
(1,3970)	1:217:B:LYS:HA	1:220:B:GLU:H	6	0.98	0.98	0.52
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD11	6	0.97	0.7	0.81
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD12	6	0.97	0.7	0.81
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD13	6	0.97	0.7	0.81
(1,506)	1:55:A:LEU:HD11	1:72:A:ALA:HA	6	0.96	0.48	1.05
(1,506)	1:55:A:LEU:HD12	1:72:A:ALA:HA	6	0.96	0.48	1.05
(1,506)	1:55:A:LEU:HD13	1:72:A:ALA:HA	6	0.96	0.48	1.05
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB2	6	0.95	0.59	0.84
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB3	6	0.95	0.59	0.84
(1,2796)	1:101:B:LYS:HA	1:104:B:ASP:H	6	0.95	0.78	0.7
(1,1313)	1:29:A:GLY:H	1:43:B:ALA:HA	6	0.95	0.52	0.9
(1,3657)	1:181:B:TYR:H	1:189:B:ALA:HA	6	0.9	0.71	0.55
(1,3252)	1:143:B:ALA:H	1:155:B:ALA:HA	6	0.85	0.48	0.9
(1,3725)	1:190:B:LEU:HD11	1:212:B:TYR:HA	6	0.84	0.44	0.89
(1,3725)	1:190:B:LEU:HD12	1:212:B:TYR:HA	6	0.84	0.44	0.89
(1,3725)	1:190:B:LEU:HD13	1:212:B:TYR:HA	6	0.84	0.44	0.89
(1,3145)	1:132:B:LEU:HD11	1:134:B:THR:H	6	0.83	0.29	0.93
(1,3145)	1:132:B:LEU:HD12	1:134:B:THR:H	6	0.83	0.29	0.93
(1,3145)	1:132:B:LEU:HD13	1:134:B:THR:H	6	0.83	0.29	0.93
(1,4027)	1:225:B:LEU:H	1:226:B:GLU:H	6	0.82	0.37	0.89
(1,2750)	1:95:B:ASP:HA	1:97:B:GLU:H	6	0.82	0.72	0.62
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	6	0.77	0.5	0.62
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	6	0.77	0.5	0.62
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB2	6	0.77	0.5	0.62
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	6	0.77	0.5	0.62
(1,1274)	1:15:A:TYR:HH	1:5:B:LYS:HA	6	0.75	0.44	0.91
(1,3256)	1:143:B:ALA:HA	1:155:B:ALA:H	6	0.74	0.52	0.6
(1,1110)	1:55:B:LEU:H	1:57:B:LYS:H	6	0.73	0.59	0.48
(1,3641)	1:180:B:LYS:H	1:189:B:ALA:HA	6	0.7	0.5	0.5
(1,3729)	1:190:B:LEU:HD21	1:216:B:LYS:HA	6	0.7	0.49	0.58
(1,3729)	1:190:B:LEU:HD22	1:216:B:LYS:HA	6	0.7	0.49	0.58

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3729)	1:190:B:LEU:HD23	1:216:B:LYS:HA	6	0.7	0.49	0.58
(1,3921)	1:211:B:ASP:HA	1:215:B:ALA:H	6	0.69	0.48	0.62
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG12	6	0.69	0.4	0.7
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG13	6	0.69	0.4	0.7
(1,3361)	1:152:B:TYR:HB2	1:183:B:GLN:H	6	0.69	0.47	0.64
(1,3361)	1:152:B:TYR:HB3	1:183:B:GLN:H	6	0.69	0.47	0.64
(1,2236)	1:170:A:PHE:HE2	1:171:A:ARG:HD2	6	0.67	0.58	0.35
(1,2236)	1:170:A:PHE:HE2	1:171:A:ARG:HD3	6	0.67	0.58	0.35
(1,2236)	1:170:A:PHE:HE1	1:171:A:ARG:HD3	6	0.67	0.58	0.35
(1,529)	1:59:A:GLU:HA	1:64:A:HIS:HA	6	0.64	0.29	0.63
(1,2469)	1:194:A:LYS:H	1:212:A:TYR:HA	6	0.63	0.38	0.66
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	6	0.63	0.59	0.31
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	6	0.63	0.59	0.31
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB2	6	0.63	0.59	0.31
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	6	0.63	0.59	0.31
(1,561)	1:63:A:GLN:HA	1:67:A:ASP:H	6	0.61	0.53	0.42
(1,2004)	1:147:A:SER:HA	1:150:A:LYS:HA	6	0.61	0.36	0.66
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG21	6	0.6	0.47	0.46
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG22	6	0.6	0.47	0.46
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG23	6	0.6	0.47	0.46
(1,1289)	1:16:A:PHE:HE1	1:12:B:ILE:HD12	6	0.59	0.4	0.42
(1,1289)	1:16:A:PHE:HE2	1:12:B:ILE:HD12	6	0.59	0.4	0.42
(1,1336)	1:36:A:ALA:H	1:36:B:ALA:HA	6	0.58	0.25	0.59
(1,3357)	1:152:B:TYR:HA	1:156:B:VAL:H	6	0.58	0.29	0.55
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB2	6	0.56	0.3	0.57
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	6	0.56	0.3	0.57
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB2	6	0.56	0.3	0.57
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB3	6	0.56	0.3	0.57
(1,3195)	1:138:B:TYR:HA	1:141:B:ASN:H	6	0.56	0.25	0.57
(1,3946)	1:214:B:SER:HA	1:217:B:LYS:H	6	0.56	0.41	0.4
(1,1321)	1:32:A:SER:HB2	1:43:B:ALA:H	6	0.55	0.31	0.48
(1,1321)	1:32:A:SER:HB3	1:43:B:ALA:H	6	0.55	0.31	0.48
(1,3091)	1:126:B:THR:HA	1:130:B:LYS:H	6	0.55	0.43	0.51
(1,1314)	1:29:A:GLY:HA2	1:43:B:ALA:H	6	0.54	0.4	0.46
(1,1314)	1:29:A:GLY:HA3	1:43:B:ALA:H	6	0.54	0.4	0.46
(1,2719)	1:224:A:ASN:HA	1:226:A:GLU:H	6	0.53	0.3	0.53
(1,1145)	1:60:B:PHE:HA	1:62:B:GLY:H	6	0.53	0.23	0.49
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD11	6	0.52	0.19	0.54
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD12	6	0.52	0.19	0.54
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD13	6	0.52	0.19	0.54
(1,2419)	1:190:A:LEU:HD11	1:212:A:TYR:HA	6	0.52	0.22	0.5
(1,2419)	1:190:A:LEU:HD12	1:212:A:TYR:HA	6	0.52	0.22	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2419)	1:190:A:LEU:HD13	1:212:A:TYR:HA	6	0.52	0.22	0.5
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB1	6	0.52	0.38	0.3
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB2	6	0.52	0.38	0.3
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB3	6	0.52	0.38	0.3
(1,1011)	1:41:B:SER:HA	1:46:B:PHE:H	6	0.51	0.27	0.44
(1,2941)	1:113:B:MET:HA	1:118:B:TYR:HA	6	0.5	0.33	0.38
(1,1946)	1:143:A:ALA:H	1:155:A:ALA:HA	6	0.5	0.3	0.5
(1,3313)	1:147:B:SER:HA	1:152:B:TYR:HA	6	0.5	0.23	0.41
(1,1951)	1:143:A:ALA:HA	1:155:A:ALA:HA	6	0.49	0.28	0.46
(1,4156)	1:248:B:GLY:H	1:249:B:LEU:H	6	0.48	0.1	0.48
(1,1278)	1:16:A:PHE:HA	1:44:B:PHE:HZ	6	0.48	0.24	0.44
(1,624)	1:4:B:SER:H	1:8:B:ILE:H	6	0.47	0.31	0.38
(1,2529)	1:200:A:GLU:HB2	1:204:A:ALA:HA	6	0.46	0.46	0.32
(1,2529)	1:200:A:GLU:HB3	1:204:A:ALA:HA	6	0.46	0.46	0.32
(1,2350)	1:181:A:TYR:H	1:189:A:ALA:H	6	0.46	0.15	0.47
(1,4077)	1:305:A:GLY:H	1:307:A:GLY:H	6	0.45	0.29	0.42
(1,2279)	1:174:A:SER:HA	1:193:A:TYR:HA	6	0.44	0.23	0.4
(1,3763)	1:193:B:TYR:HD1	1:211:B:ASP:HA	6	0.44	0.26	0.43
(1,3763)	1:193:B:TYR:HD2	1:211:B:ASP:HA	6	0.44	0.26	0.43
(1,3724)	1:190:B:LEU:HA	1:216:B:LYS:H	6	0.43	0.12	0.36
(1,3722)	1:190:B:LEU:HA	1:212:B:TYR:HA	6	0.42	0.19	0.46
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD11	6	0.42	0.17	0.43
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD12	6	0.42	0.17	0.43
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD13	6	0.42	0.17	0.43
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB2	6	0.42	0.11	0.44
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB3	6	0.42	0.11	0.44
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB2	6	0.42	0.11	0.44
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB3	6	0.42	0.11	0.44
(1,2824)	1:103:B:GLU:HA	1:106:B:LYS:H	6	0.41	0.26	0.26
(1,3075)	1:125:B:TYR:HB2	1:142:B:ARG:HA	6	0.41	0.27	0.31
(1,3075)	1:125:B:TYR:HB3	1:142:B:ARG:HA	6	0.41	0.27	0.31
(1,2555)	1:205:A:THR:H	1:209:A:LYS:H	6	0.41	0.24	0.38
(1,1518)	1:103:A:GLU:HA	1:106:A:LYS:H	6	0.4	0.23	0.3
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE1	6	0.38	0.33	0.29
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE2	6	0.38	0.33	0.29
(1,2645)	1:215:A:ALA:H	1:218:A:LYS:H	6	0.38	0.21	0.3
(1,4064)	1:256:A:LEU:H	1:257:A:GLY:H	6	0.37	0.14	0.42
(1,1054)	1:47:B:GLU:H	1:50:B:ALA:H	6	0.34	0.18	0.28
(1,1785)	1:126:A:THR:HA	1:130:A:LYS:H	6	0.34	0.18	0.34
(1,4207)	1:344:B:ASN:H	1:345:B:LYS:H	6	0.34	0.17	0.24
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG11	6	0.33	0.15	0.34
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG12	6	0.33	0.15	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG13	6	0.33	0.15	0.34
(1,1853)	1:135:A:ASN:HB2	1:138:A:TYR:H	6	0.33	0.2	0.25
(1,1853)	1:135:A:ASN:HB3	1:138:A:TYR:H	6	0.33	0.2	0.25
(1,2245)	1:171:A:ARG:HA	1:175:A:ARG:H	6	0.33	0.27	0.26
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE1	6	0.33	0.13	0.3
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE2	6	0.33	0.13	0.3
(1,4162)	1:256:B:LEU:H	1:257:B:GLY:H	6	0.32	0.08	0.32
(1,953)	1:35:B:VAL:HA	1:38:B:ASP:HA	6	0.32	0.33	0.18
(1,2694)	1:221:A:GLN:H	1:224:A:ASN:H	6	0.32	0.11	0.26
(1,3159)	1:135:B:ASN:HB2	1:138:B:TYR:H	6	0.32	0.2	0.25
(1,3159)	1:135:B:ASN:HB3	1:138:B:TYR:H	6	0.32	0.2	0.25
(1,4205)	1:342:B:ASN:H	1:343:B:GLU:H	6	0.32	0.17	0.24
(1,336)	1:34:A:ASN:HA	1:38:A:ASP:H	6	0.31	0.18	0.26
(1,2383)	1:185:A:LYS:HA	1:188:A:GLU:H	6	0.3	0.12	0.28
(1,458)	1:48:A:ARG:HA	1:50:A:ALA:H	6	0.29	0.25	0.18
(1,3148)	1:134:B:THR:H	1:135:B:ASN:HA	6	0.29	0.12	0.24
(1,616)	1:3:B:ALA:HA	1:4:B:SER:H	6	0.29	0.04	0.26
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE1	6	0.29	0.13	0.28
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE2	6	0.29	0.13	0.28
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE1	6	0.29	0.13	0.28
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE2	6	0.29	0.13	0.28
(1,3572)	1:173:B:TYR:HB2	1:196:B:VAL:H	6	0.26	0.16	0.21
(1,3572)	1:173:B:TYR:HB3	1:196:B:VAL:H	6	0.26	0.16	0.21
(1,4071)	1:300:A:GLU:H	1:301:A:GLY:H	6	0.26	0.09	0.25
(1,2979)	1:117:B:ASP:H	1:118:B:TYR:H	6	0.24	0.08	0.26
(1,2502)	1:197:A:LEU:HA	1:200:A:GLU:H	6	0.23	0.07	0.24
(1,2980)	1:117:B:ASP:H	1:118:B:TYR:HA	6	0.22	0.09	0.21
(1,587)	1:68:A:ILE:H	1:69:A:LEU:HA	6	0.16	0.04	0.16
(1,3648)	1:180:B:LYS:HB2	1:185:B:LYS:H	5	1.09	0.31	1.17
(1,3648)	1:180:B:LYS:HB3	1:185:B:LYS:H	5	1.09	0.31	1.17
(1,3279)	1:144:B:ALA:HB1	1:175:B:ARG:HE	5	1.05	0.7	0.58
(1,3279)	1:144:B:ALA:HB2	1:175:B:ARG:HE	5	1.05	0.7	0.58
(1,3279)	1:144:B:ALA:HB3	1:175:B:ARG:HE	5	1.05	0.7	0.58
(1,1544)	1:105:A:LEU:HD21	1:124:A:LYS:HA	5	1.01	0.83	0.74
(1,1544)	1:105:A:LEU:HD22	1:124:A:LYS:HA	5	1.01	0.83	0.74
(1,1544)	1:105:A:LEU:HD23	1:124:A:LYS:HA	5	1.01	0.83	0.74
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB1	5	1.01	0.88	0.7
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB2	5	1.01	0.88	0.7
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB3	5	1.01	0.88	0.7
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB1	5	1.01	0.88	0.7
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB2	5	1.01	0.88	0.7
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB3	5	1.01	0.88	0.7

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB1	5	1.01	0.88	0.7
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB2	5	1.01	0.88	0.7
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB3	5	1.01	0.88	0.7
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD21	5	1.0	0.47	0.89
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD22	5	1.0	0.47	0.89
(1,3832)	1:200:B:GLU:HA	1:203:B:ASN:H	5	0.84	0.35	0.92
(1,2933)	1:113:B:MET:H	1:121:B:ALA:HA	5	0.81	0.43	0.78
(1,2995)	1:118:B:TYR:HA	1:145:B:ALA:HA	5	0.81	0.27	0.9
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG21	5	0.81	0.26	0.75
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG22	5	0.81	0.26	0.75
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG23	5	0.81	0.26	0.75
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG11	5	0.8	0.34	0.75
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG12	5	0.8	0.34	0.75
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG13	5	0.8	0.34	0.75
(1,2942)	1:113:B:MET:HA	1:121:B:ALA:H	5	0.79	0.4	0.75
(1,3081)	1:125:B:TYR:HE1	1:142:B:ARG:HA	5	0.75	0.56	0.51
(1,3081)	1:125:B:TYR:HE2	1:142:B:ARG:HA	5	0.75	0.56	0.51
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE1	5	0.73	0.68	0.47
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE2	5	0.73	0.68	0.47
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE3	5	0.73	0.68	0.47
(1,1499)	1:102:A:ALA:HA	1:105:A:LEU:H	5	0.71	0.28	0.64
(1,2697)	1:221:A:GLN:HA	1:224:A:ASN:H	5	0.7	0.27	0.76
(1,2526)	1:200:A:GLU:HA	1:203:A:ASN:H	5	0.67	0.27	0.74
(1,3800)	1:196:B:VAL:HG11	1:208:B:MET:HA	5	0.66	0.42	0.49
(1,3800)	1:196:B:VAL:HG12	1:208:B:MET:HA	5	0.66	0.42	0.49
(1,3800)	1:196:B:VAL:HG13	1:208:B:MET:HA	5	0.66	0.42	0.49
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD2	5	0.66	0.31	0.81
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD3	5	0.66	0.31	0.81
(1,625)	1:4:B:SER:HA	1:5:B:LYS:H	5	0.66	0.31	0.71
(1,3068)	1:125:B:TYR:HA	1:138:B:TYR:HA	5	0.62	0.48	0.32
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE1	5	0.62	0.51	0.34
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE2	5	0.62	0.51	0.34
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE3	5	0.62	0.51	0.34
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE1	5	0.62	0.51	0.34
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE2	5	0.62	0.51	0.34
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE3	5	0.62	0.51	0.34
(1,3749)	1:193:B:TYR:H	1:212:B:TYR:HA	5	0.62	0.28	0.47
(1,4032)	1:226:B:GLU:HA	1:227:B:LYS:H	5	0.62	0.34	0.85
(1,835)	1:20:B:VAL:HA	1:24:B:GLU:H	5	0.62	0.25	0.51
(1,1337)	1:36:A:ALA:HA	1:36:B:ALA:H	5	0.61	0.19	0.56
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD11	5	0.6	0.46	0.45
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD12	5	0.6	0.46	0.45

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD13	5	0.6	0.46	0.45
(1,2615)	1:211:A:ASP:HA	1:215:A:ALA:H	5	0.57	0.17	0.54
(1,1353)	1:39:A:CYS:HB2	1:36:B:ALA:H	5	0.57	0.46	0.49
(1,1353)	1:39:A:CYS:HB3	1:36:B:ALA:H	5	0.57	0.46	0.49
(1,284)	1:28:A:ASP:HA	1:32:A:SER:H	5	0.56	0.36	0.58
(1,2664)	1:217:A:LYS:HA	1:220:A:GLU:H	5	0.56	0.25	0.63
(1,2343)	1:180:A:LYS:HB2	1:188:A:GLU:H	5	0.55	0.33	0.5
(1,2343)	1:180:A:LYS:HB3	1:188:A:GLU:H	5	0.55	0.33	0.5
(1,2349)	1:181:A:TYR:H	1:186:A:PRO:HA	5	0.55	0.34	0.76
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB2	5	0.55	0.24	0.6
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB3	5	0.55	0.24	0.6
(1,3310)	1:147:B:SER:HA	1:150:B:LYS:HA	5	0.54	0.22	0.67
(1,1900)	1:139:A:TYR:HA	1:158:A:ASP:HA	5	0.54	0.3	0.58
(1,2580)	1:207:A:ALA:HA	1:210:A:ARG:H	5	0.54	0.44	0.48
(1,2138)	1:160:A:GLU:HA	1:164:A:SER:H	5	0.53	0.55	0.29
(1,634)	1:5:B:LYS:HA	1:8:B:ILE:H	5	0.51	0.31	0.27
(1,3858)	1:205:B:THR:H	1:208:B:MET:H	5	0.51	0.23	0.45
(1,4208)	1:345:B:LYS:H	1:346:B:GLN:H	5	0.51	0.24	0.5
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB2	5	0.5	0.18	0.43
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB3	5	0.5	0.18	0.43
(1,3769)	1:193:B:TYR:HD2	1:211:B:ASP:HA	5	0.49	0.37	0.4
(1,3769)	1:193:B:TYR:HE2	1:211:B:ASP:HA	5	0.49	0.37	0.4
(1,1767)	1:125:A:TYR:HB2	1:139:A:TYR:H	5	0.49	0.24	0.49
(1,1767)	1:125:A:TYR:HB3	1:139:A:TYR:H	5	0.49	0.24	0.49
(1,3738)	1:191:B:GLU:HA	1:195:B:LYS:H	5	0.48	0.22	0.47
(1,2076)	1:154:A:GLN:HA	1:158:A:ASP:H	5	0.48	0.29	0.53
(1,2833)	1:104:B:ASP:HA	1:107:B:MET:H	5	0.47	0.27	0.48
(1,3808)	1:197:B:LEU:HA	1:200:B:GLU:H	5	0.46	0.22	0.42
(1,3396)	1:156:B:VAL:HA	1:176:B:LEU:HA	5	0.46	0.31	0.49
(1,2342)	1:180:A:LYS:HB2	1:185:A:LYS:H	5	0.45	0.24	0.38
(1,2342)	1:180:A:LYS:HB3	1:185:A:LYS:H	5	0.45	0.24	0.38
(1,1350)	1:39:A:CYS:HB2	1:32:B:SER:HA	5	0.45	0.18	0.41
(1,1350)	1:39:A:CYS:HB3	1:32:B:SER:HA	5	0.45	0.18	0.41
(1,2216)	1:170:A:PHE:HA	1:196:A:VAL:HA	5	0.45	0.19	0.43
(1,1973)	1:144:A:ALA:HB1	1:175:A:ARG:HE	5	0.45	0.32	0.38
(1,1973)	1:144:A:ALA:HB2	1:175:A:ARG:HE	5	0.45	0.32	0.38
(1,1973)	1:144:A:ALA:HB3	1:175:A:ARG:HE	5	0.45	0.32	0.38
(1,4050)	1:240:A:ALA:H	1:241:A:SER:H	5	0.44	0.13	0.46
(1,1325)	1:33:A:LEU:HA	1:40:B:ILE:HA	5	0.43	0.26	0.37
(1,3569)	1:173:B:TYR:HB2	1:195:B:LYS:H	5	0.43	0.17	0.51
(1,3569)	1:173:B:TYR:HB3	1:195:B:LYS:H	5	0.43	0.17	0.51
(1,2416)	1:190:A:LEU:HA	1:212:A:TYR:HA	5	0.42	0.29	0.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB2	5	0.42	0.22	0.53
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB3	5	0.42	0.22	0.53
(1,885)	1:27:B:GLU:HA	1:30:B:ALA:HA	5	0.42	0.29	0.29
(1,1266)	1:15:A:TYR:HE1	1:5:B:LYS:H	5	0.42	0.29	0.29
(1,1266)	1:15:A:TYR:HE2	1:5:B:LYS:H	5	0.42	0.29	0.29
(1,2984)	1:117:B:ASP:HA	1:120:B:LEU:H	5	0.41	0.14	0.38
(1,3225)	1:140:B:ALA:H	1:162:B:ALA:HA	5	0.41	0.18	0.42
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB2	5	0.41	0.33	0.28
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB3	5	0.41	0.33	0.28
(1,1282)	1:16:A:PHE:HE1	1:9:B:ALA:HB2	5	0.4	0.28	0.38
(1,1282)	1:16:A:PHE:HE2	1:9:B:ALA:HB2	5	0.4	0.28	0.38
(1,76)	1:10:A:ALA:HA	1:48:A:ARG:HA	5	0.4	0.18	0.33
(1,4051)	1:241:A:SER:H	1:242:A:GLN:H	5	0.4	0.17	0.34
(1,945)	1:34:B:ASN:HA	1:38:B:ASP:H	5	0.39	0.25	0.26
(1,4110)	1:345:A:LYS:H	1:346:A:GLN:H	5	0.38	0.11	0.39
(1,1535)	1:105:A:LEU:HA	1:108:A:GLN:H	5	0.38	0.34	0.16
(1,4095)	1:328:A:PHE:H	1:329:A:GLY:H	5	0.37	0.11	0.42
(1,834)	1:20:B:VAL:HA	1:23:B:LYS:HA	5	0.37	0.21	0.27
(1,2800)	1:102:B:ALA:H	1:105:B:LEU:H	5	0.36	0.28	0.18
(1,2432)	1:191:A:GLU:HA	1:195:A:LYS:H	5	0.35	0.17	0.39
(1,2390)	1:187:A:GLU:HA	1:190:A:LEU:H	5	0.35	0.19	0.35
(1,4188)	1:323:B:MET:H	1:324:B:ALA:H	5	0.35	0.08	0.38
(1,1646)	1:113:A:MET:HE1	1:145:A:ALA:HA	5	0.34	0.11	0.36
(1,1646)	1:113:A:MET:HE2	1:145:A:ALA:HA	5	0.34	0.11	0.36
(1,1646)	1:113:A:MET:HE3	1:145:A:ALA:HA	5	0.34	0.11	0.36
(1,2640)	1:214:A:SER:HA	1:217:A:LYS:H	5	0.34	0.21	0.27
(1,1553)	1:106:A:LYS:HA	1:109:A:GLY:H	5	0.34	0.11	0.27
(1,1852)	1:135:A:ASN:HA	1:138:A:TYR:H	5	0.33	0.2	0.28
(1,3420)	1:158:B:ASP:HA	1:162:B:ALA:H	5	0.33	0.19	0.28
(1,3135)	1:130:B:LYS:HA	1:132:B:LEU:H	5	0.32	0.12	0.34
(1,2163)	1:163:A:ILE:HA	1:167:A:PRO:HA	5	0.32	0.22	0.17
(1,578)	1:66:A:ALA:HA	1:68:A:ILE:H	5	0.31	0.11	0.28
(1,2243)	1:171:A:ARG:HA	1:174:A:SER:H	5	0.31	0.17	0.24
(1,3241)	1:141:B:ASN:HA	1:145:B:ALA:H	5	0.31	0.2	0.18
(1,4052)	1:242:A:GLN:H	1:243:A:GLY:H	5	0.31	0.09	0.29
(1,4068)	1:260:A:LEU:H	1:261:A:GLY:H	5	0.29	0.15	0.28
(1,2789)	1:101:B:LYS:H	1:103:B:GLU:H	5	0.28	0.14	0.21
(1,4107)	1:342:A:ASN:H	1:343:A:GLU:H	5	0.28	0.1	0.25
(1,3721)	1:190:B:LEU:HA	1:194:B:LYS:H	5	0.28	0.14	0.2
(1,2666)	1:217:A:LYS:HG2	1:218:A:LYS:H	5	0.27	0.1	0.27
(1,2666)	1:217:A:LYS:HG3	1:218:A:LYS:H	5	0.27	0.1	0.27
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	5	0.27	0.09	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	5	0.27	0.09	0.28
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE1	5	0.27	0.09	0.28
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE2	5	0.27	0.09	0.28
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB2	5	0.27	0.14	0.22
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB3	5	0.27	0.14	0.22
(1,2457)	1:193:A:TYR:HD1	1:211:A:ASP:HA	5	0.26	0.11	0.22
(1,2457)	1:193:A:TYR:HD2	1:211:A:ASP:HA	5	0.26	0.11	0.22
(1,2029)	1:150:A:LYS:HA	1:152:A:TYR:HA	5	0.26	0.1	0.3
(1,2517)	1:198:A:ASP:HA	1:201:A:GLY:H	5	0.25	0.1	0.24
(1,2359)	1:181:A:TYR:HA	1:189:A:ALA:H	5	0.23	0.1	0.21
(1,852)	1:22:B:LYS:H	1:24:B:GLU:H	5	0.23	0.16	0.16
(1,4147)	1:239:B:ASP:H	1:240:B:ALA:H	5	0.22	0.08	0.2
(1,3894)	1:208:B:MET:H	1:211:B:ASP:H	5	0.22	0.04	0.21
(1,1009)	1:41:B:SER:HA	1:44:B:PHE:H	5	0.2	0.07	0.18
(1,4199)	1:334:B:GLN:H	1:335:B:SER:H	5	0.16	0.01	0.16
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB1	4	2.01	1.51	2.13
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB2	4	2.01	1.51	2.13
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB3	4	2.01	1.51	2.13
(1,2948)	1:113:B:MET:HE1	1:142:B:ARG:HA	4	1.74	0.81	1.81
(1,2948)	1:113:B:MET:HE2	1:142:B:ARG:HA	4	1.74	0.81	1.81
(1,2948)	1:113:B:MET:HE3	1:142:B:ARG:HA	4	1.74	0.81	1.81
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD11	4	1.57	1.18	1.27
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD12	4	1.57	1.18	1.27
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD13	4	1.57	1.18	1.27
(1,3665)	1:181:B:TYR:HA	1:189:B:ALA:H	4	1.49	1.03	1.36
(1,1427)	1:69:A:LEU:HD11	1:2:B:SER:HG	4	1.31	0.89	1.08
(1,1427)	1:69:A:LEU:HD12	1:2:B:SER:HG	4	1.31	0.89	1.08
(1,1427)	1:69:A:LEU:HD13	1:2:B:SER:HG	4	1.31	0.89	1.08
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE1	4	1.27	0.63	1.17
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE2	4	1.27	0.63	1.17
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE1	4	1.27	0.63	1.17
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE2	4	1.27	0.63	1.17
(1,1113)	1:55:B:LEU:HA	1:58:B:SER:H	4	1.19	1.1	0.86
(1,3649)	1:180:B:LYS:HB2	1:188:B:GLU:H	4	1.18	0.53	1.02
(1,3649)	1:180:B:LYS:HB3	1:188:B:GLU:H	4	1.18	0.53	1.02
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG11	4	1.16	0.64	1.26
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG12	4	1.16	0.64	1.26
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG13	4	1.16	0.64	1.26
(1,3815)	1:197:B:LEU:HD21	1:209:B:LYS:H	4	1.08	0.47	1.17
(1,3815)	1:197:B:LEU:HD22	1:209:B:LYS:H	4	1.08	0.47	1.17
(1,3815)	1:197:B:LEU:HD23	1:209:B:LYS:H	4	1.08	0.47	1.17
(1,3816)	1:197:B:LEU:HD21	1:209:B:LYS:HA	4	1.0	0.43	1.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3816)	1:197:B:LEU:HD22	1:209:B:LYS:HA	4	1.0	0.43	1.12
(1,3816)	1:197:B:LEU:HD23	1:209:B:LYS:HA	4	1.0	0.43	1.12
(1,1385)	1:44:A:PHE:HA	1:25:B:ILE:HD13	4	1.0	0.64	0.84
(1,3966)	1:217:B:LYS:H	1:220:B:GLU:H	4	0.99	0.87	0.73
(1,3433)	1:159:B:ALA:HB1	1:176:B:LEU:HA	4	0.98	0.61	0.82
(1,3433)	1:159:B:ALA:HB2	1:176:B:LEU:HA	4	0.98	0.61	0.82
(1,3433)	1:159:B:ALA:HB3	1:176:B:LEU:HA	4	0.98	0.61	0.82
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE1	4	0.97	0.52	0.83
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE2	4	0.97	0.52	0.83
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE1	4	0.97	0.52	0.83
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE2	4	0.97	0.52	0.83
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE1	4	0.97	0.52	0.83
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE2	4	0.97	0.52	0.83
(1,2769)	1:98:B:THR:H	1:101:B:LYS:H	4	0.96	0.42	0.84
(1,3543)	1:170:B:PHE:HE2	1:208:B:MET:HE3	4	0.96	0.47	0.72
(1,3543)	1:170:B:PHE:HD2	1:208:B:MET:HE3	4	0.96	0.47	0.72
(1,3543)	1:170:B:PHE:HE2	1:208:B:MET:HE1	4	0.96	0.47	0.72
(1,3543)	1:170:B:PHE:HD1	1:208:B:MET:HE3	4	0.96	0.47	0.72
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD11	4	0.93	0.54	0.86
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD12	4	0.93	0.54	0.86
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD13	4	0.93	0.54	0.86
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD11	4	0.93	0.33	0.9
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD12	4	0.93	0.33	0.9
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD13	4	0.93	0.33	0.9
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD11	4	0.93	0.33	0.9
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD12	4	0.93	0.33	0.9
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD13	4	0.93	0.33	0.9
(1,2846)	1:105:B:LEU:HD11	1:128:B:ALA:HA	4	0.91	0.58	0.72
(1,2846)	1:105:B:LEU:HD12	1:128:B:ALA:HA	4	0.91	0.58	0.72
(1,2846)	1:105:B:LEU:HD13	1:128:B:ALA:HA	4	0.91	0.58	0.72
(1,3206)	1:139:B:TYR:HA	1:158:B:ASP:HA	4	0.89	0.47	0.68
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD11	4	0.83	0.43	0.9
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD12	4	0.83	0.43	0.9
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD13	4	0.83	0.43	0.9
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD21	4	0.81	0.46	0.82
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD22	4	0.81	0.46	0.82
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD23	4	0.81	0.46	0.82
(1,627)	1:4:B:SER:HA	1:6:B:GLU:H	4	0.8	0.27	0.86
(1,1293)	1:16:A:PHE:HE1	1:40:B:ILE:HG21	4	0.79	0.26	0.67
(1,1293)	1:16:A:PHE:HE2	1:40:B:ILE:HG21	4	0.79	0.26	0.67
(1,642)	1:6:B:GLU:HA	1:10:B:ALA:H	4	0.76	0.5	0.57
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD1	4	0.75	0.32	0.69

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD2	4	0.75	0.32	0.69
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD1	4	0.75	0.32	0.69
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD2	4	0.75	0.32	0.69
(1,1118)	1:56:B:GLY:H	1:58:B:SER:H	4	0.75	0.6	0.55
(1,3339)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	4	0.71	0.18	0.74
(1,3339)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	4	0.71	0.18	0.74
(1,2351)	1:181:A:TYR:H	1:189:A:ALA:HA	4	0.69	0.33	0.8
(1,3756)	1:193:B:TYR:HA	1:197:B:LEU:H	4	0.68	0.5	0.64
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE1	4	0.66	0.43	0.66
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE2	4	0.66	0.43	0.66
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE3	4	0.66	0.43	0.66
(1,3840)	1:201:B:GLY:H	1:204:B:ALA:H	4	0.65	0.34	0.56
(1,1221)	1:2:A:SER:HA	1:67:B:ASP:HA	4	0.64	0.67	0.32
(1,4016)	1:223:B:LEU:H	1:225:B:LEU:H	4	0.64	0.47	0.48
(1,3600)	1:176:B:LEU:HD11	1:180:B:LYS:H	4	0.63	0.4	0.53
(1,3600)	1:176:B:LEU:HD12	1:180:B:LYS:H	4	0.63	0.4	0.53
(1,3600)	1:176:B:LEU:HD13	1:180:B:LYS:H	4	0.63	0.4	0.53
(1,2779)	1:99:B:LYS:HA	1:101:B:LYS:H	4	0.62	0.2	0.66
(1,344)	1:35:A:VAL:HA	1:38:A:ASP:HA	4	0.61	0.22	0.52
(1,2055)	1:152:A:TYR:HB2	1:183:A:GLN:H	4	0.6	0.47	0.44
(1,2055)	1:152:A:TYR:HB3	1:183:A:GLN:H	4	0.6	0.47	0.44
(1,225)	1:20:A:VAL:HA	1:23:A:LYS:HA	4	0.59	0.37	0.58
(1,3629)	1:178:B:PHE:HB2	1:179:B:ALA:H	4	0.58	0.15	0.65
(1,3629)	1:178:B:PHE:HB3	1:179:B:ALA:H	4	0.58	0.15	0.65
(1,2146)	1:161:A:SER:HA	1:165:A:ILE:H	4	0.57	0.32	0.51
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB2	4	0.55	0.38	0.48
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB3	4	0.55	0.38	0.48
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB2	4	0.55	0.38	0.48
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB3	4	0.55	0.38	0.48
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB2	4	0.55	0.38	0.48
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB3	4	0.55	0.38	0.48
(1,2820)	1:103:B:GLU:H	1:106:B:LYS:H	4	0.55	0.2	0.55
(1,2892)	1:109:B:GLY:HA2	1:113:B:MET:H	4	0.54	0.29	0.48
(1,2892)	1:109:B:GLY:HA3	1:113:B:MET:H	4	0.54	0.29	0.48
(1,4159)	1:253:B:GLY:H	1:254:B:SER:H	4	0.54	0.18	0.57
(1,2451)	1:193:A:TYR:HA	1:212:A:TYR:HA	4	0.54	0.46	0.34
(1,1776)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	4	0.53	0.17	0.54
(1,1776)	1:125:A:TYR:HD2	1:141:A:ASN:HB3	4	0.53	0.17	0.54
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB2	4	0.53	0.39	0.38
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB3	4	0.53	0.39	0.38
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB2	4	0.53	0.39	0.38
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB3	4	0.53	0.39	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB2	4	0.53	0.39	0.38
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB3	4	0.53	0.39	0.38
(1,2816)	1:102:B:ALA:HB1	1:132:B:LEU:H	4	0.52	0.57	0.21
(1,2816)	1:102:B:ALA:HB2	1:132:B:LEU:H	4	0.52	0.57	0.21
(1,2816)	1:102:B:ALA:HB3	1:132:B:LEU:H	4	0.52	0.57	0.21
(1,2939)	1:113:B:MET:HA	1:116:B:LYS:HA	4	0.52	0.28	0.52
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB2	4	0.52	0.39	0.38
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB3	4	0.52	0.39	0.38
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB2	4	0.52	0.39	0.38
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB3	4	0.52	0.39	0.38
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB2	4	0.52	0.39	0.38
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB3	4	0.52	0.39	0.38
(1,3677)	1:182:B:ALA:HA	1:184:B:GLY:H	4	0.5	0.55	0.22
(1,1444)	1:95:A:ASP:HA	1:97:A:GLU:H	4	0.5	0.39	0.34
(1,1536)	1:105:A:LEU:HA	1:109:A:GLY:H	4	0.5	0.33	0.53
(1,1463)	1:98:A:THR:H	1:101:A:LYS:H	4	0.48	0.16	0.49
(1,1522)	1:104:A:ASP:H	1:107:A:MET:H	4	0.48	0.27	0.44
(1,3951)	1:215:B:ALA:H	1:218:B:LYS:H	4	0.48	0.09	0.44
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE1	4	0.48	0.19	0.42
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE2	4	0.48	0.19	0.42
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE3	4	0.48	0.19	0.42
(1,1882)	1:137:A:ILE:HA	1:141:A:ASN:H	4	0.48	0.12	0.46
(1,685)	1:10:B:ALA:HA	1:48:B:ARG:HA	4	0.48	0.36	0.4
(1,2358)	1:181:A:TYR:HA	1:186:A:PRO:HA	4	0.47	0.11	0.52
(1,857)	1:23:B:LYS:H	1:25:B:ILE:H	4	0.44	0.24	0.41
(1,1150)	1:60:B:PHE:HB2	1:63:B:GLN:H	4	0.42	0.24	0.34
(1,1150)	1:60:B:PHE:HB3	1:63:B:GLN:H	4	0.42	0.24	0.34
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE1	4	0.42	0.16	0.46
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE2	4	0.42	0.16	0.46
(1,2300)	1:177:A:GLY:H	1:189:A:ALA:HA	4	0.42	0.15	0.46
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG21	4	0.41	0.35	0.25
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG22	4	0.41	0.35	0.25
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG23	4	0.41	0.35	0.25
(1,1865)	1:136:A:ALA:HA	1:166:A:ASP:H	4	0.41	0.19	0.42
(1,1096)	1:53:B:GLY:H	1:56:B:GLY:H	4	0.41	0.18	0.4
(1,4003)	1:221:B:GLN:HA	1:224:B:ASN:H	4	0.41	0.11	0.45
(1,1666)	1:116:A:LYS:HA	1:118:A:TYR:H	4	0.4	0.18	0.43
(1,1490)	1:101:A:LYS:HA	1:104:A:ASP:H	4	0.4	0.19	0.34
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB2	4	0.4	0.15	0.46
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB3	4	0.4	0.15	0.46
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB2	4	0.4	0.15	0.46
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB3	4	0.4	0.15	0.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4206)	1:343:B:GLU:H	1:344:B:ASN:H	4	0.4	0.16	0.4
(1,2842)	1:105:B:LEU:HA	1:109:B:GLY:H	4	0.39	0.16	0.38
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB1	4	0.39	0.18	0.36
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB2	4	0.39	0.18	0.36
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB3	4	0.39	0.18	0.36
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB2	4	0.39	0.27	0.33
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB3	4	0.39	0.27	0.33
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB2	4	0.39	0.27	0.33
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB3	4	0.39	0.27	0.33
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB2	4	0.39	0.27	0.33
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB3	4	0.39	0.27	0.33
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE1	4	0.39	0.11	0.39
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE2	4	0.39	0.11	0.39
(1,4163)	1:257:B:GLY:H	1:258:B:GLY:H	4	0.38	0.14	0.38
(1,4189)	1:324:B:ALA:H	1:325:B:GLY:H	4	0.38	0.18	0.4
(1,3355)	1:152:B:TYR:HA	1:155:B:ALA:HA	4	0.38	0.1	0.36
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB2	4	0.36	0.1	0.36
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB3	4	0.36	0.1	0.36
(1,4073)	1:302:A:PHE:H	1:303:A:ALA:H	4	0.35	0.12	0.36
(1,3204)	1:139:B:TYR:HA	1:142:B:ARG:H	4	0.35	0.24	0.24
(1,1813)	1:129:A:ILE:HA	1:133:A:PRO:HA	4	0.34	0.27	0.21
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG11	4	0.34	0.07	0.36
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG12	4	0.34	0.07	0.36
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG13	4	0.34	0.07	0.36
(1,1121)	1:56:B:GLY:HA2	1:58:B:SER:H	4	0.34	0.16	0.28
(1,1121)	1:56:B:GLY:HA3	1:58:B:SER:H	4	0.34	0.16	0.28
(1,2660)	1:217:A:LYS:H	1:220:A:GLU:H	4	0.34	0.13	0.28
(1,2504)	1:197:A:LEU:HA	1:204:A:ALA:HA	4	0.33	0.16	0.24
(1,2573)	1:206:A:GLU:HB2	1:207:A:ALA:H	4	0.33	0.09	0.32
(1,2573)	1:206:A:GLU:HB3	1:207:A:ALA:H	4	0.33	0.09	0.32
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG2	4	0.33	0.31	0.18
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG3	4	0.33	0.31	0.18
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG2	4	0.33	0.31	0.18
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG3	4	0.33	0.31	0.18
(1,4065)	1:257:A:GLY:H	1:258:A:GLY:H	4	0.32	0.11	0.36
(1,4190)	1:325:B:GLY:H	1:326:B:ASN:H	4	0.32	0.08	0.3
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE21	4	0.32	0.14	0.29
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE22	4	0.32	0.14	0.29
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE21	4	0.32	0.14	0.29
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE22	4	0.32	0.14	0.29
(1,3727)	1:190:B:LEU:HD11	1:216:B:LYS:H	4	0.31	0.17	0.26
(1,3727)	1:190:B:LEU:HD12	1:216:B:LYS:H	4	0.31	0.17	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3727)	1:190:B:LEU:HD13	1:216:B:LYS:H	4	0.31	0.17	0.26
(1,595)	1:69:A:LEU:H	1:71:A:SER:H	4	0.3	0.05	0.3
(1,3879)	1:206:B:GLU:HB2	1:207:B:ALA:H	4	0.3	0.12	0.34
(1,3879)	1:206:B:GLU:HB3	1:207:B:ALA:H	4	0.3	0.12	0.34
(1,3825)	1:199:B:ILE:H	1:201:B:GLY:H	4	0.3	0.15	0.27
(1,1998)	1:147:A:SER:H	1:155:A:ALA:HA	4	0.3	0.07	0.34
(1,3102)	1:128:B:ALA:H	1:131:B:VAL:H	4	0.29	0.09	0.3
(1,1565)	1:107:A:MET:HA	1:110:A:ASN:H	4	0.29	0.07	0.29
(1,1214)	1:71:B:SER:H	1:72:B:ALA:HA	4	0.27	0.07	0.26
(1,2418)	1:190:A:LEU:HA	1:216:A:LYS:H	4	0.27	0.16	0.2
(1,2570)	1:206:A:GLU:HA	1:209:A:LYS:H	4	0.27	0.16	0.22
(1,245)	1:22:A:LYS:HA	1:24:A:GLU:H	4	0.27	0.06	0.26
(1,379)	1:39:A:CYS:HA	1:42:A:GLU:H	4	0.26	0.07	0.29
(1,1985)	1:146:A:HIS:H	1:155:A:ALA:HA	4	0.25	0.13	0.22
(1,3939)	1:213:B:GLU:HA	1:217:B:LYS:H	4	0.25	0.12	0.22
(1,1279)	1:16:A:PHE:HE1	1:9:B:ALA:HA	4	0.24	0.19	0.15
(1,1279)	1:16:A:PHE:HE2	1:9:B:ALA:HA	4	0.24	0.19	0.15
(1,1667)	1:116:A:LYS:HA	1:118:A:TYR:HA	4	0.24	0.1	0.2
(1,171)	1:16:A:PHE:HA	1:18:A:SER:H	4	0.23	0.13	0.2
(1,2768)	1:98:B:THR:H	1:100:B:ALA:H	4	0.23	0.09	0.24
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD1	4	0.22	0.09	0.22
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD2	4	0.22	0.09	0.22
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD1	4	0.22	0.09	0.22
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD2	4	0.22	0.09	0.22
(1,3354)	1:152:B:TYR:HA	1:155:B:ALA:H	4	0.22	0.06	0.23
(1,2632)	1:213:A:GLU:HA	1:216:A:LYS:H	4	0.22	0.09	0.24
(1,4139)	1:231:B:GLU:H	1:232:B:GLN:H	4	0.22	0.07	0.2
(1,2051)	1:152:A:TYR:HA	1:156:A:VAL:H	4	0.22	0.04	0.22
(1,567)	1:65:A:LEU:H	1:67:A:ASP:H	4	0.22	0.09	0.2
(1,248)	1:23:A:LYS:H	1:25:A:ILE:H	4	0.22	0.11	0.2
(1,1593)	1:110:A:ASN:HA	1:113:A:MET:H	4	0.2	0.05	0.22
(1,2552)	1:205:A:THR:H	1:208:A:MET:H	4	0.2	0.13	0.14
(1,26)	1:5:A:LYS:HA	1:9:A:ALA:H	4	0.15	0.05	0.14
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG21	3	2.58	0.3	2.43
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG22	3	2.58	0.3	2.43
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG23	3	2.58	0.3	2.43
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG21	3	2.58	0.3	2.43
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG22	3	2.58	0.3	2.43
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG23	3	2.58	0.3	2.43
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG21	3	2.58	0.3	2.43
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG22	3	2.58	0.3	2.43
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG23	3	2.58	0.3	2.43

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3812)	1:197:B:LEU:HD11	1:209:B:LYS:HA	3	2.4	1.15	1.78
(1,3812)	1:197:B:LEU:HD12	1:209:B:LYS:HA	3	2.4	1.15	1.78
(1,3812)	1:197:B:LEU:HD13	1:209:B:LYS:HA	3	2.4	1.15	1.78
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD21	3	2.06	1.08	2.63
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD22	3	2.06	1.08	2.63
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD23	3	2.06	1.08	2.63
(1,3650)	1:180:B:LYS:HB2	1:188:B:GLU:HB2	3	1.96	1.27	1.82
(1,3650)	1:180:B:LYS:HB2	1:188:B:GLU:HB3	3	1.96	1.27	1.82
(1,3650)	1:180:B:LYS:HB3	1:188:B:GLU:HB2	3	1.96	1.27	1.82
(1,3650)	1:180:B:LYS:HB3	1:188:B:GLU:HB3	3	1.96	1.27	1.82
(1,1856)	1:135:A:ASN:HB3	1:138:A:TYR:HE2	3	1.66	0.48	1.35
(1,1856)	1:135:A:ASN:HB2	1:138:A:TYR:HE2	3	1.66	0.48	1.35
(1,2945)	1:113:B:MET:HB2	1:125:B:TYR:HE1	3	1.38	0.61	1.57
(1,2945)	1:113:B:MET:HB2	1:125:B:TYR:HE2	3	1.38	0.61	1.57
(1,3364)	1:152:B:TYR:HE1	1:178:B:PHE:HE2	3	1.38	0.23	1.24
(1,3364)	1:152:B:TYR:HE2	1:178:B:PHE:HE2	3	1.38	0.23	1.24
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG21	3	1.27	0.91	1.12
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG22	3	1.27	0.91	1.12
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG23	3	1.27	0.91	1.12
(1,1213)	1:71:B:SER:H	1:72:B:ALA:H	3	1.23	0.15	1.14
(1,763)	1:15:B:TYR:HA	1:18:B:SER:HB2	3	1.12	0.29	1.3
(1,763)	1:15:B:TYR:HA	1:18:B:SER:HB3	3	1.12	0.29	1.3
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD11	3	1.11	0.2	1.16
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD12	3	1.11	0.2	1.16
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD13	3	1.11	0.2	1.16
(1,2813)	1:102:B:ALA:HB1	1:128:B:ALA:HA	3	1.1	0.49	0.92
(1,2813)	1:102:B:ALA:HB2	1:128:B:ALA:HA	3	1.1	0.49	0.92
(1,2813)	1:102:B:ALA:HB3	1:128:B:ALA:HA	3	1.1	0.49	0.92
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE1	3	1.1	0.94	0.81
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE2	3	1.1	0.94	0.81
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE3	3	1.1	0.94	0.81
(1,162)	1:15:A:TYR:HB2	1:70:A:ASN:HD21	3	1.08	0.27	1.16
(1,162)	1:15:A:TYR:HB2	1:70:A:ASN:HD22	3	1.08	0.27	1.16
(1,162)	1:15:A:TYR:HB3	1:70:A:ASN:HD21	3	1.08	0.27	1.16
(1,162)	1:15:A:TYR:HB3	1:70:A:ASN:HD22	3	1.08	0.27	1.16
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD21	3	0.98	0.56	0.79
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD22	3	0.98	0.56	0.79
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD23	3	0.98	0.56	0.79
(1,2264)	1:173:A:TYR:HB2	1:195:A:LYS:HB2	3	0.96	0.65	0.73
(1,2264)	1:173:A:TYR:HB2	1:195:A:LYS:HB3	3	0.96	0.65	0.73
(1,2264)	1:173:A:TYR:HB3	1:195:A:LYS:HB2	3	0.96	0.65	0.73
(1,2264)	1:173:A:TYR:HB3	1:195:A:LYS:HB3	3	0.96	0.65	0.73

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3663)	1:181:B:TYR:HA	1:185:B:LYS:H	3	0.94	0.73	0.53
(1,3130)	1:129:B:ILE:HD11	1:142:B:ARG:HB2	3	0.93	1.0	0.29
(1,3130)	1:129:B:ILE:HD11	1:142:B:ARG:HB3	3	0.93	1.0	0.29
(1,3130)	1:129:B:ILE:HD12	1:142:B:ARG:HB2	3	0.93	1.0	0.29
(1,3130)	1:129:B:ILE:HD12	1:142:B:ARG:HB3	3	0.93	1.0	0.29
(1,3130)	1:129:B:ILE:HD13	1:142:B:ARG:HB2	3	0.93	1.0	0.29
(1,3130)	1:129:B:ILE:HD13	1:142:B:ARG:HB3	3	0.93	1.0	0.29
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD11	3	0.9	0.43	0.98
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD12	3	0.9	0.43	0.98
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD13	3	0.9	0.43	0.98
(1,3536)	1:170:B:PHE:HE1	1:171:B:ARG:H	3	0.9	0.15	0.9
(1,3536)	1:170:B:PHE:HE2	1:171:B:ARG:H	3	0.9	0.15	0.9
(1,3654)	1:181:B:TYR:H	1:185:B:LYS:H	3	0.89	0.64	0.8
(1,1412)	1:67:A:ASP:HB2	1:60:B:PHE:HB2	3	0.89	0.41	0.77
(1,1412)	1:67:A:ASP:HB2	1:60:B:PHE:HB3	3	0.89	0.41	0.77
(1,1412)	1:67:A:ASP:HB3	1:60:B:PHE:HB2	3	0.89	0.41	0.77
(1,1412)	1:67:A:ASP:HB3	1:60:B:PHE:HB3	3	0.89	0.41	0.77
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE1	3	0.89	0.37	1.06
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE2	3	0.89	0.37	1.06
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE3	3	0.89	0.37	1.06
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB1	3	0.87	0.46	1.13
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB2	3	0.87	0.46	1.13
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB3	3	0.87	0.46	1.13
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB1	3	0.87	0.46	1.13
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB2	3	0.87	0.46	1.13
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB3	3	0.87	0.46	1.13
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB1	3	0.87	0.46	1.13
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB2	3	0.87	0.46	1.13
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB3	3	0.87	0.46	1.13
(1,3527)	1:170:B:PHE:HB2	1:196:B:VAL:HA	3	0.85	0.41	0.58
(1,3527)	1:170:B:PHE:HB3	1:196:B:VAL:HA	3	0.85	0.41	0.58
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD11	3	0.83	0.56	0.61
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD12	3	0.83	0.56	0.61
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD13	3	0.83	0.56	0.61
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE1	3	0.82	0.5	0.76
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE2	3	0.82	0.5	0.76
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE3	3	0.82	0.5	0.76
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE1	3	0.82	0.5	0.76
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE2	3	0.82	0.5	0.76
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE3	3	0.82	0.5	0.76
(1,3444)	1:160:B:GLU:HA	1:164:B:SER:H	3	0.81	0.48	0.6
(1,3878)	1:206:B:GLU:HA	1:210:B:ARG:H	3	0.81	0.06	0.8

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4061)	1:253:A:GLY:H	1:254:A:SER:H	3	0.77	0.39	0.96
(1,172)	1:16:A:PHE:HA	1:18:A:SER:HB2	3	0.76	0.19	0.88
(1,172)	1:16:A:PHE:HA	1:18:A:SER:HB3	3	0.76	0.19	0.88
(1,3041)	1:122:B:ILE:HA	1:126:B:THR:H	3	0.76	0.38	0.78
(1,3343)	1:150:B:LYS:HZ1	1:152:B:TYR:HE1	3	0.73	0.7	0.28
(1,3343)	1:150:B:LYS:HZ1	1:152:B:TYR:HE2	3	0.73	0.7	0.28
(1,3343)	1:150:B:LYS:HZ2	1:152:B:TYR:HE1	3	0.73	0.7	0.28
(1,3343)	1:150:B:LYS:HZ2	1:152:B:TYR:HE2	3	0.73	0.7	0.28
(1,3343)	1:150:B:LYS:HZ3	1:152:B:TYR:HE1	3	0.73	0.7	0.28
(1,3343)	1:150:B:LYS:HZ3	1:152:B:TYR:HE2	3	0.73	0.7	0.28
(1,1391)	1:44:A:PHE:HE1	1:19:B:ILE:HG12	3	0.72	0.32	0.9
(1,1391)	1:44:A:PHE:HE1	1:19:B:ILE:HG13	3	0.72	0.32	0.9
(1,1391)	1:44:A:PHE:HE2	1:19:B:ILE:HG12	3	0.72	0.32	0.9
(1,1391)	1:44:A:PHE:HE2	1:19:B:ILE:HG13	3	0.72	0.32	0.9
(1,886)	1:27:B:GLU:HA	1:31:B:ASP:H	3	0.7	0.28	0.53
(1,3668)	1:181:B:TYR:HD1	1:218:B:LYS:HB2	3	0.7	0.46	0.73
(1,3668)	1:181:B:TYR:HD1	1:218:B:LYS:HB3	3	0.7	0.46	0.73
(1,3668)	1:181:B:TYR:HD2	1:218:B:LYS:HB2	3	0.7	0.46	0.73
(1,3668)	1:181:B:TYR:HD2	1:218:B:LYS:HB3	3	0.7	0.46	0.73
(1,3205)	1:139:B:TYR:HA	1:143:B:ALA:H	3	0.69	0.79	0.14
(1,277)	1:27:A:GLU:HA	1:31:A:ASP:H	3	0.69	0.63	0.33
(1,1855)	1:135:A:ASN:HB2	1:138:A:TYR:HE1	3	0.69	0.26	0.53
(1,1855)	1:135:A:ASN:HB2	1:138:A:TYR:HE2	3	0.69	0.26	0.53
(1,1855)	1:135:A:ASN:HB3	1:138:A:TYR:HE1	3	0.69	0.26	0.53
(1,1855)	1:135:A:ASN:HB3	1:138:A:TYR:HE2	3	0.69	0.26	0.53
(1,3992)	1:220:B:GLU:H	1:222:B:SER:H	3	0.66	0.38	0.45
(1,3366)	1:152:B:TYR:HD1	1:182:B:ALA:HB1	3	0.65	0.22	0.67
(1,3366)	1:152:B:TYR:HD2	1:182:B:ALA:HB1	3	0.65	0.22	0.67
(1,3366)	1:152:B:TYR:HD1	1:182:B:ALA:HB3	3	0.65	0.22	0.67
(1,1170)	1:63:B:GLN:HA	1:67:B:ASP:H	3	0.65	0.64	0.2
(1,1393)	1:44:A:PHE:HE1	1:25:B:ILE:HD11	3	0.64	0.26	0.81
(1,1393)	1:44:A:PHE:HE2	1:25:B:ILE:HD11	3	0.64	0.26	0.81
(1,3126)	1:129:B:ILE:HD11	1:139:B:TYR:HA	3	0.64	0.55	0.34
(1,3126)	1:129:B:ILE:HD12	1:139:B:TYR:HA	3	0.64	0.55	0.34
(1,3126)	1:129:B:ILE:HD13	1:139:B:TYR:HA	3	0.64	0.55	0.34
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB1	3	0.63	0.17	0.53
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB2	3	0.63	0.17	0.53
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB3	3	0.63	0.17	0.53
(1,1950)	1:143:A:ALA:HA	1:155:A:ALA:H	3	0.62	0.01	0.63
(1,726)	1:13:B:VAL:HA	1:17:B:SER:H	3	0.61	0.36	0.48
(1,1411)	1:67:A:ASP:HA	1:62:B:GLY:H	3	0.61	0.2	0.55
(1,1117)	1:56:B:GLY:H	1:57:B:LYS:H	3	0.61	0.18	0.69

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1106)	1:54:B:ILE:HA	1:57:B:LYS:HG2	3	0.6	0.36	0.8
(1,1106)	1:54:B:ILE:HA	1:57:B:LYS:HG3	3	0.6	0.36	0.8
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD11	3	0.6	0.32	0.78
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD12	3	0.6	0.32	0.78
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD13	3	0.6	0.32	0.78
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD11	3	0.59	0.48	0.31
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD12	3	0.59	0.48	0.31
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD13	3	0.59	0.48	0.31
(1,1418)	1:68:A:ILE:HG21	1:2:B:SER:HA	3	0.59	0.45	0.31
(1,1418)	1:68:A:ILE:HG22	1:2:B:SER:HA	3	0.59	0.45	0.31
(1,1418)	1:68:A:ILE:HG23	1:2:B:SER:HA	3	0.59	0.45	0.31
(1,2713)	1:223:A:LEU:HA	1:225:A:LEU:H	3	0.58	0.3	0.68
(1,2232)	1:170:A:PHE:HE1	1:171:A:ARG:HD2	3	0.57	0.3	0.56
(1,2232)	1:170:A:PHE:HE1	1:171:A:ARG:HD3	3	0.57	0.3	0.56
(1,2232)	1:170:A:PHE:HE2	1:171:A:ARG:HD2	3	0.57	0.3	0.56
(1,2232)	1:170:A:PHE:HE2	1:171:A:ARG:HD3	3	0.57	0.3	0.56
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD11	3	0.56	0.19	0.51
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD12	3	0.56	0.19	0.51
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD13	3	0.56	0.19	0.51
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD11	3	0.55	0.26	0.61
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD12	3	0.55	0.26	0.61
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD13	3	0.55	0.26	0.61
(1,3532)	1:170:B:PHE:HD1	1:171:B:ARG:HD2	3	0.55	0.32	0.38
(1,3532)	1:170:B:PHE:HD1	1:171:B:ARG:HD3	3	0.55	0.32	0.38
(1,3532)	1:170:B:PHE:HD2	1:171:B:ARG:HD2	3	0.55	0.32	0.38
(1,3532)	1:170:B:PHE:HD2	1:171:B:ARG:HD3	3	0.55	0.32	0.38
(1,1761)	1:125:A:TYR:HA	1:129:A:ILE:H	3	0.54	0.28	0.61
(1,3044)	1:122:B:ILE:HD11	1:146:B:HIS:HA	3	0.54	0.36	0.37
(1,3044)	1:122:B:ILE:HD12	1:146:B:HIS:HA	3	0.54	0.36	0.37
(1,3044)	1:122:B:ILE:HD13	1:146:B:HIS:HA	3	0.54	0.36	0.37
(1,3912)	1:210:B:ARG:HA	1:213:B:GLU:H	3	0.54	0.32	0.32
(1,2003)	1:147:A:SER:HA	1:150:A:LYS:H	3	0.54	0.09	0.51
(1,2572)	1:206:A:GLU:HA	1:210:A:ARG:H	3	0.53	0.24	0.6
(1,4202)	1:337:B:ASP:H	1:338:B:GLU:H	3	0.52	0.16	0.59
(1,3809)	1:197:B:LEU:HA	1:201:B:GLY:H	3	0.5	0.34	0.33
(1,1991)	1:146:A:HIS:HA	1:151:A:GLU:H	3	0.49	0.07	0.5
(1,3521)	1:170:B:PHE:HA	1:174:B:SER:H	3	0.49	0.34	0.44
(1,3593)	1:175:B:ARG:HA	1:178:B:PHE:H	3	0.49	0.27	0.32
(1,2244)	1:171:A:ARG:HA	1:174:A:SER:HA	3	0.49	0.3	0.33
(1,2230)	1:170:A:PHE:HE1	1:171:A:ARG:H	3	0.49	0.14	0.51
(1,2230)	1:170:A:PHE:HE2	1:171:A:ARG:H	3	0.49	0.14	0.51
(1,764)	1:15:B:TYR:HA	1:19:B:ILE:H	3	0.48	0.19	0.47

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1165)	1:62:B:GLY:H	1:64:B:HIS:H	3	0.48	0.45	0.19
(1,836)	1:20:B:VAL:HA	1:30:B:ALA:HA	3	0.48	0.45	0.16
(1,4158)	1:252:B:LEU:H	1:253:B:GLY:H	3	0.47	0.17	0.56
(1,445)	1:47:A:GLU:H	1:50:A:ALA:H	3	0.47	0.29	0.4
(1,1507)	1:102:A:ALA:HB1	1:128:A:ALA:HA	3	0.47	0.26	0.48
(1,1507)	1:102:A:ALA:HB2	1:128:A:ALA:HA	3	0.47	0.26	0.48
(1,1507)	1:102:A:ALA:HB3	1:128:A:ALA:HA	3	0.47	0.26	0.48
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD11	3	0.47	0.32	0.38
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD12	3	0.47	0.32	0.38
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD13	3	0.47	0.32	0.38
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD11	3	0.47	0.32	0.38
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD12	3	0.47	0.32	0.38
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD13	3	0.47	0.32	0.38
(1,2919)	1:112:B:ALA:HA	1:117:B:ASP:H	3	0.47	0.38	0.21
(1,163)	1:15:A:TYR:HD1	1:18:A:SER:HB2	3	0.46	0.19	0.55
(1,163)	1:15:A:TYR:HD1	1:18:A:SER:HB3	3	0.46	0.19	0.55
(1,163)	1:15:A:TYR:HD2	1:18:A:SER:HB2	3	0.46	0.19	0.55
(1,163)	1:15:A:TYR:HD2	1:18:A:SER:HB3	3	0.46	0.19	0.55
(1,560)	1:63:A:GLN:HA	1:65:A:LEU:H	3	0.46	0.23	0.54
(1,537)	1:60:A:PHE:HA	1:63:A:GLN:H	3	0.45	0.41	0.19
(1,77)	1:10:A:ALA:HA	1:51:A:VAL:HA	3	0.44	0.17	0.51
(1,3533)	1:170:B:PHE:HD1	1:196:B:VAL:HA	3	0.44	0.11	0.47
(1,3533)	1:170:B:PHE:HD2	1:196:B:VAL:HA	3	0.44	0.11	0.47
(1,2978)	1:116:B:LYS:HB2	1:118:B:TYR:HE1	3	0.42	0.12	0.45
(1,2978)	1:116:B:LYS:HB2	1:118:B:TYR:HE2	3	0.42	0.12	0.45
(1,2978)	1:116:B:LYS:HB3	1:118:B:TYR:HE1	3	0.42	0.12	0.45
(1,2978)	1:116:B:LYS:HB3	1:118:B:TYR:HE2	3	0.42	0.12	0.45
(1,3626)	1:178:B:PHE:HA	1:182:B:ALA:H	3	0.42	0.25	0.28
(1,3158)	1:135:B:ASN:HA	1:138:B:TYR:H	3	0.42	0.25	0.38
(1,2628)	1:213:A:GLU:H	1:216:A:LYS:H	3	0.42	0.14	0.37
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB1	3	0.41	0.31	0.26
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB2	3	0.41	0.31	0.26
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB3	3	0.41	0.31	0.26
(1,2265)	1:173:A:TYR:HB2	1:195:A:LYS:HG2	3	0.41	0.18	0.47
(1,2265)	1:173:A:TYR:HB2	1:195:A:LYS:HG3	3	0.41	0.18	0.47
(1,2265)	1:173:A:TYR:HB3	1:195:A:LYS:HG2	3	0.41	0.18	0.47
(1,2265)	1:173:A:TYR:HB3	1:195:A:LYS:HG3	3	0.41	0.18	0.47
(1,2305)	1:177:A:GLY:HA2	1:189:A:ALA:HA	3	0.41	0.06	0.45
(1,2305)	1:177:A:GLY:HA3	1:189:A:ALA:HA	3	0.41	0.06	0.45
(1,3002)	1:118:B:TYR:HB2	1:148:B:SER:HB2	3	0.41	0.35	0.19
(1,3002)	1:118:B:TYR:HB2	1:148:B:SER:HB3	3	0.41	0.35	0.19
(1,3002)	1:118:B:TYR:HB3	1:148:B:SER:HB2	3	0.41	0.35	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3002)	1:118:B:TYR:HB3	1:148:B:SER:HB3	3	0.41	0.35	0.19
(1,2287)	1:175:A:ARG:HA	1:178:A:PHE:H	3	0.4	0.18	0.41
(1,2756)	1:96:B:ALA:H	1:98:B:THR:H	3	0.4	0.16	0.46
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB1	3	0.4	0.26	0.32
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB2	3	0.4	0.26	0.32
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB3	3	0.4	0.26	0.32
(1,2009)	1:147:A:SER:HA	1:179:A:ALA:HA	3	0.39	0.29	0.27
(1,2992)	1:118:B:TYR:HA	1:121:B:ALA:H	3	0.39	0.31	0.18
(1,2067)	1:153:A:ASP:HA	1:156:A:VAL:H	3	0.39	0.32	0.18
(1,3108)	1:128:B:ALA:HA	1:132:B:LEU:H	3	0.39	0.2	0.41
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG21	3	0.38	0.15	0.48
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG22	3	0.38	0.15	0.48
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG23	3	0.38	0.15	0.48
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG21	3	0.38	0.15	0.48
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG22	3	0.38	0.15	0.48
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG23	3	0.38	0.15	0.48
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG21	3	0.38	0.15	0.48
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG22	3	0.38	0.15	0.48
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG23	3	0.38	0.15	0.48
(1,3312)	1:147:B:SER:HA	1:152:B:TYR:H	3	0.38	0.15	0.42
(1,4151)	1:243:B:GLY:H	1:244:B:ALA:H	3	0.38	0.0	0.38
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD21	3	0.37	0.3	0.19
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD22	3	0.37	0.3	0.19
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD23	3	0.37	0.3	0.19
(1,4167)	1:294:B:SER:H	1:295:B:ILE:H	3	0.37	0.18	0.31
(1,1146)	1:60:B:PHE:HA	1:63:B:GLN:H	3	0.37	0.13	0.37
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB1	3	0.36	0.23	0.32
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB2	3	0.36	0.23	0.32
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB3	3	0.36	0.23	0.32
(1,2534)	1:201:A:GLY:H	1:204:A:ALA:H	3	0.36	0.13	0.44
(1,3882)	1:207:B:ALA:H	1:210:B:ARG:H	3	0.36	0.16	0.36
(1,4108)	1:343:A:GLU:H	1:344:A:ASN:H	3	0.36	0.14	0.29
(1,174)	1:16:A:PHE:HA	1:19:A:ILE:HA	3	0.36	0.04	0.34
(1,1239)	1:8:A:ILE:HG21	1:12:B:ILE:HA	3	0.35	0.18	0.38
(1,1239)	1:8:A:ILE:HG22	1:12:B:ILE:HA	3	0.35	0.18	0.38
(1,1239)	1:8:A:ILE:HG23	1:12:B:ILE:HA	3	0.35	0.18	0.38
(1,4060)	1:252:A:LEU:H	1:253:A:GLY:H	3	0.35	0.1	0.35
(1,889)	1:28:B:ASP:H	1:31:B:ASP:H	3	0.35	0.18	0.33
(1,781)	1:16:B:PHE:HA	1:18:B:SER:HB2	3	0.35	0.24	0.2
(1,781)	1:16:B:PHE:HA	1:18:B:SER:HB3	3	0.35	0.24	0.2
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB1	3	0.34	0.25	0.17
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB2	3	0.34	0.25	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB3	3	0.34	0.25	0.17
(1,2940)	1:113:B:MET:HA	1:117:B:ASP:H	3	0.34	0.05	0.31
(1,1358)	1:40:A:ILE:HA	1:33:B:LEU:HA	3	0.34	0.16	0.41
(1,1689)	1:118:A:TYR:HA	1:145:A:ALA:HA	3	0.33	0.21	0.21
(1,550)	1:61:A:LYS:H	1:63:A:GLN:H	3	0.33	0.09	0.39
(1,4197)	1:332:B:GLY:H	1:333:B:ALA:H	3	0.33	0.06	0.37
(1,173)	1:16:A:PHE:HA	1:19:A:ILE:H	3	0.33	0.1	0.3
(1,3801)	1:196:B:VAL:HG11	1:208:B:MET:HB2	3	0.33	0.17	0.22
(1,3801)	1:196:B:VAL:HG11	1:208:B:MET:HB3	3	0.33	0.17	0.22
(1,3801)	1:196:B:VAL:HG12	1:208:B:MET:HB2	3	0.33	0.17	0.22
(1,3801)	1:196:B:VAL:HG12	1:208:B:MET:HB3	3	0.33	0.17	0.22
(1,3801)	1:196:B:VAL:HG13	1:208:B:MET:HB2	3	0.33	0.17	0.22
(1,3801)	1:196:B:VAL:HG13	1:208:B:MET:HB3	3	0.33	0.17	0.22
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB1	3	0.33	0.11	0.3
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB2	3	0.33	0.11	0.3
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB3	3	0.33	0.11	0.3
(1,2588)	1:208:A:MET:H	1:211:A:ASP:H	3	0.32	0.11	0.38
(1,2977)	1:116:B:LYS:HB2	1:118:B:TYR:HD1	3	0.32	0.1	0.35
(1,2977)	1:116:B:LYS:HB2	1:118:B:TYR:HD2	3	0.32	0.1	0.35
(1,2977)	1:116:B:LYS:HB3	1:118:B:TYR:HD1	3	0.32	0.1	0.35
(1,2977)	1:116:B:LYS:HB3	1:118:B:TYR:HD2	3	0.32	0.1	0.35
(1,626)	1:4:B:SER:HA	1:5:B:LYS:HA	3	0.32	0.11	0.35
(1,2819)	1:103:B:GLU:H	1:105:B:LEU:H	3	0.32	0.25	0.15
(1,1829)	1:130:A:LYS:HA	1:132:A:LEU:H	3	0.32	0.15	0.36
(1,2938)	1:113:B:MET:HA	1:116:B:LYS:H	3	0.32	0.1	0.25
(1,3079)	1:125:B:TYR:HB2	1:142:B:ARG:HD2	3	0.32	0.14	0.22
(1,3079)	1:125:B:TYR:HB2	1:142:B:ARG:HD3	3	0.32	0.14	0.22
(1,3079)	1:125:B:TYR:HB3	1:142:B:ARG:HD2	3	0.32	0.14	0.22
(1,3079)	1:125:B:TYR:HB3	1:142:B:ARG:HD3	3	0.32	0.14	0.22
(1,3704)	1:188:B:GLU:HA	1:191:B:GLU:H	3	0.31	0.1	0.29
(1,3595)	1:176:B:LEU:H	1:178:B:PHE:H	3	0.31	0.15	0.25
(1,4171)	1:302:B:PHE:H	1:303:B:ALA:H	3	0.31	0.19	0.25
(1,3411)	1:157:B:LYS:HA	1:160:B:GLU:H	3	0.31	0.16	0.28
(1,4176)	1:307:B:GLY:H	1:308:B:THR:H	3	0.31	0.06	0.33
(1,2231)	1:170:A:PHE:HE1	1:171:A:ARG:HA	3	0.3	0.24	0.16
(1,2231)	1:170:A:PHE:HE2	1:171:A:ARG:HA	3	0.3	0.24	0.16
(1,2837)	1:105:B:LEU:H	1:108:B:GLN:H	3	0.3	0.07	0.31
(1,2010)	1:147:A:SER:HB2	1:178:A:PHE:HB2	3	0.3	0.09	0.3
(1,2010)	1:147:A:SER:HB2	1:178:A:PHE:HB3	3	0.3	0.09	0.3
(1,2010)	1:147:A:SER:HB3	1:178:A:PHE:HB2	3	0.3	0.09	0.3
(1,2010)	1:147:A:SER:HB3	1:178:A:PHE:HB3	3	0.3	0.09	0.3
(1,2633)	1:213:A:GLU:HA	1:217:A:LYS:H	3	0.3	0.13	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4143)	1:235:B:ASP:H	1:236:B:ALA:H	3	0.29	0.02	0.3
(1,2335)	1:180:A:LYS:H	1:189:A:ALA:HA	3	0.29	0.09	0.26
(1,884)	1:27:B:GLU:HA	1:30:B:ALA:H	3	0.29	0.07	0.25
(1,1773)	1:125:A:TYR:HB2	1:142:A:ARG:HD2	3	0.28	0.1	0.22
(1,1773)	1:125:A:TYR:HB2	1:142:A:ARG:HD3	3	0.28	0.1	0.22
(1,1773)	1:125:A:TYR:HB3	1:142:A:ARG:HD2	3	0.28	0.1	0.22
(1,1773)	1:125:A:TYR:HB3	1:142:A:ARG:HD3	3	0.28	0.1	0.22
(1,2136)	1:160:A:GLU:HA	1:163:A:ILE:H	3	0.28	0.07	0.29
(1,211)	1:18:A:SER:HA	1:22:A:LYS:H	3	0.28	0.12	0.2
(1,2485)	1:195:A:LYS:HA	1:199:A:ILE:H	3	0.28	0.02	0.27
(1,1283)	1:16:A:PHE:HE1	1:12:B:ILE:HB	3	0.27	0.09	0.28
(1,1283)	1:16:A:PHE:HE2	1:12:B:ILE:HB	3	0.27	0.09	0.28
(1,1163)	1:62:B:GLY:H	1:63:B:GLN:H	3	0.27	0.14	0.18
(1,1678)	1:117:A:ASP:HA	1:120:A:LEU:H	3	0.27	0.12	0.24
(1,4187)	1:322:B:ASN:H	1:323:B:MET:H	3	0.26	0.15	0.16
(1,3171)	1:136:B:ALA:HA	1:166:B:ASP:H	3	0.26	0.12	0.26
(1,2522)	1:199:A:ILE:HA	1:201:A:GLY:H	3	0.26	0.13	0.21
(1,3507)	1:169:B:TYR:HE1	1:171:B:ARG:HB2	3	0.25	0.09	0.25
(1,3507)	1:169:B:TYR:HE1	1:171:B:ARG:HB3	3	0.25	0.09	0.25
(1,3507)	1:169:B:TYR:HE2	1:171:B:ARG:HB2	3	0.25	0.09	0.25
(1,3507)	1:169:B:TYR:HE2	1:171:B:ARG:HB3	3	0.25	0.09	0.25
(1,1862)	1:136:A:ALA:HA	1:162:A:ALA:HA	3	0.25	0.05	0.22
(1,2175)	1:164:A:SER:HA	1:166:A:ASP:H	3	0.24	0.04	0.23
(1,2320)	1:178:A:PHE:HA	1:182:A:ALA:H	3	0.24	0.16	0.16
(1,3337)	1:150:B:LYS:HB2	1:152:B:TYR:HD1	3	0.24	0.06	0.22
(1,3337)	1:150:B:LYS:HB2	1:152:B:TYR:HD2	3	0.24	0.06	0.22
(1,3337)	1:150:B:LYS:HB3	1:152:B:TYR:HD1	3	0.24	0.06	0.22
(1,3337)	1:150:B:LYS:HB3	1:152:B:TYR:HD2	3	0.24	0.06	0.22
(1,669)	1:9:B:ALA:HA	1:13:B:VAL:H	3	0.24	0.06	0.24
(1,339)	1:35:A:VAL:H	1:38:A:ASP:H	3	0.23	0.08	0.29
(1,2380)	1:185:A:LYS:H	1:186:A:PRO:HA	3	0.23	0.1	0.21
(1,1962)	1:143:A:ALA:HB1	1:175:A:ARG:HB2	3	0.23	0.13	0.16
(1,1962)	1:143:A:ALA:HB1	1:175:A:ARG:HB3	3	0.23	0.13	0.16
(1,1962)	1:143:A:ALA:HB2	1:175:A:ARG:HB2	3	0.23	0.13	0.16
(1,1962)	1:143:A:ALA:HB2	1:175:A:ARG:HB3	3	0.23	0.13	0.16
(1,1962)	1:143:A:ALA:HB3	1:175:A:ARG:HB2	3	0.23	0.13	0.16
(1,1962)	1:143:A:ALA:HB3	1:175:A:ARG:HB3	3	0.23	0.13	0.16
(1,2991)	1:118:B:TYR:HA	1:120:B:LEU:H	3	0.23	0.05	0.25
(1,1894)	1:139:A:TYR:H	1:162:A:ALA:HA	3	0.23	0.1	0.23
(1,3938)	1:213:B:GLU:HA	1:216:B:LYS:H	3	0.22	0.03	0.22
(1,251)	1:23:A:LYS:HA	1:25:A:ILE:H	3	0.22	0.04	0.22
(1,276)	1:27:A:GLU:HA	1:30:A:ALA:HA	3	0.22	0.12	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2277)	1:174:A:SER:HA	1:177:A:GLY:H	3	0.21	0.08	0.16
(1,1191)	1:67:B:ASP:H	1:68:B:ILE:H	3	0.2	0.07	0.19
(1,4042)	1:232:A:GLN:H	1:233:A:SER:H	3	0.2	0.08	0.16
(1,495)	1:54:A:ILE:HA	1:57:A:LYS:H	3	0.2	0.04	0.18
(1,1898)	1:139:A:TYR:HA	1:142:A:ARG:H	3	0.2	0.04	0.18
(1,3512)	1:169:B:TYR:HE1	1:171:B:ARG:HB3	3	0.2	0.06	0.24
(1,3512)	1:169:B:TYR:HE2	1:171:B:ARG:HB2	3	0.2	0.06	0.24
(1,3512)	1:169:B:TYR:HE1	1:171:B:ARG:HB2	3	0.2	0.06	0.24
(1,2201)	1:169:A:TYR:HE1	1:171:A:ARG:HB2	3	0.2	0.09	0.14
(1,2201)	1:169:A:TYR:HE1	1:171:A:ARG:HB3	3	0.2	0.09	0.14
(1,2201)	1:169:A:TYR:HE2	1:171:A:ARG:HB2	3	0.2	0.09	0.14
(1,2201)	1:169:A:TYR:HE2	1:171:A:ARG:HB3	3	0.2	0.09	0.14
(1,1889)	1:138:A:TYR:HA	1:141:A:ASN:H	3	0.19	0.03	0.19
(1,3067)	1:125:B:TYR:HA	1:129:B:ILE:H	3	0.19	0.02	0.2
(1,3106)	1:128:B:ALA:HA	1:131:B:VAL:H	3	0.19	0.1	0.14
(1,3481)	1:164:B:SER:HA	1:166:B:ASP:H	3	0.19	0.05	0.17
(1,3807)	1:197:B:LEU:HA	1:199:B:ILE:H	3	0.19	0.08	0.15
(1,599)	1:70:A:ASN:H	1:71:A:SER:H	3	0.18	0.08	0.12
(1,1179)	1:65:B:LEU:HA	1:67:B:ASP:H	3	0.18	0.05	0.15
(1,1181)	1:65:B:LEU:HD21	1:66:B:ALA:H	3	0.17	0.04	0.18
(1,1181)	1:65:B:LEU:HD22	1:66:B:ALA:H	3	0.17	0.04	0.18
(1,1181)	1:65:B:LEU:HD23	1:66:B:ALA:H	3	0.17	0.04	0.18
(1,431)	1:45:A:GLY:H	1:46:A:PHE:HD1	3	0.17	0.04	0.15
(1,3377)	1:154:B:GLN:H	1:157:B:LYS:H	3	0.17	0.06	0.14
(1,401)	1:41:A:SER:HA	1:45:A:GLY:H	3	0.17	0.02	0.16
(1,25)	1:5:A:LYS:HA	1:8:A:ILE:H	3	0.16	0.07	0.12
(1,3765)	1:193:B:TYR:HD1	1:212:B:TYR:H	3	0.16	0.04	0.19
(1,3765)	1:193:B:TYR:HD2	1:212:B:TYR:H	3	0.16	0.04	0.19
(1,4045)	1:235:A:ASP:H	1:236:A:ALA:H	3	0.16	0.02	0.16
(1,362)	1:37:A:MET:HA	1:40:A:ILE:H	3	0.15	0.03	0.14
(1,21)	1:5:A:LYS:H	1:8:A:ILE:H	3	0.14	0.01	0.13
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE1	2	1.98	1.14	1.98
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE2	2	1.98	1.14	1.98
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE3	2	1.98	1.14	1.98
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE1	2	1.98	1.14	1.98
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE2	2	1.98	1.14	1.98
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE3	2	1.98	1.14	1.98
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE1	2	1.58	0.58	1.58
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE2	2	1.58	0.58	1.58
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE3	2	1.58	0.58	1.58
(1,1417)	1:68:A:ILE:HA	1:2:B:SER:HB2	2	1.51	0.86	1.51
(1,1417)	1:68:A:ILE:HA	1:2:B:SER:HB3	2	1.51	0.86	1.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD11	2	1.37	0.77	1.37
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD12	2	1.37	0.77	1.37
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD13	2	1.37	0.77	1.37
(1,2263)	1:173:A:TYR:HB2	1:195:A:LYS:H	2	1.31	0.4	1.31
(1,2263)	1:173:A:TYR:HB3	1:195:A:LYS:H	2	1.31	0.4	1.31
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD11	2	1.29	0.13	1.29
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD12	2	1.29	0.13	1.29
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD13	2	1.29	0.13	1.29
(1,2783)	1:100:B:ALA:H	1:102:B:ALA:H	2	1.28	0.47	1.28
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG21	2	1.28	0.78	1.28
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG22	2	1.28	0.78	1.28
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG23	2	1.28	0.78	1.28
(1,1025)	1:43:B:ALA:HA	1:45:B:GLY:H	2	1.27	1.06	1.27
(1,1010)	1:41:B:SER:HA	1:45:B:GLY:H	2	1.25	0.38	1.25
(1,507)	1:55:A:LEU:HD21	1:71:A:SER:HA	2	1.25	0.17	1.25
(1,507)	1:55:A:LEU:HD22	1:71:A:SER:HA	2	1.25	0.17	1.25
(1,507)	1:55:A:LEU:HD23	1:71:A:SER:HA	2	1.25	0.17	1.25
(1,1308)	1:25:A:ILE:HD11	1:43:B:ALA:HA	2	1.19	0.39	1.19
(1,1308)	1:25:A:ILE:HD12	1:43:B:ALA:HA	2	1.19	0.39	1.19
(1,1308)	1:25:A:ILE:HD13	1:43:B:ALA:HA	2	1.19	0.39	1.19
(1,1387)	1:44:A:PHE:HE1	1:16:B:PHE:HE1	2	1.16	0.5	1.16
(1,1387)	1:44:A:PHE:HE2	1:16:B:PHE:HE1	2	1.16	0.5	1.16
(1,2788)	1:101:B:LYS:H	1:102:B:ALA:H	2	1.12	0.27	1.12
(1,1386)	1:44:A:PHE:HE1	1:16:B:PHE:HD1	2	1.08	0.28	1.08
(1,1386)	1:44:A:PHE:HE2	1:16:B:PHE:HD1	2	1.08	0.28	1.08
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB1	2	1.07	0.26	1.07
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB2	2	1.07	0.26	1.07
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB3	2	1.07	0.26	1.07
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB1	2	1.07	0.26	1.07
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB2	2	1.07	0.26	1.07
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB3	2	1.07	0.26	1.07
(1,2421)	1:190:A:LEU:HD11	1:216:A:LYS:H	2	1.01	0.16	1.01
(1,2421)	1:190:A:LEU:HD12	1:216:A:LYS:H	2	1.01	0.16	1.01
(1,2421)	1:190:A:LEU:HD13	1:216:A:LYS:H	2	1.01	0.16	1.01
(1,2755)	1:96:B:ALA:H	1:97:B:GLU:H	2	1.01	0.34	1.01
(1,3931)	1:212:B:TYR:HD1	1:213:B:GLU:HA	2	1.01	0.15	1.01
(1,3931)	1:212:B:TYR:HD2	1:213:B:GLU:HA	2	1.01	0.15	1.01
(1,2773)	1:98:B:THR:HA	1:101:B:LYS:H	2	1.0	0.7	1.0
(1,3196)	1:138:B:TYR:HA	1:142:B:ARG:H	2	0.97	0.71	0.97
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD11	2	0.94	0.74	0.94
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD12	2	0.94	0.74	0.94
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD13	2	0.94	0.74	0.94

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD11	2	0.92	0.1	0.92
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD12	2	0.92	0.1	0.92
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD13	2	0.92	0.1	0.92
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG21	2	0.92	0.66	0.92
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG22	2	0.92	0.66	0.92
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG23	2	0.92	0.66	0.92
(1,2266)	1:173:A:TYR:HB2	1:196:A:VAL:H	2	0.92	0.24	0.92
(1,2266)	1:173:A:TYR:HB3	1:196:A:VAL:H	2	0.92	0.24	0.92
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD11	2	0.9	0.38	0.9
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD12	2	0.9	0.38	0.9
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD13	2	0.9	0.38	0.9
(1,1134)	1:59:B:GLU:H	1:60:B:PHE:H	2	0.9	0.23	0.9
(1,878)	1:27:B:GLU:H	1:28:B:ASP:H	2	0.87	0.02	0.87
(1,3848)	1:203:B:ASN:H	1:204:B:ALA:H	2	0.87	0.15	0.87
(1,280)	1:28:A:ASP:H	1:31:A:ASP:H	2	0.85	0.11	0.85
(1,1231)	1:5:A:LYS:H	1:15:B:TYR:HE1	2	0.82	0.57	0.82
(1,1231)	1:5:A:LYS:H	1:15:B:TYR:HE2	2	0.82	0.57	0.82
(1,1839)	1:132:A:LEU:HD11	1:134:A:THR:H	2	0.78	0.2	0.78
(1,1839)	1:132:A:LEU:HD12	1:134:A:THR:H	2	0.78	0.2	0.78
(1,1839)	1:132:A:LEU:HD13	1:134:A:THR:H	2	0.78	0.2	0.78
(1,2340)	1:180:A:LYS:HA	1:185:A:LYS:H	2	0.78	0.52	0.78
(1,3819)	1:198:B:ASP:H	1:201:B:GLY:H	2	0.76	0.41	0.76
(1,3298)	1:146:B:HIS:HB2	1:151:B:GLU:HB2	2	0.75	0.18	0.75
(1,3298)	1:146:B:HIS:HB2	1:151:B:GLU:HB3	2	0.75	0.18	0.75
(1,3298)	1:146:B:HIS:HB3	1:151:B:GLU:HB2	2	0.75	0.18	0.75
(1,3298)	1:146:B:HIS:HB3	1:151:B:GLU:HB3	2	0.75	0.18	0.75
(1,1527)	1:104:A:ASP:HA	1:107:A:MET:H	2	0.72	0.16	0.72
(1,752)	1:14:B:ASN:HA	1:18:B:SER:H	2	0.71	0.47	0.71
(1,1467)	1:98:A:THR:HA	1:101:A:LYS:H	2	0.69	0.43	0.69
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE1	2	0.68	0.26	0.68
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE2	2	0.68	0.26	0.68
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE3	2	0.68	0.26	0.68
(1,2443)	1:193:A:TYR:H	1:212:A:TYR:HA	2	0.66	0.48	0.66
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD11	2	0.66	0.08	0.66
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD12	2	0.66	0.08	0.66
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD13	2	0.66	0.08	0.66
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE1	2	0.66	0.03	0.66
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE2	2	0.66	0.03	0.66
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE3	2	0.66	0.03	0.66
(1,1177)	1:65:B:LEU:HA	1:66:B:ALA:H	2	0.65	0.0	0.65
(1,4019)	1:223:B:LEU:HA	1:225:B:LEU:H	2	0.64	0.18	0.64
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD11	2	0.62	0.29	0.62

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD12	2	0.62	0.29	0.62
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD13	2	0.62	0.29	0.62
(1,1576)	1:109:A:GLY:H	1:121:A:ALA:HA	2	0.62	0.33	0.62
(1,772)	1:15:B:TYR:HD1	1:18:B:SER:HB2	2	0.6	0.17	0.6
(1,772)	1:15:B:TYR:HD1	1:18:B:SER:HB3	2	0.6	0.17	0.6
(1,772)	1:15:B:TYR:HD2	1:18:B:SER:HB2	2	0.6	0.17	0.6
(1,772)	1:15:B:TYR:HD2	1:18:B:SER:HB3	2	0.6	0.17	0.6
(1,3846)	1:202:B:ASP:HA	1:204:B:ALA:H	2	0.6	0.26	0.6
(1,4021)	1:224:B:ASN:H	1:225:B:LEU:H	2	0.59	0.42	0.59
(1,544)	1:60:A:PHE:HB2	1:63:A:GLN:HG2	2	0.57	0.46	0.57
(1,544)	1:60:A:PHE:HB2	1:63:A:GLN:HG3	2	0.57	0.46	0.57
(1,544)	1:60:A:PHE:HB3	1:63:A:GLN:HG2	2	0.57	0.46	0.57
(1,544)	1:60:A:PHE:HB3	1:63:A:GLN:HG3	2	0.57	0.46	0.57
(1,1135)	1:59:B:GLU:H	1:60:B:PHE:HA	2	0.57	0.24	0.57
(1,1202)	1:69:B:LEU:H	1:70:B:ASN:H	2	0.57	0.44	0.57
(1,3188)	1:137:B:ILE:HA	1:141:B:ASN:H	2	0.57	0.34	0.57
(1,1572)	1:108:A:GLN:HA	1:111:A:LYS:H	2	0.57	0.34	0.57
(1,1268)	1:15:A:TYR:HE1	1:5:B:LYS:HB2	2	0.56	0.22	0.56
(1,1268)	1:15:A:TYR:HE1	1:5:B:LYS:HB3	2	0.56	0.22	0.56
(1,1268)	1:15:A:TYR:HE2	1:5:B:LYS:HB2	2	0.56	0.22	0.56
(1,1268)	1:15:A:TYR:HE2	1:5:B:LYS:HB3	2	0.56	0.22	0.56
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD11	2	0.56	0.36	0.56
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD12	2	0.56	0.36	0.56
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD13	2	0.56	0.36	0.56
(1,1228)	1:2:A:SER:HB2	1:68:B:ILE:HA	2	0.54	0.2	0.54
(1,1228)	1:2:A:SER:HB3	1:68:B:ILE:HA	2	0.54	0.2	0.54
(1,861)	1:24:B:GLU:H	1:25:B:ILE:H	2	0.53	0.06	0.53
(1,2871)	1:107:B:MET:HA	1:110:B:ASN:H	2	0.53	0.34	0.53
(1,758)	1:15:B:TYR:H	1:18:B:SER:H	2	0.52	0.15	0.52
(1,1142)	1:60:B:PHE:HA	1:61:B:LYS:H	2	0.52	0.03	0.52
(1,2367)	1:181:A:TYR:HE1	1:218:A:LYS:HE2	2	0.52	0.16	0.52
(1,2367)	1:181:A:TYR:HE1	1:218:A:LYS:HE3	2	0.52	0.16	0.52
(1,2367)	1:181:A:TYR:HE2	1:218:A:LYS:HE2	2	0.52	0.16	0.52
(1,2367)	1:181:A:TYR:HE2	1:218:A:LYS:HE3	2	0.52	0.16	0.52
(1,2215)	1:170:A:PHE:HA	1:174:A:SER:H	2	0.52	0.29	0.52
(1,3575)	1:173:B:TYR:HE2	1:199:B:ILE:HD13	2	0.52	0.08	0.52
(1,2033)	1:150:A:LYS:HB2	1:152:A:TYR:HE2	2	0.51	0.38	0.51
(1,2226)	1:170:A:PHE:HD1	1:171:A:ARG:HD2	2	0.51	0.13	0.51
(1,2226)	1:170:A:PHE:HD1	1:171:A:ARG:HD3	2	0.51	0.13	0.51
(1,2226)	1:170:A:PHE:HD2	1:171:A:ARG:HD2	2	0.51	0.13	0.51
(1,2226)	1:170:A:PHE:HD2	1:171:A:ARG:HD3	2	0.51	0.13	0.51
(1,3077)	1:125:B:TYR:HB2	1:138:B:TYR:HB2	2	0.51	0.01	0.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3077)	1:125:B:TYR:HB2	1:138:B:TYR:HB3	2	0.51	0.01	0.51
(1,3077)	1:125:B:TYR:HB3	1:138:B:TYR:HB2	2	0.51	0.01	0.51
(1,3077)	1:125:B:TYR:HB3	1:138:B:TYR:HB3	2	0.51	0.01	0.51
(1,1913)	1:139:A:TYR:HE1	1:161:A:SER:HB2	2	0.5	0.01	0.5
(1,1913)	1:139:A:TYR:HE1	1:161:A:SER:HB3	2	0.5	0.01	0.5
(1,1913)	1:139:A:TYR:HE2	1:161:A:SER:HB2	2	0.5	0.01	0.5
(1,1913)	1:139:A:TYR:HE2	1:161:A:SER:HB3	2	0.5	0.01	0.5
(1,3782)	1:194:B:LYS:HB2	1:212:B:TYR:HD1	2	0.5	0.01	0.5
(1,3782)	1:194:B:LYS:HB2	1:212:B:TYR:HD2	2	0.5	0.01	0.5
(1,3782)	1:194:B:LYS:HB3	1:212:B:TYR:HD1	2	0.5	0.01	0.5
(1,3782)	1:194:B:LYS:HB3	1:212:B:TYR:HD2	2	0.5	0.01	0.5
(1,1154)	1:60:B:PHE:HB2	1:63:B:GLN:HE21	2	0.5	0.1	0.5
(1,1154)	1:60:B:PHE:HB2	1:63:B:GLN:HE22	2	0.5	0.1	0.5
(1,1154)	1:60:B:PHE:HB3	1:63:B:GLN:HE21	2	0.5	0.1	0.5
(1,1154)	1:60:B:PHE:HB3	1:63:B:GLN:HE22	2	0.5	0.1	0.5
(1,2872)	1:107:B:MET:HA	1:111:B:LYS:H	2	0.49	0.39	0.49
(1,1075)	1:50:B:ALA:H	1:51:B:VAL:H	2	0.48	0.38	0.48
(1,1494)	1:102:A:ALA:H	1:105:A:LEU:H	2	0.48	0.02	0.48
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG21	2	0.48	0.05	0.48
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG22	2	0.48	0.05	0.48
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG23	2	0.48	0.05	0.48
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG21	2	0.48	0.05	0.48
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG22	2	0.48	0.05	0.48
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG23	2	0.48	0.05	0.48
(1,1364)	1:40:A:ILE:HG12	1:36:B:ALA:HA	2	0.48	0.26	0.48
(1,1364)	1:40:A:ILE:HG13	1:36:B:ALA:HA	2	0.48	0.26	0.48
(1,1064)	1:48:B:ARG:H	1:50:B:ALA:H	2	0.47	0.26	0.47
(1,1814)	1:129:A:ILE:HA	1:135:A:ASN:H	2	0.47	0.23	0.47
(1,3168)	1:136:B:ALA:HA	1:162:B:ALA:HA	2	0.47	0.06	0.47
(1,2356)	1:181:A:TYR:HA	1:184:A:GLY:H	2	0.46	0.08	0.46
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD11	2	0.46	0.12	0.46
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD12	2	0.46	0.12	0.46
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD13	2	0.46	0.12	0.46
(1,1403)	1:62:A:GLY:H	1:67:B:ASP:HA	2	0.45	0.01	0.45
(1,1735)	1:122:A:ILE:HA	1:126:A:THR:H	2	0.45	0.11	0.45
(1,1394)	1:44:A:PHE:HE1	1:25:B:ILE:HD12	2	0.45	0.04	0.45
(1,1394)	1:44:A:PHE:HE2	1:25:B:ILE:HD12	2	0.45	0.04	0.45
(1,2227)	1:170:A:PHE:HD1	1:196:A:VAL:HA	2	0.45	0.24	0.45
(1,2227)	1:170:A:PHE:HD2	1:196:A:VAL:HA	2	0.45	0.24	0.45
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD11	2	0.44	0.09	0.44
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD12	2	0.44	0.09	0.44
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD13	2	0.44	0.09	0.44

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD11	2	0.44	0.09	0.44
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD12	2	0.44	0.09	0.44
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD13	2	0.44	0.09	0.44
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD11	2	0.44	0.29	0.44
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD12	2	0.44	0.29	0.44
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD13	2	0.44	0.29	0.44
(1,3781)	1:194:B:LYS:HA	1:198:B:ASP:H	2	0.44	0.19	0.44
(1,1201)	1:68:B:ILE:HA	1:70:B:ASN:H	2	0.44	0.03	0.44
(1,1483)	1:101:A:LYS:H	1:103:A:GLU:H	2	0.44	0.03	0.44
(1,2450)	1:193:A:TYR:HA	1:197:A:LEU:H	2	0.44	0.32	0.44
(1,2635)	1:214:A:SER:H	1:216:A:LYS:H	2	0.44	0.08	0.44
(1,1633)	1:113:A:MET:HA	1:116:A:LYS:HA	2	0.43	0.32	0.43
(1,1820)	1:129:A:ILE:HD11	1:139:A:TYR:HA	2	0.43	0.22	0.43
(1,1820)	1:129:A:ILE:HD12	1:139:A:TYR:HA	2	0.43	0.22	0.43
(1,1820)	1:129:A:ILE:HD13	1:139:A:TYR:HA	2	0.43	0.22	0.43
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB1	2	0.43	0.04	0.43
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB2	2	0.43	0.04	0.43
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB3	2	0.43	0.04	0.43
(1,14)	1:4:A:SER:H	1:7:A:GLU:H	2	0.43	0.13	0.43
(1,155)	1:15:A:TYR:HA	1:19:A:ILE:H	2	0.42	0.28	0.42
(1,226)	1:20:A:VAL:HA	1:24:A:GLU:H	2	0.42	0.26	0.42
(1,2164)	1:163:A:ILE:HA	1:169:A:TYR:H	2	0.42	0.16	0.42
(1,3549)	1:171:B:ARG:HA	1:174:B:SER:H	2	0.42	0.28	0.42
(1,2114)	1:158:A:ASP:HA	1:162:A:ALA:H	2	0.42	0.15	0.42
(1,1587)	1:109:A:GLY:HA2	1:121:A:ALA:H	2	0.42	0.28	0.42
(1,1587)	1:109:A:GLY:HA3	1:121:A:ALA:H	2	0.42	0.28	0.42
(1,1696)	1:118:A:TYR:HB2	1:148:A:SER:HB2	2	0.41	0.21	0.41
(1,1696)	1:118:A:TYR:HB2	1:148:A:SER:HB3	2	0.41	0.21	0.41
(1,1696)	1:118:A:TYR:HB3	1:148:A:SER:HB2	2	0.41	0.21	0.41
(1,1696)	1:118:A:TYR:HB3	1:148:A:SER:HB3	2	0.41	0.21	0.41
(1,1890)	1:138:A:TYR:HA	1:142:A:ARG:H	2	0.41	0.11	0.41
(1,2357)	1:181:A:TYR:HA	1:185:A:LYS:H	2	0.41	0.16	0.41
(1,1880)	1:137:A:ILE:HA	1:140:A:ALA:H	2	0.4	0.06	0.4
(1,3461)	1:162:B:ALA:HB1	1:172:B:GLY:H	2	0.4	0.19	0.4
(1,3461)	1:162:B:ALA:HB2	1:172:B:GLY:H	2	0.4	0.19	0.4
(1,3461)	1:162:B:ALA:HB3	1:172:B:GLY:H	2	0.4	0.19	0.4
(1,1398)	1:44:A:PHE:HE1	1:33:B:LEU:HD11	2	0.4	0.24	0.4
(1,1398)	1:44:A:PHE:HE2	1:33:B:LEU:HD11	2	0.4	0.24	0.4
(1,3303)	1:147:B:SER:H	1:151:B:GLU:H	2	0.4	0.1	0.4
(1,2591)	1:208:A:MET:HA	1:210:A:ARG:H	2	0.4	0.01	0.4
(1,4149)	1:241:B:SER:H	1:242:B:GLN:H	2	0.4	0.24	0.4
(1,762)	1:15:B:TYR:HA	1:18:B:SER:H	2	0.39	0.15	0.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3334)	1:150:B:LYS:HA	1:152:B:TYR:H	2	0.39	0.27	0.39
(1,3876)	1:206:B:GLU:HA	1:209:B:LYS:H	2	0.39	0.2	0.39
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD11	2	0.38	0.05	0.38
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD12	2	0.38	0.05	0.38
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD13	2	0.38	0.05	0.38
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD11	2	0.38	0.08	0.38
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD12	2	0.38	0.08	0.38
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD13	2	0.38	0.08	0.38
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD21	2	0.38	0.17	0.38
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD22	2	0.38	0.17	0.38
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD23	2	0.38	0.17	0.38
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG21	2	0.38	0.2	0.38
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG22	2	0.38	0.2	0.38
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG23	2	0.38	0.2	0.38
(1,776)	1:16:B:PHE:H	1:18:B:SER:H	2	0.38	0.26	0.38
(1,1390)	1:44:A:PHE:HE1	1:25:B:ILE:HB	2	0.38	0.01	0.38
(1,1390)	1:44:A:PHE:HE2	1:25:B:ILE:HB	2	0.38	0.01	0.38
(1,2007)	1:147:A:SER:HA	1:152:A:TYR:HA	2	0.38	0.08	0.38
(1,2090)	1:156:A:VAL:HA	1:176:A:LEU:HA	2	0.38	0.26	0.38
(1,3098)	1:127:B:GLU:HA	1:130:B:LYS:H	2	0.38	0.22	0.38
(1,3114)	1:129:B:ILE:H	1:138:B:TYR:HB2	2	0.38	0.18	0.38
(1,3114)	1:129:B:ILE:H	1:138:B:TYR:HB3	2	0.38	0.18	0.38
(1,3584)	1:174:B:SER:HA	1:178:B:PHE:H	2	0.38	0.26	0.38
(1,1534)	1:105:A:LEU:HA	1:107:A:MET:H	2	0.37	0.12	0.37
(1,1762)	1:125:A:TYR:HA	1:138:A:TYR:HA	2	0.37	0.18	0.37
(1,1074)	1:49:B:GLU:HA	1:51:B:VAL:H	2	0.36	0.01	0.36
(1,1641)	1:113:A:MET:HE1	1:141:A:ASN:HA	2	0.36	0.24	0.36
(1,1641)	1:113:A:MET:HE2	1:141:A:ASN:HA	2	0.36	0.24	0.36
(1,1641)	1:113:A:MET:HE3	1:141:A:ASN:HA	2	0.36	0.24	0.36
(1,3474)	1:163:B:ILE:HD11	1:176:B:LEU:H	2	0.36	0.12	0.36
(1,3474)	1:163:B:ILE:HD12	1:176:B:LEU:H	2	0.36	0.12	0.36
(1,3474)	1:163:B:ILE:HD13	1:176:B:LEU:H	2	0.36	0.12	0.36
(1,2294)	1:176:A:LEU:HD11	1:180:A:LYS:H	2	0.36	0.12	0.36
(1,2294)	1:176:A:LEU:HD12	1:180:A:LYS:H	2	0.36	0.12	0.36
(1,2294)	1:176:A:LEU:HD13	1:180:A:LYS:H	2	0.36	0.12	0.36
(1,948)	1:35:B:VAL:H	1:38:B:ASP:H	2	0.35	0.23	0.35
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG11	2	0.35	0.02	0.35
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG12	2	0.35	0.02	0.35
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG13	2	0.35	0.02	0.35
(1,2675)	1:218:A:LYS:HB2	1:219:A:VAL:H	2	0.35	0.06	0.35
(1,2675)	1:218:A:LYS:HB3	1:219:A:VAL:H	2	0.35	0.06	0.35
(1,3442)	1:160:B:GLU:HA	1:163:B:ILE:H	2	0.35	0.1	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB1	2	0.35	0.04	0.35
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB2	2	0.35	0.04	0.35
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB3	2	0.35	0.04	0.35
(1,1405)	1:63:A:GLN:H	1:67:B:ASP:HB2	2	0.34	0.04	0.34
(1,1405)	1:63:A:GLN:H	1:67:B:ASP:HB3	2	0.34	0.04	0.34
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE1	2	0.34	0.24	0.34
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE2	2	0.34	0.24	0.34
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE3	2	0.34	0.24	0.34
(1,1636)	1:113:A:MET:HA	1:121:A:ALA:H	2	0.34	0.08	0.34
(1,4041)	1:231:A:GLU:H	1:232:A:GLN:H	2	0.34	0.02	0.34
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD21	2	0.34	0.19	0.34
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD22	2	0.34	0.19	0.34
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD23	2	0.34	0.19	0.34
(1,2032)	1:150:A:LYS:HB2	1:152:A:TYR:HE1	2	0.34	0.2	0.34
(1,2032)	1:150:A:LYS:HB2	1:152:A:TYR:HE2	2	0.34	0.2	0.34
(1,2032)	1:150:A:LYS:HB3	1:152:A:TYR:HE1	2	0.34	0.2	0.34
(1,2032)	1:150:A:LYS:HB3	1:152:A:TYR:HE2	2	0.34	0.2	0.34
(1,3753)	1:193:B:TYR:HA	1:196:B:VAL:H	2	0.34	0.12	0.34
(1,1112)	1:55:B:LEU:HA	1:57:B:LYS:H	2	0.34	0.13	0.34
(1,4109)	1:344:A:ASN:H	1:345:A:LYS:H	2	0.34	0.14	0.34
(1,992)	1:40:B:ILE:H	1:42:B:GLU:H	2	0.33	0.01	0.33
(1,1638)	1:113:A:MET:HB2	1:125:A:TYR:HE1	2	0.33	0.08	0.33
(1,1638)	1:113:A:MET:HB2	1:125:A:TYR:HE2	2	0.33	0.08	0.33
(1,1638)	1:113:A:MET:HB3	1:125:A:TYR:HE1	2	0.33	0.08	0.33
(1,1638)	1:113:A:MET:HB3	1:125:A:TYR:HE2	2	0.33	0.08	0.33
(1,2894)	1:110:B:ASN:H	1:113:B:MET:H	2	0.33	0.04	0.33
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD21	2	0.32	0.12	0.32
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD22	2	0.32	0.12	0.32
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD23	2	0.32	0.12	0.32
(1,1635)	1:113:A:MET:HA	1:118:A:TYR:HA	2	0.32	0.08	0.32
(1,3597)	1:176:B:LEU:HA	1:178:B:PHE:H	2	0.32	0.12	0.32
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD11	2	0.32	0.14	0.32
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD12	2	0.32	0.14	0.32
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD13	2	0.32	0.14	0.32
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD11	2	0.32	0.15	0.32
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD12	2	0.32	0.15	0.32
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD13	2	0.32	0.15	0.32
(1,2836)	1:105:B:LEU:H	1:107:B:MET:H	2	0.32	0.04	0.32
(1,2304)	1:177:A:GLY:HA2	1:189:A:ALA:H	2	0.31	0.11	0.31
(1,2304)	1:177:A:GLY:HA3	1:189:A:ALA:H	2	0.31	0.11	0.31
(1,3748)	1:193:B:TYR:H	1:196:B:VAL:H	2	0.31	0.04	0.31
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD11	2	0.3	0.01	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD12	2	0.3	0.01	0.3
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD13	2	0.3	0.01	0.3
(1,1178)	1:65:B:LEU:HA	1:66:B:ALA:HA	2	0.3	0.01	0.3
(1,1909)	1:139:A:TYR:HD1	1:162:A:ALA:H	2	0.3	0.08	0.3
(1,1909)	1:139:A:TYR:HD2	1:162:A:ALA:H	2	0.3	0.08	0.3
(1,2105)	1:157:A:LYS:HA	1:160:A:GLU:H	2	0.3	0.15	0.3
(1,1229)	1:2:A:SER:HB2	1:69:B:LEU:H	2	0.29	0.15	0.29
(1,1229)	1:2:A:SER:HB3	1:69:B:LEU:H	2	0.29	0.15	0.29
(1,1768)	1:125:A:TYR:HB2	1:142:A:ARG:H	2	0.29	0.15	0.29
(1,1768)	1:125:A:TYR:HB3	1:142:A:ARG:H	2	0.29	0.15	0.29
(1,3194)	1:138:B:TYR:HA	1:140:B:ALA:H	2	0.29	0.11	0.29
(1,3605)	1:177:B:GLY:H	1:180:B:LYS:H	2	0.29	0.04	0.29
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD11	2	0.29	0.08	0.29
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD12	2	0.29	0.08	0.29
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD13	2	0.29	0.08	0.29
(1,1627)	1:113:A:MET:H	1:121:A:ALA:HA	2	0.29	0.12	0.29
(1,728)	1:13:B:VAL:HA	1:37:B:MET:HB2	2	0.28	0.1	0.28
(1,728)	1:13:B:VAL:HA	1:37:B:MET:HB3	2	0.28	0.1	0.28
(1,876)	1:26:B:SER:HA	1:28:B:ASP:H	2	0.28	0.01	0.28
(1,1802)	1:128:A:ALA:HA	1:132:A:LEU:H	2	0.28	0.16	0.28
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB1	2	0.27	0.14	0.27
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB2	2	0.27	0.14	0.27
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB3	2	0.27	0.14	0.27
(1,3054)	1:124:B:LYS:H	1:127:B:GLU:H	2	0.27	0.16	0.27
(1,482)	1:52:A:SER:HA	1:55:A:LEU:H	2	0.26	0.14	0.26
(1,1290)	1:16:A:PHE:HE1	1:12:B:ILE:HD13	2	0.26	0.06	0.26
(1,1290)	1:16:A:PHE:HE2	1:12:B:ILE:HD13	2	0.26	0.06	0.26
(1,2398)	1:188:A:GLU:HA	1:191:A:GLU:H	2	0.26	0.09	0.26
(1,3671)	1:181:B:TYR:HE1	1:218:B:LYS:HB2	2	0.26	0.06	0.26
(1,3671)	1:181:B:TYR:HE1	1:218:B:LYS:HB3	2	0.26	0.06	0.26
(1,3671)	1:181:B:TYR:HE2	1:218:B:LYS:HB2	2	0.26	0.06	0.26
(1,3671)	1:181:B:TYR:HE2	1:218:B:LYS:HB3	2	0.26	0.06	0.26
(1,4062)	1:254:A:SER:H	1:255:A:LEU:H	2	0.26	0.1	0.26
(1,984)	1:39:B:CYS:H	1:42:B:GLU:H	2	0.26	0.14	0.26
(1,1552)	1:106:A:LYS:HA	1:108:A:GLN:H	2	0.26	0.12	0.26
(1,3058)	1:124:B:LYS:HA	1:127:B:GLU:H	2	0.26	0.02	0.26
(1,3262)	1:143:B:ALA:HB1	1:155:B:ALA:HA	2	0.26	0.08	0.26
(1,3262)	1:143:B:ALA:HB2	1:155:B:ALA:HA	2	0.26	0.08	0.26
(1,3262)	1:143:B:ALA:HB3	1:155:B:ALA:HA	2	0.26	0.08	0.26
(1,505)	1:55:A:LEU:HD11	1:71:A:SER:HA	2	0.25	0.15	0.25
(1,505)	1:55:A:LEU:HD12	1:71:A:SER:HA	2	0.25	0.15	0.25
(1,505)	1:55:A:LEU:HD13	1:71:A:SER:HA	2	0.25	0.15	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1164)	1:62:B:GLY:H	1:63:B:GLN:HA	2	0.25	0.03	0.25
(1,178)	1:16:A:PHE:HA	1:20:A:VAL:H	2	0.24	0.03	0.24
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD11	2	0.24	0.06	0.24
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD12	2	0.24	0.06	0.24
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD13	2	0.24	0.06	0.24
(1,1301)	1:19:A:ILE:HD11	1:5:B:LYS:HA	2	0.24	0.03	0.24
(1,1301)	1:19:A:ILE:HD12	1:5:B:LYS:HA	2	0.24	0.03	0.24
(1,1301)	1:19:A:ILE:HD13	1:5:B:LYS:HA	2	0.24	0.03	0.24
(1,3124)	1:129:B:ILE:HD11	1:138:B:TYR:HD2	2	0.24	0.02	0.24
(1,3124)	1:129:B:ILE:HD12	1:138:B:TYR:HD2	2	0.24	0.02	0.24
(1,3124)	1:129:B:ILE:HD13	1:138:B:TYR:HD2	2	0.24	0.02	0.24
(1,4089)	1:322:A:ASN:H	1:323:A:MET:H	2	0.24	0.03	0.24
(1,3248)	1:142:B:ARG:HA	1:145:B:ALA:H	2	0.24	0.04	0.24
(1,3186)	1:137:B:ILE:HA	1:140:B:ALA:H	2	0.24	0.11	0.24
(1,224)	1:20:A:VAL:HA	1:23:A:LYS:H	2	0.24	0.05	0.24
(1,1752)	1:124:A:LYS:HA	1:127:A:GLU:H	2	0.24	0.06	0.24
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD11	2	0.23	0.11	0.23
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD12	2	0.23	0.11	0.23
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD13	2	0.23	0.11	0.23
(1,2558)	1:205:A:THR:HA	1:207:A:ALA:H	2	0.23	0.04	0.23
(1,3583)	1:174:B:SER:HA	1:177:B:GLY:H	2	0.23	0.0	0.23
(1,3509)	1:169:B:TYR:HE1	1:172:B:GLY:H	2	0.23	0.06	0.23
(1,3509)	1:169:B:TYR:HE2	1:172:B:GLY:H	2	0.23	0.06	0.23
(1,3627)	1:178:B:PHE:HA	1:193:B:TYR:HE1	2	0.22	0.05	0.22
(1,3627)	1:178:B:PHE:HA	1:193:B:TYR:HE2	2	0.22	0.05	0.22
(1,3948)	1:214:B:SER:HB2	1:215:B:ALA:H	2	0.22	0.05	0.22
(1,3948)	1:214:B:SER:HB3	1:215:B:ALA:H	2	0.22	0.05	0.22
(1,725)	1:13:B:VAL:HA	1:16:B:PHE:H	2	0.22	0.02	0.22
(1,2206)	1:169:A:TYR:HE2	1:171:A:ARG:HB2	2	0.22	0.1	0.22
(1,2206)	1:169:A:TYR:HE2	1:171:A:ARG:HB3	2	0.22	0.1	0.22
(1,3118)	1:129:B:ILE:HA	1:132:B:LEU:H	2	0.22	0.02	0.22
(1,3822)	1:198:B:ASP:HA	1:200:B:GLU:H	2	0.22	0.08	0.22
(1,3325)	1:149:B:LEU:H	1:151:B:GLU:H	2	0.22	0.12	0.22
(1,896)	1:29:B:GLY:H	1:32:B:SER:H	2	0.22	0.08	0.22
(1,286)	1:29:A:GLY:H	1:31:A:ASP:H	2	0.21	0.05	0.21
(1,854)	1:22:B:LYS:HA	1:24:B:GLU:H	2	0.21	0.07	0.21
(1,1680)	1:118:A:TYR:H	1:120:A:LEU:H	2	0.21	0.01	0.21
(1,4091)	1:324:A:ALA:H	1:325:A:GLY:H	2	0.21	0.06	0.21
(1,310)	1:31:A:ASP:HA	1:35:A:VAL:H	2	0.21	0.09	0.21
(1,375)	1:39:A:CYS:H	1:42:A:GLU:H	2	0.21	0.1	0.21
(1,325)	1:33:A:LEU:HA	1:37:A:MET:H	2	0.2	0.03	0.2
(1,381)	1:39:A:CYS:HA	1:43:A:ALA:H	2	0.2	0.06	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1311)	1:25:A:ILE:HD11	1:44:B:PHE:HA	2	0.2	0.03	0.2
(1,1311)	1:25:A:ILE:HD12	1:44:B:PHE:HA	2	0.2	0.03	0.2
(1,1311)	1:25:A:ILE:HD13	1:44:B:PHE:HA	2	0.2	0.03	0.2
(1,1755)	1:125:A:TYR:H	1:128:A:ALA:H	2	0.2	0.06	0.2
(1,3419)	1:158:B:ASP:HA	1:161:B:SER:H	2	0.2	0.0	0.2
(1,4074)	1:303:A:ALA:H	1:304:A:SER:H	2	0.2	0.02	0.2
(1,1440)	1:95:A:ASP:H	1:96:A:ALA:H	2	0.2	0.02	0.2
(1,4044)	1:234:A:ARG:H	1:235:A:ASP:H	2	0.2	0.02	0.2
(1,1642)	1:113:A:MET:HE1	1:142:A:ARG:HA	2	0.19	0.02	0.19
(1,1642)	1:113:A:MET:HE2	1:142:A:ARG:HA	2	0.19	0.02	0.19
(1,1642)	1:113:A:MET:HE3	1:142:A:ARG:HA	2	0.19	0.02	0.19
(1,2512)	1:198:A:ASP:H	1:200:A:GLU:H	2	0.19	0.02	0.19
(1,524)	1:58:A:SER:HB2	1:60:A:PHE:H	2	0.18	0.02	0.18
(1,524)	1:58:A:SER:HB3	1:60:A:PHE:H	2	0.18	0.02	0.18
(1,1713)	1:120:A:LEU:HA	1:123:A:ASN:H	2	0.18	0.02	0.18
(1,3645)	1:180:B:LYS:HA	1:183:B:GLN:H	2	0.18	0.04	0.18
(1,2278)	1:174:A:SER:HA	1:178:A:PHE:H	2	0.18	0.04	0.18
(1,536)	1:60:A:PHE:HA	1:62:A:GLY:H	2	0.17	0.0	0.17
(1,1796)	1:128:A:ALA:H	1:131:A:VAL:H	2	0.17	0.01	0.17
(1,4054)	1:244:A:ALA:H	1:245:A:SER:H	2	0.17	0.04	0.17
(1,201)	1:17:A:SER:HA	1:21:A:GLU:H	2	0.16	0.04	0.16
(1,1721)	1:121:A:ALA:HA	1:125:A:TYR:H	2	0.16	0.04	0.16
(1,2642)	1:214:A:SER:HB2	1:215:A:ALA:H	2	0.16	0.02	0.16
(1,2642)	1:214:A:SER:HB3	1:215:A:ALA:H	2	0.16	0.02	0.16
(1,2795)	1:101:B:LYS:HA	1:103:B:GLU:H	2	0.16	0.01	0.16
(1,1125)	1:57:B:LYS:HB2	1:58:B:SER:H	2	0.15	0.02	0.15
(1,1125)	1:57:B:LYS:HB3	1:58:B:SER:H	2	0.15	0.02	0.15
(1,2061)	1:152:A:TYR:HD2	1:183:A:GLN:HG2	2	0.15	0.01	0.15
(1,2648)	1:215:A:ALA:HA	1:217:A:LYS:H	2	0.15	0.01	0.15
(1,4063)	1:255:A:LEU:H	1:256:A:LEU:H	2	0.15	0.01	0.15
(1,503)	1:55:A:LEU:HA	1:57:A:LYS:H	2	0.15	0.04	0.15
(1,2501)	1:197:A:LEU:HA	1:199:A:ILE:H	2	0.15	0.02	0.15
(1,2562)	1:205:A:THR:HG21	1:208:A:MET:HG2	2	0.15	0.0	0.15
(1,2562)	1:205:A:THR:HG21	1:208:A:MET:HG3	2	0.15	0.0	0.15
(1,2562)	1:205:A:THR:HG22	1:208:A:MET:HG2	2	0.15	0.0	0.15
(1,2562)	1:205:A:THR:HG22	1:208:A:MET:HG3	2	0.15	0.0	0.15
(1,2562)	1:205:A:THR:HG23	1:208:A:MET:HG2	2	0.15	0.0	0.15
(1,2562)	1:205:A:THR:HG23	1:208:A:MET:HG3	2	0.15	0.0	0.15
(1,2716)	1:224:A:ASN:H	1:226:A:GLU:H	2	0.14	0.03	0.14
(1,3502)	1:169:B:TYR:HD1	1:170:B:PHE:H	2	0.14	0.04	0.14
(1,3502)	1:169:B:TYR:HD2	1:170:B:PHE:H	2	0.14	0.04	0.14
(1,239)	1:21:A:GLU:HB2	1:22:A:LYS:H	2	0.14	0.02	0.14

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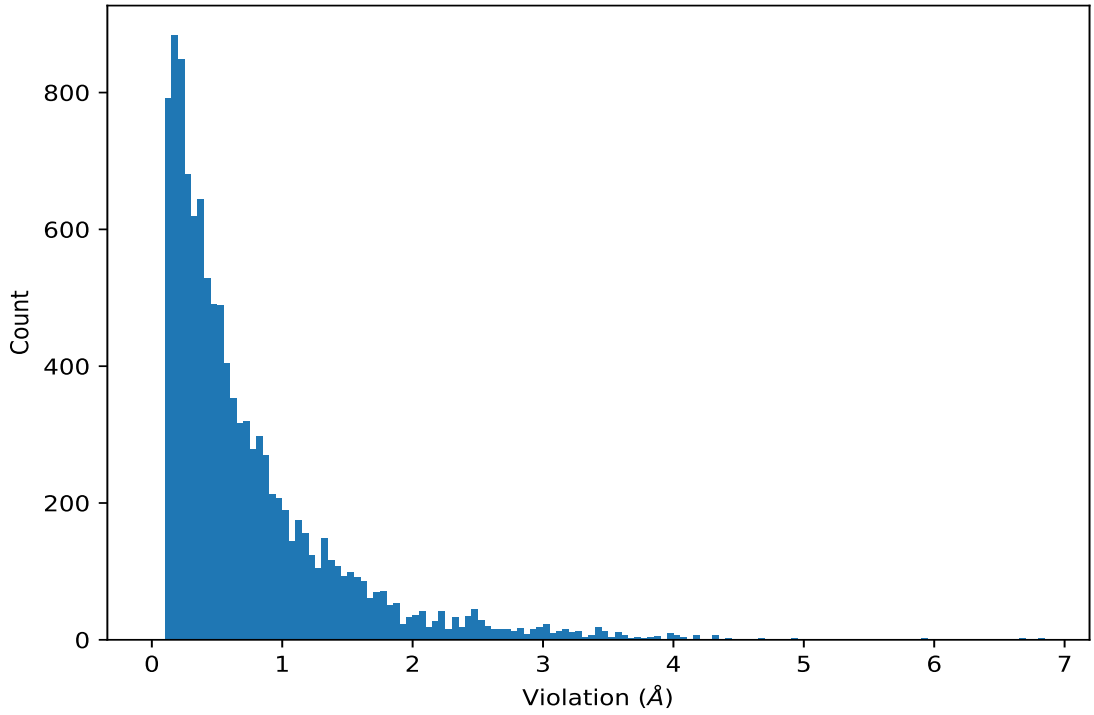
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,239)	1:21:A:GLU:HB3	1:22:A:LYS:H	2	0.14	0.02	0.14
(1,275)	1:27:A:GLU:HA	1:30:A:ALA:H	2	0.14	0.04	0.14
(1,1517)	1:103:A:GLU:HA	1:105:A:LEU:H	2	0.12	0.02	0.12
(1,2039)	1:151:A:GLU:H	1:152:A:TYR:HA	2	0.12	0.0	0.12
(1,1157)	1:60:B:PHE:HD1	1:61:B:LYS:H	2	0.11	0.0	0.11
(1,1157)	1:60:B:PHE:HD2	1:61:B:LYS:H	2	0.11	0.0	0.11
(1,2899)	1:110:B:ASN:HA	1:113:B:MET:H	2	0.11	0.0	0.11
(1,3089)	1:126:B:THR:HA	1:129:B:ILE:H	2	0.11	0.0	0.11
(1,3400)	1:156:B:VAL:HG11	1:160:B:GLU:H	2	0.11	0.0	0.11
(1,3400)	1:156:B:VAL:HG12	1:160:B:GLU:H	2	0.11	0.0	0.11
(1,3400)	1:156:B:VAL:HG13	1:160:B:GLU: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 (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	19	6.83
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	19	6.83
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	10	6.65
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	10	6.65
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	2	5.93
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	2	5.93
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	9	5.19
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	19	5.01
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	7	4.9
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	7	4.9
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	18	4.7
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	12	4.67
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	17	4.66
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	5	4.44
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	5	4.44
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	18	4.34
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	18	4.34
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	9	4.34
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	9	4.34
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	9	4.34
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	19	4.32
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	14	4.18
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	10	4.17
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	10	4.17
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	8	4.15
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	8	4.15
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	5	4.15
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	5	4.15
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	3	4.09
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	3	4.09
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	3	4.09
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	19	4.03
(1,3812)	1:197:B:LEU:HD11	1:209:B:LYS:HA	18	4.01
(1,3812)	1:197:B:LEU:HD12	1:209:B:LYS:HA	18	4.01
(1,3812)	1:197:B:LEU:HD13	1:209:B:LYS:HA	18	4.01
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	14	4.01
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	14	4.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	2	4.01
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	8	3.98
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	2	3.97
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	2	3.97
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	2	3.97
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	12	3.95
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	12	3.95
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	10	3.95
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	10	3.95
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	10	3.95
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	10	3.95
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	9	3.89
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	9	3.89
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	9	3.89
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	10	3.87
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	10	3.87
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	3	3.82
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	3	3.82
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	1	3.8
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	1	3.8
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	2	3.78
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	3	3.75
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	20	3.74
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	9	3.74
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	2	3.73
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	2	3.73
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	18	3.67
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	18	3.67
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	3	3.62
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	3	3.62
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	3	3.62
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	18	3.6
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	18	3.6
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	18	3.6
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB1	19	3.59
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB2	19	3.59
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB3	19	3.59
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	7	3.59
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	7	3.59
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	7	3.59
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	7	3.59
(1,3650)	1:180:B:LYS:HB2	1:188:B:GLU:HB2	11	3.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3650)	1:180:B:LYS:HB2	1:188:B:GLU:HB3	11	3.58
(1,3650)	1:180:B:LYS:HB3	1:188:B:GLU:HB2	11	3.58
(1,3650)	1:180:B:LYS:HB3	1:188:B:GLU:HB3	11	3.58
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	19	3.52
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	3	3.51
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	3	3.51
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	9	3.49
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	9	3.49
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD11	11	3.48
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD12	11	3.48
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD13	11	3.48
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	17	3.47
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	17	3.47
(1,2952)	1:113:B:MET:HE1	1:145:B:ALA:HA	3	3.46
(1,2952)	1:113:B:MET:HE2	1:145:B:ALA:HA	3	3.46
(1,2952)	1:113:B:MET:HE3	1:145:B:ALA:HA	3	3.46
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	15	3.46
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	2	3.45
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	2	3.45
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	8	3.44
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	8	3.44
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	20	3.43
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	20	3.43
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	15	3.42
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	15	3.42
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	15	3.42
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	12	3.41
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	12	3.41
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB1	5	3.41
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB2	5	3.41
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB3	5	3.41
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	9	3.41
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	9	3.41
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	9	3.41
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	19	3.4
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	15	3.4
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	2	3.4
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	12	3.39
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	20	3.38
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	20	3.38
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	19	3.38
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	12	3.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	12	3.36
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	3	3.33
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	2	3.31
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	9	3.3
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	9	3.3
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	9	3.28
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	9	3.28
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	9	3.28
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	5	3.27
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	3	3.26
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	14	3.26
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	14	3.26
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	17	3.26
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	17	3.26
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	17	3.26
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	17	3.26
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	8	3.25
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	8	3.24
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	10	3.24
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	10	3.24
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	6	3.24
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	6	3.24
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	2	3.23
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	2	3.23
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	6	3.22
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	6	3.22
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	1	3.2
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	1	3.2
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB2	2	3.19
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB3	2	3.19
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB2	2	3.19
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB3	2	3.19
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	15	3.19
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	15	3.19
(1,2850)	1:105:B:LEU:HD21	1:124:B:LYS:HA	3	3.17
(1,2850)	1:105:B:LEU:HD22	1:124:B:LYS:HA	3	3.17
(1,2850)	1:105:B:LEU:HD23	1:124:B:LYS:HA	3	3.17
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	17	3.17
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	17	3.17
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	14	3.16
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	14	3.15
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	14	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	14	3.15
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	14	3.15
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	2	3.14
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	12	3.13
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE1	7	3.12
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE2	7	3.12
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE3	7	3.12
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE1	7	3.12
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE2	7	3.12
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE3	7	3.12
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	5	3.12
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	5	3.12
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	18	3.12
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	11	3.11
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	11	3.11
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	16	3.09
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	16	3.09
(1,3665)	1:181:B:TYR:HA	1:189:B:ALA:H	11	3.07
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	17	3.07
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	13	3.07
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	13	3.07
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	2	3.07
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	2	3.07
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	9	3.05
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	18	3.04
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	18	3.04
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	18	3.04
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	2	3.02
(1,1248)	1:9:A:ALA:H	1:16:B:PHE:HZ	3	3.02
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	15	3.02
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	15	3.02
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	15	3.02
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	3	3.01
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	3	3.01
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	3	3.01
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	17	3.0
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	13	3.0
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG21	8	3.0
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG22	8	3.0
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG23	8	3.0
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG21	8	3.0
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG22	8	3.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG23	8	3.0
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG21	8	3.0
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG22	8	3.0
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG23	8	3.0
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD21	3	2.99
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD22	3	2.99
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD23	3	2.99
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	13	2.99
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	13	2.98
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	6	2.98
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	6	2.98
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	6	2.98
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	12	2.97
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	12	2.97
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	12	2.97
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB2	3	2.97
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB3	3	2.97
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB2	3	2.97
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB3	3	2.97
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	13	2.96
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	13	2.96
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	13	2.96
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	4	2.94
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	6	2.94
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	6	2.94
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	6	2.94
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	6	2.94
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	7	2.93
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	7	2.93
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	11	2.92
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	9	2.92
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	9	2.92
(1,1113)	1:55:B:LEU:HA	1:58:B:SER:H	17	2.91
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	12	2.9
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	12	2.9
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	19	2.9
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	19	2.9
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	2	2.87
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	2	2.87
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	3	2.87
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	3	2.87
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	3	2.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	3	2.87
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	16	2.86
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	16	2.86
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	19	2.84
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	15	2.83
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	15	2.83
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	15	2.83
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	5	2.82
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	15	2.82
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	1	2.82
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	1	2.82
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	18	2.82
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	2	2.82
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	2	2.82
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	2	2.82
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	9	2.81
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	12	2.8
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	12	2.8
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	12	2.8
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	12	2.8
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	6	2.79
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	6	2.79
(1,3970)	1:217:B:LYS:HA	1:220:B:GLU:H	3	2.78
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	14	2.78
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	11	2.77
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	8	2.77
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	8	2.77
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	18	2.77
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	12	2.76
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	12	2.76
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	13	2.75
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	13	2.75
(1,1427)	1:69:A:LEU:HD11	1:2:B:SER:HG	10	2.74
(1,1427)	1:69:A:LEU:HD12	1:2:B:SER:HG	10	2.74
(1,1427)	1:69:A:LEU:HD13	1:2:B:SER:HG	10	2.74
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	7	2.73
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	7	2.73
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	18	2.72
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	18	2.72
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	16	2.71
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	16	2.71
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	10	2.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	3	2.7
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	3	2.7
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	3	2.7
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	19	2.7
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	19	2.7
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	19	2.7
(1,3656)	1:181:B:TYR:H	1:189:B:ALA:H	11	2.69
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	16	2.67
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	16	2.67
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	16	2.67
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	15	2.67
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	15	2.67
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	16	2.66
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	16	2.66
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	18	2.66
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	9	2.65
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	9	2.65
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	9	2.65
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	9	2.65
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	12	2.65
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	3	2.65
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	14	2.64
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	14	2.64
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD21	11	2.63
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD22	11	2.63
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD23	11	2.63
(1,1544)	1:105:A:LEU:HD21	1:124:A:LYS:HA	3	2.63
(1,1544)	1:105:A:LEU:HD22	1:124:A:LYS:HA	3	2.63
(1,1544)	1:105:A:LEU:HD23	1:124:A:LYS:HA	3	2.63
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	6	2.62
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	6	2.62
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	18	2.61
(1,2796)	1:101:B:LYS:HA	1:104:B:ASP:H	19	2.61
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	1	2.61
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	1	2.61
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	8	2.61
(1,3542)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	10	2.6
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	13	2.59
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	13	2.59
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	13	2.58
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	20	2.58
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	20	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	4	2.58
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	4	2.58
(1,2948)	1:113:B:MET:HE1	1:142:B:ARG:HA	3	2.57
(1,2948)	1:113:B:MET:HE2	1:142:B:ARG:HA	3	2.57
(1,2948)	1:113:B:MET:HE3	1:142:B:ARG:HA	3	2.57
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	18	2.57
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB2	10	2.57
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB3	10	2.57
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	9	2.56
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	9	2.56
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	9	2.56
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	9	2.56
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	2	2.55
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	4	2.55
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	4	2.55
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	18	2.54
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	2	2.54
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	4	2.54
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	4	2.54
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG11	12	2.53
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG12	12	2.53
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG13	12	2.53
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	19	2.53
(1,2948)	1:113:B:MET:HE1	1:142:B:ARG:HA	15	2.52
(1,2948)	1:113:B:MET:HE2	1:142:B:ARG:HA	15	2.52
(1,2948)	1:113:B:MET:HE3	1:142:B:ARG:HA	15	2.52
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	8	2.52
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	8	2.52
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	17	2.52
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	17	2.52
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB1	3	2.51
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB2	3	2.51
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB3	3	2.51
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB1	3	2.51
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB2	3	2.51
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB3	3	2.51
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB1	3	2.51
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB2	3	2.51
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB3	3	2.51
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	3	2.5
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	3	2.5
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	3	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	8	2.5
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	3	2.49
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	3	2.49
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	16	2.49
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	16	2.49
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	16	2.49
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	16	2.49
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	11	2.48
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	13	2.48
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	13	2.48
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	13	2.48
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	13	2.48
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	13	2.48
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	13	2.48
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	15	2.48
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	15	2.48
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD11	11	2.48
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD12	11	2.48
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD13	11	2.48
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	8	2.48
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	1	2.48
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	1	2.48
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	4	2.48
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	4	2.48
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	16	2.47
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	16	2.47
(1,1022)	1:43:B:ALA:H	1:45:B:GLY:H	16	2.47
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	15	2.47
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	15	2.47
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	10	2.46
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	13	2.46
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	13	2.46
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	13	2.46
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	5	2.46
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	5	2.46
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG21	11	2.45
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG22	11	2.45
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG23	11	2.45
(1,2952)	1:113:B:MET:HE1	1:145:B:ALA:HA	15	2.45
(1,2952)	1:113:B:MET:HE2	1:145:B:ALA:HA	15	2.45
(1,2952)	1:113:B:MET:HE3	1:145:B:ALA:HA	15	2.45
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	7	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	15	2.45
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	15	2.45
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	1	2.45
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	11	2.43
(1,2844)	1:105:B:LEU:HD11	1:127:B:GLU:HA	3	2.43
(1,2844)	1:105:B:LEU:HD12	1:127:B:GLU:HA	3	2.43
(1,2844)	1:105:B:LEU:HD13	1:127:B:GLU:HA	3	2.43
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG21	3	2.43
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG22	3	2.43
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG23	3	2.43
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG21	3	2.43
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG22	3	2.43
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG23	3	2.43
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG21	3	2.43
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG22	3	2.43
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG23	3	2.43
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	1	2.43
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	1	2.43
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	16	2.43
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	16	2.43
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	16	2.43
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	16	2.43
(1,1248)	1:9:A:ALA:H	1:16:B:PHE:HZ	17	2.43
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	1	2.43
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	1	2.43
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	1	2.43
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	19	2.42
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	18	2.42
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	18	2.42
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	7	2.41
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	7	2.41
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	17	2.4
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	17	2.4
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	3	2.4
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	20	2.4
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	20	2.4
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	3	2.4
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	12	2.39
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	11	2.39
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	11	2.39
(1,2750)	1:95:B:ASP:HA	1:97:B:GLU:H	20	2.38
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	18	2.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	11	2.37
(1,1417)	1:68:A:ILE:HA	1:2:B:SER:HB2	10	2.37
(1,1417)	1:68:A:ILE:HA	1:2:B:SER:HB3	10	2.37
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE1	17	2.36
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE2	17	2.36
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE3	17	2.36
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	10	2.36
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	10	2.36
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB2	20	2.36
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB3	20	2.36
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	19	2.36
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	19	2.36
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	19	2.36
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	20	2.36
(1,3130)	1:129:B:ILE:HD11	1:142:B:ARG:HB2	19	2.34
(1,3130)	1:129:B:ILE:HD11	1:142:B:ARG:HB3	19	2.34
(1,3130)	1:129:B:ILE:HD12	1:142:B:ARG:HB2	19	2.34
(1,3130)	1:129:B:ILE:HD12	1:142:B:ARG:HB3	19	2.34
(1,3130)	1:129:B:ILE:HD13	1:142:B:ARG:HB2	19	2.34
(1,3130)	1:129:B:ILE:HD13	1:142:B:ARG:HB3	19	2.34
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	9	2.34
(1,1856)	1:135:A:ASN:HB3	1:138:A:TYR:HE2	14	2.34
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	10	2.34
(1,1025)	1:43:B:ALA:HA	1:45:B:GLY:H	16	2.34
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	11	2.33
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	8	2.33
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	17	2.33
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	17	2.33
(1,3966)	1:217:B:LYS:H	1:220:B:GLU:H	3	2.31
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	12	2.31
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	8	2.31
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	8	2.31
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	8	2.31
(1,2261)	1:173:A:TYR:HA	1:192:A:ALA:HA	8	2.31
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	6	2.31
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	17	2.31
(1,3657)	1:181:B:TYR:H	1:189:B:ALA:HA	11	2.3
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG2	3	2.3
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG21	7	2.3
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG22	7	2.3
(1,2424)	1:190:A:LEU:HD21	1:219:A:VAL:HG23	7	2.3
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG21	7	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG22	7	2.3
(1,2424)	1:190:A:LEU:HD22	1:219:A:VAL:HG23	7	2.3
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG21	7	2.3
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG22	7	2.3
(1,2424)	1:190:A:LEU:HD23	1:219:A:VAL:HG23	7	2.3
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	14	2.29
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	14	2.29
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	14	2.29
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	3	2.29
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	9	2.28
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	9	2.28
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	9	2.28
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	9	2.28
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	13	2.28
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	9	2.27
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	12	2.27
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	3	2.26
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	3	2.26
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	19	2.26
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	11	2.25
(1,1537)	1:105:A:LEU:HA	1:124:A:LYS:HA	3	2.25
(1,2850)	1:105:B:LEU:HD21	1:124:B:LYS:HA	18	2.24
(1,2850)	1:105:B:LEU:HD22	1:124:B:LYS:HA	18	2.24
(1,2850)	1:105:B:LEU:HD23	1:124:B:LYS:HA	18	2.24
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	7	2.24
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	7	2.24
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	2	2.24
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	2	2.24
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	11	2.23
(1,1288)	1:16:A:PHE:HE1	1:12:B:ILE:HD11	20	2.23
(1,1288)	1:16:A:PHE:HE2	1:12:B:ILE:HD11	20	2.23
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE1	12	2.22
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE2	12	2.22
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE1	12	2.22
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE2	12	2.22
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	2	2.22
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	2	2.22
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	12	2.22
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	12	2.22
(1,1140)	1:59:B:GLU:HB2	1:64:B:HIS:HA	5	2.22
(1,1140)	1:59:B:GLU:HB3	1:64:B:HIS:HA	5	2.22
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	2	2.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	2	2.22
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	2	2.22
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	18	2.22
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	18	2.22
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	5	2.21
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	8	2.21
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	9	2.21
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	9	2.21
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	9	2.21
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	15	2.21
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	15	2.21
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	10	2.21
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	10	2.21
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	10	2.21
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	7	2.21
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	7	2.21
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	3	2.2
(1,2423)	1:190:A:LEU:HD21	1:216:A:LYS:HA	8	2.2
(1,2423)	1:190:A:LEU:HD22	1:216:A:LYS:HA	8	2.2
(1,2423)	1:190:A:LEU:HD23	1:216:A:LYS:HA	8	2.2
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	1	2.2
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	5	2.19
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	17	2.18
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	13	2.17
(1,2423)	1:190:A:LEU:HD21	1:216:A:LYS:HA	7	2.17
(1,2423)	1:190:A:LEU:HD22	1:216:A:LYS:HA	7	2.17
(1,2423)	1:190:A:LEU:HD23	1:216:A:LYS:HA	7	2.17
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	2	2.17
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	11	2.17
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	11	2.17
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	11	2.17
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE1	7	2.16
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE2	7	2.16
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE3	7	2.16
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	13	2.16
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	13	2.16
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	13	2.16
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	3	2.16
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	3	2.16
(1,2845)	1:105:B:LEU:HD11	1:128:B:ALA:H	3	2.15
(1,2845)	1:105:B:LEU:HD12	1:128:B:ALA:H	3	2.15
(1,2845)	1:105:B:LEU:HD13	1:128:B:ALA:H	3	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	4	2.15
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	4	2.15
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	20	2.15
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	20	2.15
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	6	2.15
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	6	2.15
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD11	11	2.14
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD12	11	2.14
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD13	11	2.14
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG11	7	2.12
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG12	7	2.12
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG13	7	2.12
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	16	2.12
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	16	2.11
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	16	2.11
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	16	2.11
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	13	2.11
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	15	2.11
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	10	2.11
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	6	2.11
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	12	2.1
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	8	2.1
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	13	2.1
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	3	2.1
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	19	2.09
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	19	2.09
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	19	2.09
(1,1424)	1:69:A:LEU:HD11	1:2:B:SER:H	10	2.09
(1,1424)	1:69:A:LEU:HD12	1:2:B:SER:H	10	2.09
(1,1424)	1:69:A:LEU:HD13	1:2:B:SER:H	10	2.09
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	9	2.09
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	9	2.09
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	4	2.08
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG21	3	2.08
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG22	3	2.08
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG23	3	2.08
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	8	2.08
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	8	2.08
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	8	2.08
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	2	2.07
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	10	2.07
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	2	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	19	2.07
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG21	11	2.06
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG22	11	2.06
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG23	11	2.06
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE1	17	2.06
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE2	17	2.06
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE3	17	2.06
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	2	2.06
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	2	2.06
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	3	2.06
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	3	2.06
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	3	2.06
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	4	2.06
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	4	2.06
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	2	2.05
(1,3689)	1:185:B:LYS:HA	1:188:B:GLU:H	11	2.05
(1,3649)	1:180:B:LYS:HB2	1:188:B:GLU:H	2	2.05
(1,3649)	1:180:B:LYS:HB3	1:188:B:GLU:H	2	2.05
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	2	2.05
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	2	2.05
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	2	2.05
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	19	2.05
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	18	2.05
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	18	2.05
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	1	2.04
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG21	17	2.04
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG22	17	2.04
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG23	17	2.04
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	19	2.04
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	8	2.04
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	19	2.03
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	19	2.03
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	3	2.03
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	13	2.03
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	13	2.03
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	13	2.02
(1,2945)	1:113:B:MET:HB2	1:125:B:TYR:HE2	12	2.02
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	20	2.02
(1,1288)	1:16:A:PHE:HE1	1:12:B:ILE:HD11	10	2.02
(1,1288)	1:16:A:PHE:HE2	1:12:B:ILE:HD11	10	2.02
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	12	2.01
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	12	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	12	2.01
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	14	2.01
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	14	2.01
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	14	2.01
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	14	2.01
(1,3655)	1:181:B:TYR:H	1:186:B:PRO:HA	10	2.01
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	2	2.01
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	16	2.01
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	10	2.01
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	10	2.01
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	10	2.01
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	12	2.01
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	15	2.01
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	15	2.01
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	15	2.01
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	18	2.01
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	5	2.0
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	5	2.0
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	13	1.99
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	13	1.99
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	7	1.99
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	7	1.99
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	14	1.99
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	16	1.99
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	16	1.99
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	17	1.98
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	15	1.98
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	8	1.98
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB2	9	1.98
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB3	9	1.98
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	15	1.98
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	15	1.98
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	3	1.97
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	11	1.97
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	11	1.97
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	4	1.97
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	4	1.97
(1,3279)	1:144:B:ALA:HB1	1:175:B:ARG:HE	2	1.97
(1,3279)	1:144:B:ALA:HB2	1:175:B:ARG:HE	2	1.97
(1,3279)	1:144:B:ALA:HB3	1:175:B:ARG:HE	2	1.97
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	11	1.97
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	5	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	19	1.97
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	19	1.96
(1,3663)	1:181:B:TYR:HA	1:185:B:LYS:H	10	1.96
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	3	1.96
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	7	1.96
(1,1385)	1:44:A:PHE:HA	1:25:B:ILE:HD13	7	1.96
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	5	1.95
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	18	1.95
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	18	1.95
(1,3770)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	1	1.93
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	18	1.93
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	19	1.93
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	19	1.93
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	20	1.93
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	20	1.93
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	20	1.93
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	12	1.92
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	16	1.92
(1,3770)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	5	1.92
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	2	1.92
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	2	1.92
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	2	1.92
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	2	1.92
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	9	1.92
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	8	1.91
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	18	1.91
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	12	1.91
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	3	1.91
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	17	1.91
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	1	1.9
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	14	1.9
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	14	1.9
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	2	1.89
(1,3433)	1:159:B:ALA:HB1	1:176:B:LEU:HA	9	1.89
(1,3433)	1:159:B:ALA:HB2	1:176:B:LEU:HA	9	1.89
(1,3433)	1:159:B:ALA:HB3	1:176:B:LEU:HA	9	1.89
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	19	1.89
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	10	1.89
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	10	1.89
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	16	1.89
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	16	1.89
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	16	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	16	1.89
(1,3599)	1:176:B:LEU:HA	1:180:B:LYS:H	17	1.88
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	3	1.88
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	3	1.88
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	3	1.88
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	3	1.88
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	8	1.88
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	8	1.88
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	8	1.88
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG11	7	1.87
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG12	7	1.87
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG13	7	1.87
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	4	1.87
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	4	1.87
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG21	8	1.87
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG22	8	1.87
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG23	8	1.87
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	13	1.87
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	13	1.87
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	18	1.87
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	18	1.87
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	3	1.87
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	3	1.87
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	3	1.87
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	8	1.87
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	8	1.87
(1,2846)	1:105:B:LEU:HD11	1:128:B:ALA:HA	3	1.86
(1,2846)	1:105:B:LEU:HD12	1:128:B:ALA:HA	3	1.86
(1,2846)	1:105:B:LEU:HD13	1:128:B:ALA:HA	3	1.86
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	14	1.86
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	14	1.86
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	20	1.86
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	20	1.86
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	8	1.86
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	8	1.86
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	17	1.86
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	17	1.86
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	16	1.85
(1,1313)	1:29:A:GLY:H	1:43:B:ALA:HA	9	1.85
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	4	1.85
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	13	1.85
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	10	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	10	1.85
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	18	1.84
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	18	1.84
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	19	1.84
(1,2264)	1:173:A:TYR:HB2	1:195:A:LYS:HB2	8	1.84
(1,2264)	1:173:A:TYR:HB2	1:195:A:LYS:HB3	8	1.84
(1,2264)	1:173:A:TYR:HB3	1:195:A:LYS:HB2	8	1.84
(1,2264)	1:173:A:TYR:HB3	1:195:A:LYS:HB3	8	1.84
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	2	1.83
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	1	1.83
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	16	1.83
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	16	1.83
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	15	1.83
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	17	1.83
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	11	1.83
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	13	1.83
(1,3655)	1:181:B:TYR:H	1:186:B:PRO:HA	1	1.82
(1,3650)	1:180:B:LYS:HB2	1:188:B:GLU:HB2	2	1.82
(1,3650)	1:180:B:LYS:HB2	1:188:B:GLU:HB3	2	1.82
(1,3650)	1:180:B:LYS:HB3	1:188:B:GLU:HB2	2	1.82
(1,3650)	1:180:B:LYS:HB3	1:188:B:GLU:HB3	2	1.82
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	8	1.82
(1,3279)	1:144:B:ALA:HB1	1:175:B:ARG:HE	12	1.82
(1,3279)	1:144:B:ALA:HB2	1:175:B:ARG:HE	12	1.82
(1,3279)	1:144:B:ALA:HB3	1:175:B:ARG:HE	12	1.82
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	3	1.82
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	14	1.82
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	11	1.82
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	11	1.82
(1,635)	1:5:B:LYS:HA	1:9:B:ALA:H	17	1.82
(1,3205)	1:139:B:TYR:HA	1:143:B:ALA:H	13	1.81
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	12	1.81
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	12	1.81
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	13	1.81
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	2	1.81
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	2	1.81
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG2	2	1.8
(1,3081)	1:125:B:TYR:HE1	1:142:B:ARG:HA	1	1.8
(1,3081)	1:125:B:TYR:HE2	1:142:B:ARG:HA	1	1.8
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	19	1.8
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	12	1.8
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	12	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE1	17	1.8
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE2	17	1.8
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE1	17	1.8
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE2	17	1.8
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE1	17	1.8
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE2	17	1.8
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	17	1.8
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	19	1.8
(1,1221)	1:2:A:SER:HA	1:67:B:ASP:HA	3	1.8
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	1	1.79
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	1	1.79
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	1	1.79
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	1	1.79
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	13	1.79
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	13	1.79
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	10	1.79
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	10	1.79
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	9	1.79
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	13	1.79
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	13	1.79
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	8	1.79
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	8	1.79
(1,3970)	1:217:B:LYS:HA	1:220:B:GLU:H	11	1.78
(1,3812)	1:197:B:LEU:HD11	1:209:B:LYS:HA	17	1.78
(1,3812)	1:197:B:LEU:HD12	1:209:B:LYS:HA	17	1.78
(1,3812)	1:197:B:LEU:HD13	1:209:B:LYS:HA	17	1.78
(1,2813)	1:102:B:ALA:HB1	1:128:B:ALA:HA	8	1.78
(1,2813)	1:102:B:ALA:HB2	1:128:B:ALA:HA	8	1.78
(1,2813)	1:102:B:ALA:HB3	1:128:B:ALA:HA	8	1.78
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	5	1.78
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	5	1.78
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	5	1.78
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	8	1.78
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	8	1.78
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	2	1.78
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	3	1.78
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	3	1.78
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	7	1.78
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	7	1.78
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	5	1.77
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	5	1.77
(1,3543)	1:170:B:PHE:HD1	1:208:B:MET:HE3	7	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	15	1.77
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	15	1.77
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	15	1.77
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	3	1.77
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	3	1.77
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	3	1.77
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	19	1.77
(1,3641)	1:180:B:LYS:H	1:189:B:ALA:HA	11	1.76
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	1	1.76
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	3	1.76
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	11	1.76
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	2	1.76
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	2	1.76
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	17	1.76
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	16	1.76
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	16	1.76
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	17	1.76
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	17	1.76
(1,1250)	1:12:A:ILE:HA	1:8:B:ILE:HG21	17	1.76
(1,1250)	1:12:A:ILE:HA	1:8:B:ILE:HG22	17	1.76
(1,1250)	1:12:A:ILE:HA	1:8:B:ILE:HG23	17	1.76
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	18	1.76
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	18	1.76
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	18	1.76
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	9	1.76
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	9	1.76
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	6	1.76
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	6	1.76
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	16	1.76
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	16	1.76
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD21	9	1.75
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD22	9	1.75
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD23	9	1.75
(1,2783)	1:100:B:ALA:H	1:102:B:ALA:H	5	1.75
(1,2236)	1:170:A:PHE:HE2	1:171:A:ARG:HD3	3	1.75
(1,1118)	1:56:B:GLY:H	1:58:B:SER:H	17	1.75
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	1	1.75
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	1	1.75
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	12	1.74
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	12	1.74
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	12	1.74
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	12	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	12	1.74
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	12	1.74
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	9	1.74
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	6	1.73
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	15	1.73
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	12	1.73
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	12	1.73
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	12	1.73
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	12	1.73
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	14	1.73
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	14	1.73
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	14	1.73
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	14	1.73
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	9	1.73
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	9	1.73
(1,561)	1:63:A:GLN:HA	1:67:A:ASP:H	19	1.73
(1,3729)	1:190:B:LEU:HD21	1:216:B:LYS:HA	12	1.72
(1,3729)	1:190:B:LEU:HD22	1:216:B:LYS:HA	12	1.72
(1,3729)	1:190:B:LEU:HD23	1:216:B:LYS:HA	12	1.72
(1,3654)	1:181:B:TYR:H	1:185:B:LYS:H	10	1.72
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	20	1.72
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	20	1.72
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	20	1.72
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	8	1.72
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	5	1.72
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	5	1.72
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	11	1.72
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	11	1.72
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	11	1.72
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	11	1.72
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	9	1.72
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	9	1.72
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	9	1.72
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	9	1.72
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	19	1.72
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	10	1.72
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	9	1.72
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	1	1.71
(1,3343)	1:150:B:LYS:HZ1	1:152:B:TYR:HE1	10	1.71
(1,3343)	1:150:B:LYS:HZ1	1:152:B:TYR:HE2	10	1.71
(1,3343)	1:150:B:LYS:HZ2	1:152:B:TYR:HE1	10	1.71
(1,3343)	1:150:B:LYS:HZ2	1:152:B:TYR:HE2	10	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3343)	1:150:B:LYS:HZ3	1:152:B:TYR:HE1	10	1.71
(1,3343)	1:150:B:LYS:HZ3	1:152:B:TYR:HE2	10	1.71
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	7	1.71
(1,2263)	1:173:A:TYR:HB2	1:195:A:LYS:H	8	1.71
(1,2263)	1:173:A:TYR:HB3	1:195:A:LYS:H	8	1.71
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	15	1.71
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	18	1.71
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	18	1.71
(1,3364)	1:152:B:TYR:HE1	1:178:B:PHE:HE2	4	1.7
(1,3364)	1:152:B:TYR:HE2	1:178:B:PHE:HE2	4	1.7
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	3	1.7
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	3	1.7
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	13	1.7
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	7	1.7
(1,2773)	1:98:B:THR:HA	1:101:B:LYS:H	9	1.7
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	3	1.7
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	9	1.7
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	4	1.7
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	4	1.7
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	5	1.7
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	5	1.7
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	13	1.7
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	13	1.7
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	5	1.69
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	11	1.69
(1,3206)	1:139:B:TYR:HA	1:158:B:ASP:HA	4	1.69
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	11	1.69
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	12	1.69
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	12	1.69
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	17	1.68
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	17	1.68
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	17	1.68
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	17	1.68
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD2	10	1.68
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD3	10	1.68
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	10	1.68
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD3	10	1.68
(1,3196)	1:138:B:TYR:HA	1:142:B:ARG:H	13	1.68
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	9	1.68
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD11	19	1.68
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD12	19	1.68
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD13	19	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	9	1.68
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	9	1.68
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	9	1.68
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	9	1.68
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	15	1.68
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	15	1.67
(1,2714)	1:223:A:LEU:HA	1:226:A:GLU:H	8	1.67
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	13	1.67
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	13	1.67
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	13	1.67
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	1	1.67
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	1	1.67
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	10	1.67
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	10	1.67
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	4	1.66
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	11	1.66
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	9	1.66
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	9	1.66
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	9	1.66
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	9	1.66
(1,1387)	1:44:A:PHE:HE1	1:16:B:PHE:HE1	8	1.66
(1,1387)	1:44:A:PHE:HE2	1:16:B:PHE:HE1	8	1.66
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	3	1.66
(1,3770)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	19	1.65
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	19	1.65
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	19	1.65
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	19	1.65
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	19	1.65
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	6	1.65
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB2	16	1.65
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB3	16	1.65
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB2	16	1.65
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB3	16	1.65
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	9	1.65
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	9	1.65
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	9	1.65
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	9	1.65
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	2	1.65
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	2	1.65
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	2	1.65
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	2	1.65
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	7	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	5	1.64
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	5	1.64
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	5	1.64
(1,3730)	1:190:B:LEU:HD21	1:219:B:VAL:HG21	12	1.64
(1,3730)	1:190:B:LEU:HD21	1:219:B:VAL:HG22	12	1.64
(1,3730)	1:190:B:LEU:HD21	1:219:B:VAL:HG23	12	1.64
(1,3730)	1:190:B:LEU:HD22	1:219:B:VAL:HG21	12	1.64
(1,3730)	1:190:B:LEU:HD22	1:219:B:VAL:HG22	12	1.64
(1,3730)	1:190:B:LEU:HD22	1:219:B:VAL:HG23	12	1.64
(1,3730)	1:190:B:LEU:HD23	1:219:B:VAL:HG21	12	1.64
(1,3730)	1:190:B:LEU:HD23	1:219:B:VAL:HG22	12	1.64
(1,3730)	1:190:B:LEU:HD23	1:219:B:VAL:HG23	12	1.64
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	17	1.64
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	17	1.64
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	17	1.64
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	17	1.64
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	14	1.64
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	14	1.64
(1,2769)	1:98:B:THR:H	1:101:B:LYS:H	9	1.64
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	8	1.64
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB2	5	1.64
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB3	5	1.64
(1,2714)	1:223:A:LEU:HA	1:226:A:GLU:H	17	1.64
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	15	1.64
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	15	1.64
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	15	1.64
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	18	1.64
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	18	1.64
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	18	1.64
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	18	1.64
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	7	1.63
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	2	1.63
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	2	1.63
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	1	1.63
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	5	1.63
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	5	1.63
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	5	1.63
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	5	1.63
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	19	1.63
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	10	1.63
(1,1010)	1:41:B:SER:HA	1:45:B:GLY:H	16	1.63
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	2	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	2	1.63
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD11	5	1.62
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD12	5	1.62
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD13	5	1.62
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	19	1.62
(1,2138)	1:160:A:GLU:HA	1:164:A:SER:H	12	1.62
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	12	1.62
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	16	1.62
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	16	1.62
(1,3256)	1:143:B:ALA:HA	1:155:B:ALA:H	8	1.61
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	9	1.61
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	9	1.61
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG11	12	1.61
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG12	12	1.61
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG13	12	1.61
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	11	1.61
(1,1519)	1:103:A:GLU:HA	1:107:A:MET:H	5	1.61
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	7	1.61
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	7	1.61
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	16	1.61
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	16	1.6
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	10	1.6
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	10	1.6
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	10	1.6
(1,3815)	1:197:B:LEU:HD21	1:209:B:LYS:H	18	1.6
(1,3815)	1:197:B:LEU:HD22	1:209:B:LYS:H	18	1.6
(1,3815)	1:197:B:LEU:HD23	1:209:B:LYS:H	18	1.6
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE1	7	1.6
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE2	7	1.6
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE3	7	1.6
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE1	7	1.6
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE2	7	1.6
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE3	7	1.6
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD11	9	1.6
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD12	9	1.6
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD13	9	1.6
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	2	1.6
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	20	1.6
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	4	1.6
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	13	1.6
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	13	1.6
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	12	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	12	1.6
(1,642)	1:6:B:GLU:HA	1:10:B:ALA:H	17	1.6
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	14	1.59
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	20	1.59
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	11	1.59
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	11	1.59
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	5	1.59
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	20	1.59
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	20	1.59
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD21	9	1.59
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD22	9	1.59
(1,3651)	1:180:B:LYS:HB2	1:189:B:ALA:H	2	1.58
(1,3651)	1:180:B:LYS:HB3	1:189:B:ALA:H	2	1.58
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG21	11	1.58
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG22	11	1.58
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG23	11	1.58
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	13	1.58
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	13	1.58
(1,2464)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	8	1.58
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	18	1.58
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	18	1.58
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	18	1.58
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	18	1.58
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	14	1.58
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	7	1.58
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	11	1.58
(1,1308)	1:25:A:ILE:HD11	1:43:B:ALA:HA	9	1.58
(1,1308)	1:25:A:ILE:HD12	1:43:B:ALA:HA	9	1.58
(1,1308)	1:25:A:ILE:HD13	1:43:B:ALA:HA	9	1.58
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	18	1.58
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	17	1.58
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	19	1.57
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	19	1.57
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	19	1.57
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	19	1.57
(1,3252)	1:143:B:ALA:H	1:155:B:ALA:HA	8	1.57
(1,2945)	1:113:B:MET:HB2	1:125:B:TYR:HE1	2	1.57
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG21	12	1.57
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG22	12	1.57
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG23	12	1.57
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG21	12	1.57
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG22	12	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG23	12	1.57
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB2	13	1.57
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB3	13	1.57
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB2	13	1.57
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB3	13	1.57
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	10	1.57
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	10	1.57
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	4	1.57
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	4	1.57
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	4	1.57
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	4	1.57
(1,277)	1:27:A:GLU:HA	1:31:A:ASP:H	6	1.57
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	12	1.56
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	9	1.56
(1,3921)	1:211:B:ASP:HA	1:215:B:ALA:H	5	1.56
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	8	1.56
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	17	1.56
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	17	1.56
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	5	1.56
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	5	1.56
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	16	1.56
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	16	1.56
(1,2464)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	3	1.56
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	5	1.56
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	5	1.56
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	5	1.56
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	5	1.56
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	16	1.56
(1,1170)	1:63:B:GLN:HA	1:67:B:ASP:H	19	1.56
(1,1169)	1:63:B:GLN:HA	1:65:B:LEU:H	19	1.56
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	3	1.55
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	17	1.55
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	17	1.55
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	17	1.55
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	13	1.55
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	13	1.55
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	13	1.55
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	13	1.55
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	19	1.55
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	3	1.55
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB2	15	1.55
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB3	15	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB2	15	1.55
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB3	15	1.55
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	13	1.55
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	13	1.55
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	10	1.55
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	11	1.55
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	8	1.55
(1,1110)	1:55:B:LEU:H	1:57:B:LYS:H	17	1.55
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	19	1.55
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	19	1.55
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	12	1.54
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	10	1.54
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	10	1.54
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	10	1.54
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	10	1.54
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	13	1.54
(1,3361)	1:152:B:TYR:HB2	1:183:B:GLN:H	16	1.54
(1,3361)	1:152:B:TYR:HB3	1:183:B:GLN:H	16	1.54
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	8	1.54
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	3	1.54
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	7	1.54
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	7	1.54
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	20	1.54
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	20	1.54
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	15	1.54
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	4	1.54
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	4	1.54
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	16	1.54
(1,623)	1:4:B:SER:H	1:7:B:GLU:H	10	1.54
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	5	1.53
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	5	1.53
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB2	5	1.53
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	5	1.53
(1,3725)	1:190:B:LEU:HD11	1:212:B:TYR:HA	6	1.53
(1,3725)	1:190:B:LEU:HD12	1:212:B:TYR:HA	6	1.53
(1,3725)	1:190:B:LEU:HD13	1:212:B:TYR:HA	6	1.53
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	1	1.53
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	7	1.53
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	18	1.53
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB2	1	1.53
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB3	1	1.53
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	15	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	15	1.53
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	17	1.53
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	17	1.53
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	17	1.53
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	17	1.53
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	1	1.53
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	17	1.52
(1,3651)	1:180:B:LYS:HB2	1:189:B:ALA:H	11	1.52
(1,3651)	1:180:B:LYS:HB3	1:189:B:ALA:H	11	1.52
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	10	1.52
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	12	1.52
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	5	1.52
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	16	1.52
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	16	1.52
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	15	1.52
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	15	1.52
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	15	1.52
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	15	1.52
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	6	1.52
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	6	1.52
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	6	1.52
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	6	1.52
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	12	1.52
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	12	1.52
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	12	1.52
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	10	1.52
(1,1110)	1:55:B:LEU:H	1:57:B:LYS:H	1	1.52
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	19	1.52
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	19	1.52
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	14	1.51
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	14	1.51
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	14	1.51
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	14	1.51
(1,3648)	1:180:B:LYS:HB2	1:185:B:LYS:H	7	1.51
(1,3648)	1:180:B:LYS:HB3	1:185:B:LYS:H	7	1.51
(1,3068)	1:125:B:TYR:HA	1:138:B:TYR:HA	17	1.51
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	8	1.51
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	11	1.51
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG21	4	1.51
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG22	4	1.51
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG23	4	1.51
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG21	4	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG22	4	1.51
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG23	4	1.51
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	8	1.51
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	8	1.51
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	17	1.51
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	13	1.51
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	3	1.51
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	17	1.51
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	9	1.51
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	9	1.51
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	15	1.51
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	15	1.51
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	3	1.5
(1,2816)	1:102:B:ALA:HB1	1:132:B:LEU:H	12	1.5
(1,2816)	1:102:B:ALA:HB2	1:132:B:LEU:H	12	1.5
(1,2816)	1:102:B:ALA:HB3	1:132:B:LEU:H	12	1.5
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	14	1.5
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	17	1.5
(1,1307)	1:25:A:ILE:HG12	1:44:B:PHE:HA	9	1.5
(1,1307)	1:25:A:ILE:HG13	1:44:B:PHE:HA	9	1.5
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	19	1.5
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	17	1.5
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	17	1.5
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	5	1.5
(1,3828)	1:199:B:ILE:HA	1:201:B:GLY:H	7	1.49
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG21	17	1.49
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG22	17	1.49
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG23	17	1.49
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	14	1.49
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	16	1.49
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	16	1.49
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	14	1.49
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	14	1.48
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	10	1.48
(1,3816)	1:197:B:LEU:HD21	1:209:B:LYS:HA	18	1.48
(1,3816)	1:197:B:LEU:HD22	1:209:B:LYS:HA	18	1.48
(1,3816)	1:197:B:LEU:HD23	1:209:B:LYS:HA	18	1.48
(1,3444)	1:160:B:GLU:HA	1:164:B:SER:H	3	1.48
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	20	1.48
(1,2952)	1:113:B:MET:HE1	1:145:B:ALA:HA	7	1.48
(1,2952)	1:113:B:MET:HE2	1:145:B:ALA:HA	7	1.48
(1,2952)	1:113:B:MET:HE3	1:145:B:ALA:HA	7	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	6	1.48
(1,2850)	1:105:B:LEU:HD21	1:124:B:LYS:HA	12	1.48
(1,2850)	1:105:B:LEU:HD22	1:124:B:LYS:HA	12	1.48
(1,2850)	1:105:B:LEU:HD23	1:124:B:LYS:HA	12	1.48
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	15	1.48
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG2	18	1.48
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG3	18	1.48
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	11	1.48
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	11	1.48
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	14	1.48
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	14	1.48
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	14	1.48
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	14	1.48
(1,1030)	1:44:B:PHE:H	1:45:B:GLY:H	16	1.48
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	4	1.47
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	4	1.47
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE1	11	1.47
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE2	11	1.47
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE3	11	1.47
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE1	11	1.47
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE2	11	1.47
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE3	11	1.47
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	17	1.47
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	17	1.47
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	1	1.47
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	3	1.47
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	3	1.47
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB2	3	1.47
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	3	1.47
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	17	1.47
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	17	1.47
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	17	1.47
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	17	1.47
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	19	1.47
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	19	1.47
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	19	1.47
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	19	1.47
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	19	1.47
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	19	1.47
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	5	1.47
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	5	1.47
(1,2529)	1:200:A:GLU:HB2	1:204:A:ALA:HA	8	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2529)	1:200:A:GLU:HB3	1:204:A:ALA:HA	8	1.46
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	17	1.46
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	3	1.46
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	17	1.46
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	17	1.46
(1,3677)	1:182:B:ALA:HA	1:184:B:GLY:H	15	1.45
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	7	1.45
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB1	15	1.45
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB2	15	1.45
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB3	15	1.45
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB1	15	1.45
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB2	15	1.45
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB3	15	1.45
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB1	15	1.45
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB2	15	1.45
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB3	15	1.45
(1,2942)	1:113:B:MET:HA	1:121:B:ALA:H	2	1.45
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	9	1.45
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	10	1.45
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	10	1.45
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	10	1.45
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	10	1.45
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	18	1.45
(1,1412)	1:67:A:ASP:HB2	1:60:B:PHE:HB2	19	1.45
(1,1412)	1:67:A:ASP:HB2	1:60:B:PHE:HB3	19	1.45
(1,1412)	1:67:A:ASP:HB3	1:60:B:PHE:HB2	19	1.45
(1,1412)	1:67:A:ASP:HB3	1:60:B:PHE:HB3	19	1.45
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	2	1.45
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	2	1.45
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	2	1.45
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD11	12	1.45
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD12	12	1.45
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD13	12	1.45
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	16	1.44
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	15	1.44
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	15	1.44
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	7	1.44
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	7	1.44
(1,1374)	1:43:A:ALA:HA	1:32:B:SER:H	7	1.44
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	2	1.44
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	2	1.44
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	2	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	2	1.44
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	18	1.44
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	18	1.44
(1,1213)	1:71:B:SER:H	1:72:B:ALA:H	2	1.44
(1,1114)	1:55:B:LEU:HD11	1:71:B:SER:HA	2	1.44
(1,1114)	1:55:B:LEU:HD12	1:71:B:SER:HA	2	1.44
(1,1114)	1:55:B:LEU:HD13	1:71:B:SER:HA	2	1.44
(1,811)	1:17:B:SER:HA	1:37:B:MET:HE1	3	1.44
(1,811)	1:17:B:SER:HA	1:37:B:MET:HE2	3	1.44
(1,811)	1:17:B:SER:HA	1:37:B:MET:HE3	3	1.44
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	19	1.44
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	19	1.44
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	2	1.44
(1,506)	1:55:A:LEU:HD11	1:72:A:ALA:HA	2	1.44
(1,506)	1:55:A:LEU:HD12	1:72:A:ALA:HA	2	1.44
(1,506)	1:55:A:LEU:HD13	1:72:A:ALA:HA	2	1.44
(1,506)	1:55:A:LEU:HD11	1:72:A:ALA:HA	14	1.44
(1,506)	1:55:A:LEU:HD12	1:72:A:ALA:HA	14	1.44
(1,506)	1:55:A:LEU:HD13	1:72:A:ALA:HA	14	1.44
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	8	1.43
(1,3665)	1:181:B:TYR:HA	1:189:B:ALA:H	3	1.43
(1,3527)	1:170:B:PHE:HB2	1:196:B:VAL:HA	1	1.43
(1,3527)	1:170:B:PHE:HB3	1:196:B:VAL:HA	1	1.43
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	18	1.43
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	19	1.43
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	8	1.43
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	8	1.43
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB2	8	1.43
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	8	1.43
(1,1353)	1:39:A:CYS:HB2	1:36:B:ALA:H	3	1.43
(1,1353)	1:39:A:CYS:HB3	1:36:B:ALA:H	3	1.43
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	17	1.43
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	3	1.43
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	3	1.43
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	15	1.43
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	15	1.43
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	16	1.42
(1,3812)	1:197:B:LEU:HD11	1:209:B:LYS:HA	4	1.42
(1,3812)	1:197:B:LEU:HD12	1:209:B:LYS:HA	4	1.42
(1,3812)	1:197:B:LEU:HD13	1:209:B:LYS:HA	4	1.42
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	10	1.42
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	1	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	1	1.42
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	5	1.42
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	5	1.42
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	8	1.42
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	8	1.42
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	8	1.42
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	8	1.42
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD11	20	1.42
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD12	20	1.42
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD13	20	1.42
(1,507)	1:55:A:LEU:HD21	1:71:A:SER:HA	14	1.42
(1,507)	1:55:A:LEU:HD22	1:71:A:SER:HA	14	1.42
(1,507)	1:55:A:LEU:HD23	1:71:A:SER:HA	14	1.42
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	11	1.41
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	20	1.41
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG2	7	1.41
(1,3126)	1:129:B:ILE:HD11	1:139:B:TYR:HA	19	1.41
(1,3126)	1:129:B:ILE:HD12	1:139:B:TYR:HA	19	1.41
(1,3126)	1:129:B:ILE:HD13	1:139:B:TYR:HA	19	1.41
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	10	1.41
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	10	1.41
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	10	1.41
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE1	2	1.41
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE2	2	1.41
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE1	2	1.41
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE2	2	1.41
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	3	1.41
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	3	1.41
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	19	1.41
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	4	1.41
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	4	1.41
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	4	1.41
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	19	1.41
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	19	1.41
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	19	1.41
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	19	1.41
(1,623)	1:4:B:SER:H	1:7:B:GLU:H	5	1.41
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD21	2	1.41
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD22	2	1.41
(1,3689)	1:185:B:LYS:HA	1:188:B:GLU:H	3	1.4
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	8	1.4
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	3	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	3	1.4
(1,1307)	1:25:A:ILE:HG12	1:44:B:PHE:HA	5	1.4
(1,1307)	1:25:A:ILE:HG13	1:44:B:PHE:HA	5	1.4
(1,1307)	1:25:A:ILE:HG12	1:44:B:PHE:HA	13	1.4
(1,1307)	1:25:A:ILE:HG13	1:44:B:PHE:HA	13	1.4
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	19	1.4
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	19	1.4
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	18	1.4
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	8	1.4
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	5	1.4
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	5	1.4
(1,506)	1:55:A:LEU:HD11	1:72:A:ALA:HA	4	1.4
(1,506)	1:55:A:LEU:HD12	1:72:A:ALA:HA	4	1.4
(1,506)	1:55:A:LEU:HD13	1:72:A:ALA:HA	4	1.4
(1,3689)	1:185:B:LYS:HA	1:188:B:GLU:H	7	1.39
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	11	1.39
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	11	1.39
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD11	8	1.39
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD12	8	1.39
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD13	8	1.39
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	3	1.39
(1,2933)	1:113:B:MET:H	1:121:B:ALA:HA	9	1.39
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	11	1.39
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	17	1.39
(1,2788)	1:101:B:LYS:H	1:102:B:ALA:H	5	1.39
(1,2055)	1:152:A:TYR:HB2	1:183:A:GLN:H	19	1.39
(1,2055)	1:152:A:TYR:HB3	1:183:A:GLN:H	19	1.39
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	1	1.39
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	1	1.39
(1,1231)	1:5:A:LYS:H	1:15:B:TYR:HE1	12	1.39
(1,1231)	1:5:A:LYS:H	1:15:B:TYR:HE2	12	1.39
(1,4016)	1:223:B:LEU:H	1:225:B:LEU:H	17	1.38
(1,3815)	1:197:B:LEU:HD21	1:209:B:LYS:H	17	1.38
(1,3815)	1:197:B:LEU:HD22	1:209:B:LYS:H	17	1.38
(1,3815)	1:197:B:LEU:HD23	1:209:B:LYS:H	17	1.38
(1,3655)	1:181:B:TYR:H	1:186:B:PRO:HA	17	1.38
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	10	1.38
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	20	1.38
(1,3091)	1:126:B:THR:HA	1:130:B:LYS:H	8	1.38
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	4	1.38
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	7	1.38
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	7	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	18	1.38
(1,1537)	1:105:A:LEU:HA	1:124:A:LYS:HA	20	1.38
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	1	1.38
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	2	1.38
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	2	1.38
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	19	1.38
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	19	1.38
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD11	6	1.38
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD12	6	1.38
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD13	6	1.38
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD11	6	1.38
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD12	6	1.38
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD13	6	1.38
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	1	1.38
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	1	1.38
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	10	1.37
(1,3321)	1:148:B:SER:HA	1:150:B:LYS:H	10	1.37
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD11	6	1.37
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD12	6	1.37
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD13	6	1.37
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG2	3	1.37
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG3	3	1.37
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	6	1.37
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	6	1.37
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	6	1.37
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	6	1.37
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	2	1.37
(1,1140)	1:59:B:GLU:HB2	1:64:B:HIS:HA	17	1.37
(1,1140)	1:59:B:GLU:HB3	1:64:B:HIS:HA	17	1.37
(1,1113)	1:55:B:LEU:HA	1:58:B:SER:H	7	1.37
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	13	1.37
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	13	1.37
(1,162)	1:15:A:TYR:HB2	1:70:A:ASN:HD21	2	1.37
(1,162)	1:15:A:TYR:HB2	1:70:A:ASN:HD22	2	1.37
(1,162)	1:15:A:TYR:HB3	1:70:A:ASN:HD21	2	1.37
(1,162)	1:15:A:TYR:HB3	1:70:A:ASN:HD22	2	1.37
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD2	11	1.36
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD3	11	1.36
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	11	1.36
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD3	11	1.36
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	20	1.36
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	11	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	15	1.36
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	15	1.36
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	15	1.36
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	15	1.36
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB2	4	1.36
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB3	4	1.36
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB2	4	1.36
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB3	4	1.36
(1,1386)	1:44:A:PHE:HE1	1:16:B:PHE:HD1	8	1.36
(1,1386)	1:44:A:PHE:HE2	1:16:B:PHE:HD1	8	1.36
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	7	1.36
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	19	1.36
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	19	1.36
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	4	1.36
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	4	1.36
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	12	1.36
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	13	1.36
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	13	1.36
(1,763)	1:15:B:TYR:HA	1:18:B:SER:HB2	7	1.36
(1,763)	1:15:B:TYR:HA	1:18:B:SER:HB3	7	1.36
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	12	1.35
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	12	1.35
(1,3834)	1:200:B:GLU:HB2	1:204:B:ALA:H	4	1.35
(1,3834)	1:200:B:GLU:HB3	1:204:B:ALA:H	4	1.35
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	6	1.35
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	19	1.35
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	19	1.35
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	19	1.35
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	19	1.35
(1,2973)	1:116:B:LYS:HA	1:118:B:TYR:HA	15	1.35
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	1	1.35
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	2	1.35
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	2	1.35
(1,2755)	1:96:B:ALA:H	1:97:B:GLU:H	20	1.35
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	12	1.35
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	12	1.35
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	12	1.35
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	12	1.35
(1,1856)	1:135:A:ASN:HB2	1:138:A:TYR:HE2	13	1.35
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	3	1.35
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	3	1.35
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	5	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	2	1.35
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	2	1.35
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	14	1.35
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	14	1.35
(1,4027)	1:225:B:LEU:H	1:226:B:GLU:H	2	1.34
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	1	1.34
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	1	1.34
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB2	1	1.34
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	1	1.34
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	5	1.34
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	5	1.34
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	5	1.34
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	5	1.34
(1,3342)	1:150:B:LYS:HD2	1:152:B:TYR:HE1	10	1.34
(1,3342)	1:150:B:LYS:HD2	1:152:B:TYR:HE2	10	1.34
(1,3342)	1:150:B:LYS:HD3	1:152:B:TYR:HE1	10	1.34
(1,3342)	1:150:B:LYS:HD3	1:152:B:TYR:HE2	10	1.34
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	3	1.34
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	3	1.34
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	12	1.34
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	2	1.34
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	11	1.34
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG2	4	1.34
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG3	4	1.34
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	12	1.34
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	2	1.34
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	2	1.34
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	2	1.34
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB2	7	1.34
(1,1408)	1:63:A:GLN:HE21	1:67:B:ASP:HB3	7	1.34
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB2	7	1.34
(1,1408)	1:63:A:GLN:HE22	1:67:B:ASP:HB3	7	1.34
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	9	1.34
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	9	1.34
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB2	11	1.34
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB3	11	1.34
(1,1281)	1:16:A:PHE:HE1	1:9:B:ALA:HB1	9	1.34
(1,1281)	1:16:A:PHE:HE2	1:9:B:ALA:HB1	9	1.34
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	6	1.34
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	6	1.34
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	6	1.34
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	6	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	9	1.34
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	2	1.34
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	6	1.34
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	19	1.33
(1,3657)	1:181:B:TYR:H	1:189:B:ALA:HA	17	1.33
(1,3656)	1:181:B:TYR:H	1:189:B:ALA:H	3	1.33
(1,3599)	1:176:B:LEU:HA	1:180:B:LYS:H	15	1.33
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB1	3	1.33
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB2	3	1.33
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB3	3	1.33
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB1	3	1.33
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB2	3	1.33
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB3	3	1.33
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	19	1.33
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	15	1.33
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	15	1.33
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	15	1.33
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG12	12	1.33
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG13	12	1.33
(1,3974)	1:218:B:LYS:H	1:220:B:GLU:H	3	1.32
(1,3855)	1:204:B:ALA:HA	1:208:B:MET:HB2	7	1.32
(1,3855)	1:204:B:ALA:HA	1:208:B:MET:HB3	7	1.32
(1,3800)	1:196:B:VAL:HG11	1:208:B:MET:HA	3	1.32
(1,3800)	1:196:B:VAL:HG12	1:208:B:MET:HA	3	1.32
(1,3800)	1:196:B:VAL:HG13	1:208:B:MET:HA	3	1.32
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD11	12	1.32
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD12	12	1.32
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD13	12	1.32
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	2	1.32
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	14	1.32
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	19	1.32
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	9	1.32
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	9	1.32
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	9	1.32
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	9	1.32
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	3	1.32
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	3	1.32
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	3	1.32
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	3	1.32
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	15	1.32
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	15	1.32
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	15	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	15	1.32
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	13	1.32
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	8	1.32
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	12	1.32
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	12	1.32
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	3	1.32
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	3	1.32
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	3	1.32
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	3	1.32
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	2	1.32
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	2	1.32
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	2	1.32
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	2	1.32
(1,3756)	1:193:B:TYR:HA	1:197:B:LEU:H	4	1.31
(1,3648)	1:180:B:LYS:HB2	1:185:B:LYS:H	2	1.31
(1,3648)	1:180:B:LYS:HB3	1:185:B:LYS:H	2	1.31
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	3	1.31
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	5	1.31
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	5	1.31
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	5	1.31
(1,2580)	1:207:A:ALA:HA	1:210:A:ARG:H	8	1.31
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	9	1.31
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	9	1.31
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	20	1.31
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	3	1.31
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	3	1.31
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	3	1.31
(1,1338)	1:36:A:ALA:HA	1:36:B:ALA:HA	3	1.31
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	5	1.31
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	5	1.31
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	4	1.31
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	5	1.31
(1,3810)	1:197:B:LEU:HA	1:204:B:ALA:HA	6	1.3
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG21	8	1.3
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG22	8	1.3
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG23	8	1.3
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	8	1.3
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	14	1.3
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	3	1.3
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	3	1.3
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	3	1.3
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	18	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2451)	1:193:A:TYR:HA	1:212:A:TYR:HA	15	1.3
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD21	14	1.3
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD22	14	1.3
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD23	14	1.3
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	11	1.3
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	11	1.3
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	11	1.3
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	11	1.3
(1,2340)	1:180:A:LYS:HA	1:185:A:LYS:H	3	1.3
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	3	1.3
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	5	1.3
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	5	1.3
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	5	1.3
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	5	1.3
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	7	1.3
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	12	1.3
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	12	1.3
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	12	1.3
(1,763)	1:15:B:TYR:HA	1:18:B:SER:HB2	4	1.3
(1,763)	1:15:B:TYR:HA	1:18:B:SER:HB3	4	1.3
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	8	1.3
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	8	1.3
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	12	1.3
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	9	1.3
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	9	1.3
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	11	1.3
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	11	1.3
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD11	8	1.29
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD12	8	1.29
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD13	8	1.29
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	10	1.29
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	2	1.29
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	9	1.29
(1,2746)	1:95:B:ASP:H	1:96:B:ALA:H	19	1.29
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	9	1.29
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	12	1.29
(1,1856)	1:135:A:ASN:HB3	1:138:A:TYR:HE2	10	1.29
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB2	9	1.29
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB3	9	1.29
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	9	1.29
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD11	20	1.29
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD12	20	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD13	20	1.29
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	17	1.29
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	1	1.28
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD11	2	1.28
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD12	2	1.28
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD13	2	1.28
(1,3665)	1:181:B:TYR:HA	1:189:B:ALA:H	17	1.28
(1,3600)	1:176:B:LEU:HD11	1:180:B:LYS:H	17	1.28
(1,3600)	1:176:B:LEU:HD12	1:180:B:LYS:H	17	1.28
(1,3600)	1:176:B:LEU:HD13	1:180:B:LYS:H	17	1.28
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	4	1.28
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	17	1.28
(1,2952)	1:113:B:MET:HE1	1:145:B:ALA:HA	17	1.28
(1,2952)	1:113:B:MET:HE2	1:145:B:ALA:HA	17	1.28
(1,2952)	1:113:B:MET:HE3	1:145:B:ALA:HA	17	1.28
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	11	1.28
(1,2746)	1:95:B:ASP:H	1:96:B:ALA:H	14	1.28
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	8	1.28
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	8	1.28
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	17	1.28
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	17	1.28
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	17	1.28
(1,1289)	1:16:A:PHE:HE1	1:12:B:ILE:HD12	20	1.28
(1,1289)	1:16:A:PHE:HE2	1:12:B:ILE:HD12	20	1.28
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	11	1.28
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	6	1.27
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD11	17	1.27
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD12	17	1.27
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD13	17	1.27
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	6	1.27
(1,1313)	1:29:A:GLY:H	1:43:B:ALA:HA	11	1.27
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	10	1.27
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	1	1.27
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	1	1.27
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	20	1.27
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	20	1.27
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	14	1.27
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	20	1.27
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	20	1.27
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	14	1.26
(1,3656)	1:181:B:TYR:H	1:189:B:ALA:H	17	1.26
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB1	3	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB2	3	1.26
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB3	3	1.26
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB1	3	1.26
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB2	3	1.26
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB3	3	1.26
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB1	3	1.26
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB2	3	1.26
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB3	3	1.26
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	7	1.26
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	7	1.26
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	7	1.26
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	17	1.26
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	17	1.26
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	17	1.26
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	3	1.26
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD11	6	1.26
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD12	6	1.26
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD13	6	1.26
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	19	1.26
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD11	10	1.26
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD12	10	1.26
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD13	10	1.26
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD11	10	1.26
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD12	10	1.26
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD13	10	1.26
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	14	1.25
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	14	1.25
(1,3966)	1:217:B:LYS:H	1:220:B:GLU:H	11	1.25
(1,3542)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	13	1.25
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	11	1.25
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	20	1.25
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	7	1.25
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	7	1.25
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	7	1.25
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	1	1.25
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	1	1.25
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	14	1.25
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	2	1.25
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	6	1.25
(1,2469)	1:194:A:LYS:H	1:212:A:TYR:HA	15	1.25
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD1	14	1.25
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD2	14	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD1	14	1.25
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD2	14	1.25
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	16	1.25
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	16	1.25
(1,1314)	1:29:A:GLY:HA2	1:43:B:ALA:H	9	1.25
(1,1314)	1:29:A:GLY:HA3	1:43:B:ALA:H	9	1.25
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	3	1.24
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	3	1.24
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	3	1.24
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	3	1.24
(1,3668)	1:181:B:TYR:HD1	1:218:B:LYS:HB2	8	1.24
(1,3668)	1:181:B:TYR:HD1	1:218:B:LYS:HB3	8	1.24
(1,3668)	1:181:B:TYR:HD2	1:218:B:LYS:HB2	8	1.24
(1,3668)	1:181:B:TYR:HD2	1:218:B:LYS:HB3	8	1.24
(1,3364)	1:152:B:TYR:HE1	1:178:B:PHE:HE2	17	1.24
(1,3364)	1:152:B:TYR:HE2	1:178:B:PHE:HE2	17	1.24
(1,3291)	1:146:B:HIS:H	1:155:B:ALA:HA	8	1.24
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	15	1.24
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG11	17	1.24
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG12	17	1.24
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG13	17	1.24
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	15	1.24
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	18	1.24
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD21	13	1.24
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD22	13	1.24
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD23	13	1.24
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	11	1.24
(1,1274)	1:15:A:TYR:HH	1:5:B:LYS:HA	4	1.24
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	19	1.24
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	10	1.24
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	7	1.24
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	7	1.24
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	7	1.23
(1,3646)	1:180:B:LYS:HA	1:185:B:LYS:H	10	1.23
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	15	1.23
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	18	1.23
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	1	1.23
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	1	1.23
(1,1499)	1:102:A:ALA:HA	1:105:A:LEU:H	5	1.23
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	2	1.23
(1,1293)	1:16:A:PHE:HE1	1:40:B:ILE:HG21	9	1.23
(1,1293)	1:16:A:PHE:HE2	1:40:B:ILE:HG21	9	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE1	15	1.23
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE2	15	1.23
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE3	15	1.23
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	4	1.23
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	3	1.22
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	3	1.22
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	8	1.22
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	8	1.22
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	11	1.22
(1,2973)	1:116:B:LYS:HA	1:118:B:TYR:HA	7	1.22
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	13	1.22
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	13	1.22
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	13	1.22
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB2	5	1.22
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB3	5	1.22
(1,1418)	1:68:A:ILE:HG21	1:2:B:SER:HA	10	1.22
(1,1418)	1:68:A:ILE:HG22	1:2:B:SER:HA	10	1.22
(1,1418)	1:68:A:ILE:HG23	1:2:B:SER:HA	10	1.22
(1,1349)	1:39:A:CYS:HA	1:32:B:SER:HA	3	1.22
(1,1307)	1:25:A:ILE:HG12	1:44:B:PHE:HA	15	1.22
(1,1307)	1:25:A:ILE:HG13	1:44:B:PHE:HA	15	1.22
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	10	1.22
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	10	1.22
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	10	1.22
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	10	1.22
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	10	1.22
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	10	1.22
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	14	1.22
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	14	1.22
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	14	1.22
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	14	1.22
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	3	1.22
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	2	1.21
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	2	1.21
(1,3542)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	19	1.21
(1,3041)	1:122:B:ILE:HA	1:126:B:THR:H	18	1.21
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	10	1.21
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	6	1.21
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	6	1.21
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	6	1.21
(1,1427)	1:69:A:LEU:HD11	1:2:B:SER:HG	19	1.21
(1,1427)	1:69:A:LEU:HD12	1:2:B:SER:HG	19	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	1:69:A:LEU:HD13	1:2:B:SER:HG	19	1.21
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	17	1.21
(1,1155)	1:60:B:PHE:HB2	1:64:B:HIS:H	14	1.21
(1,1155)	1:60:B:PHE:HB3	1:64:B:HIS:H	14	1.21
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	14	1.21
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	14	1.21
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	14	1.21
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE1	15	1.21
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE2	15	1.21
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE3	15	1.21
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	20	1.2
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	20	1.2
(1,3992)	1:220:B:GLU:H	1:222:B:SER:H	9	1.2
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	5	1.2
(1,3655)	1:181:B:TYR:H	1:186:B:PRO:HA	11	1.2
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	10	1.2
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	10	1.2
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD2	1	1.2
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD3	1	1.2
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	1	1.2
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD3	1	1.2
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	19	1.2
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	1	1.2
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	1	1.2
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	11	1.2
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	11	1.2
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	10	1.2
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	7	1.2
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	12	1.2
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	18	1.2
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	20	1.2
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	20	1.2
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	17	1.2
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	18	1.2
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	11	1.2
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	10	1.2
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	10	1.2
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	10	1.2
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	10	1.2
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	1	1.2
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	10	1.2
(1,1140)	1:59:B:GLU:HB2	1:64:B:HIS:HA	11	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:59:B:GLU:HB3	1:64:B:HIS:HA	11	1.2
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	6	1.2
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	6	1.2
(1,3364)	1:152:B:TYR:HE1	1:178:B:PHE:HE2	12	1.19
(1,3364)	1:152:B:TYR:HE2	1:178:B:PHE:HE2	12	1.19
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	4	1.19
(1,2828)	1:104:B:ASP:H	1:107:B:MET:H	19	1.19
(1,2805)	1:102:B:ALA:HA	1:105:B:LEU:H	6	1.19
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	8	1.19
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	8	1.19
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	8	1.19
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB2	3	1.19
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB3	3	1.19
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB2	3	1.19
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB3	3	1.19
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB2	3	1.19
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB3	3	1.19
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	3	1.19
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	3	1.19
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	3	1.19
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	3	1.19
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	11	1.19
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	11	1.19
(1,3946)	1:214:B:SER:HA	1:217:B:LYS:H	4	1.18
(1,3832)	1:200:B:GLU:HA	1:203:B:ASN:H	18	1.18
(1,3816)	1:197:B:LEU:HD21	1:209:B:LYS:HA	4	1.18
(1,3816)	1:197:B:LEU:HD22	1:209:B:LYS:HA	4	1.18
(1,3816)	1:197:B:LEU:HD23	1:209:B:LYS:HA	4	1.18
(1,3433)	1:159:B:ALA:HB1	1:176:B:LEU:HA	13	1.18
(1,3433)	1:159:B:ALA:HB2	1:176:B:LEU:HA	13	1.18
(1,3433)	1:159:B:ALA:HB3	1:176:B:LEU:HA	13	1.18
(1,3252)	1:143:B:ALA:H	1:155:B:ALA:HA	2	1.18
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE1	11	1.18
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE2	11	1.18
(1,2952)	1:113:B:MET:HE1	1:145:B:ALA:HA	6	1.18
(1,2952)	1:113:B:MET:HE2	1:145:B:ALA:HA	6	1.18
(1,2952)	1:113:B:MET:HE3	1:145:B:ALA:HA	6	1.18
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	13	1.18
(1,2421)	1:190:A:LEU:HD11	1:216:A:LYS:H	13	1.18
(1,2421)	1:190:A:LEU:HD12	1:216:A:LYS:H	13	1.18
(1,2421)	1:190:A:LEU:HD13	1:216:A:LYS:H	13	1.18
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	13	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	13	1.18
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	13	1.18
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	13	1.18
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	3	1.18
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	4	1.18
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	4	1.18
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	4	1.18
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	3	1.18
(1,1385)	1:44:A:PHE:HA	1:25:B:ILE:HD13	12	1.18
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	5	1.18
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	15	1.18
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	15	1.18
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	15	1.18
(1,752)	1:14:B:ASN:HA	1:18:B:SER:H	3	1.18
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	16	1.18
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	16	1.18
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	10	1.17
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	10	1.17
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	5	1.17
(1,3819)	1:198:B:ASP:H	1:201:B:GLY:H	10	1.17
(1,3648)	1:180:B:LYS:HB2	1:185:B:LYS:H	10	1.17
(1,3648)	1:180:B:LYS:HB3	1:185:B:LYS:H	10	1.17
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB1	12	1.17
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB2	12	1.17
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB3	12	1.17
(1,2583)	1:207:A:ALA:HA	1:211:A:ASP:H	12	1.17
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	2	1.17
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	2	1.17
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	2	1.17
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	2	1.17
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	1	1.17
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	1	1.17
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	1	1.17
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	17	1.17
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	19	1.17
(1,284)	1:28:A:ASP:HA	1:32:A:SER:H	4	1.17
(1,3931)	1:212:B:TYR:HD1	1:213:B:GLU:HA	4	1.16
(1,3931)	1:212:B:TYR:HD2	1:213:B:GLU:HA	4	1.16
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	11	1.16
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD11	8	1.16
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD12	8	1.16
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD13	8	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	14	1.16
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	16	1.16
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	16	1.16
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	16	1.16
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	16	1.16
(1,2933)	1:113:B:MET:H	1:121:B:ALA:HA	2	1.16
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG11	10	1.16
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG12	10	1.16
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG13	10	1.16
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	13	1.16
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	13	1.16
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	13	1.16
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG21	7	1.16
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG22	7	1.16
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG23	7	1.16
(1,2266)	1:173:A:TYR:HB2	1:196:A:VAL:H	8	1.16
(1,2266)	1:173:A:TYR:HB3	1:196:A:VAL:H	8	1.16
(1,1338)	1:36:A:ALA:HA	1:36:B:ALA:HA	16	1.16
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	5	1.16
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	17	1.16
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	17	1.16
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	9	1.16
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	9	1.16
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	9	1.16
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	9	1.16
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	8	1.16
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD11	11	1.16
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD12	11	1.16
(1,1200)	1:68:B:ILE:HA	1:69:B:LEU:HD13	11	1.16
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	12	1.16
(1,162)	1:15:A:TYR:HB2	1:70:A:ASN:HD21	12	1.16
(1,162)	1:15:A:TYR:HB2	1:70:A:ASN:HD22	12	1.16
(1,162)	1:15:A:TYR:HB3	1:70:A:ASN:HD21	12	1.16
(1,162)	1:15:A:TYR:HB3	1:70:A:ASN:HD22	12	1.16
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	8	1.16
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	19	1.15
(1,3840)	1:201:B:GLY:H	1:204:B:ALA:H	10	1.15
(1,3828)	1:199:B:ILE:HA	1:201:B:GLY:H	4	1.15
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	6	1.15
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	1	1.15
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	1	1.15
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	1	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	1	1.15
(1,2746)	1:95:B:ASP:H	1:96:B:ALA:H	15	1.15
(1,1444)	1:95:A:ASP:HA	1:97:A:GLU:H	1	1.15
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB2	10	1.15
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB3	10	1.15
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB2	10	1.15
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB3	10	1.15
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB2	10	1.15
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB3	10	1.15
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	8	1.15
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	8	1.15
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	8	1.15
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	8	1.15
(1,1248)	1:9:A:ALA:H	1:16:B:PHE:HZ	16	1.15
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	20	1.15
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	20	1.15
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	20	1.15
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	20	1.15
(1,1230)	1:2:A:SER:HB2	1:69:B:LEU:HD11	11	1.15
(1,1230)	1:2:A:SER:HB2	1:69:B:LEU:HD12	11	1.15
(1,1230)	1:2:A:SER:HB2	1:69:B:LEU:HD13	11	1.15
(1,1230)	1:2:A:SER:HB3	1:69:B:LEU:HD11	11	1.15
(1,1230)	1:2:A:SER:HB3	1:69:B:LEU:HD12	11	1.15
(1,1230)	1:2:A:SER:HB3	1:69:B:LEU:HD13	11	1.15
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG21	19	1.15
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG22	19	1.15
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG23	19	1.15
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	2	1.15
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	12	1.15
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	17	1.15
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	11	1.15
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	11	1.15
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	6	1.15
(1,3813)	1:197:B:LEU:HD21	1:204:B:ALA:HA	2	1.14
(1,3813)	1:197:B:LEU:HD22	1:204:B:ALA:HA	2	1.14
(1,3813)	1:197:B:LEU:HD23	1:204:B:ALA:HA	2	1.14
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	5	1.14
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	6	1.14
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	6	1.14
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	6	1.14
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB2	7	1.14
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB3	7	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	12	1.14
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	12	1.14
(1,2443)	1:193:A:TYR:H	1:212:A:TYR:HA	15	1.14
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	17	1.14
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	17	1.14
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	17	1.14
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	17	1.14
(1,2236)	1:170:A:PHE:HE2	1:171:A:ARG:HD2	10	1.14
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	10	1.14
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	10	1.14
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	14	1.14
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	12	1.14
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	9	1.14
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	10	1.14
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	10	1.14
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	12	1.14
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	12	1.14
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	12	1.14
(1,1274)	1:15:A:TYR:HH	1:5:B:LYS:HA	20	1.14
(1,1213)	1:71:B:SER:H	1:72:B:ALA:H	17	1.14
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	19	1.14
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	19	1.14
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	19	1.14
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	3	1.14
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	3	1.14
(1,3770)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	15	1.13
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB2	12	1.13
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB3	12	1.13
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB2	12	1.13
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB3	12	1.13
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB2	12	1.13
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB3	12	1.13
(1,2995)	1:118:B:TYR:HA	1:145:B:ALA:HA	3	1.13
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB1	15	1.13
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB2	15	1.13
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB3	15	1.13
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB1	15	1.13
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB2	15	1.13
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB3	15	1.13
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB1	15	1.13
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB2	15	1.13
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB3	15	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	14	1.13
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	19	1.13
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	14	1.13
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	14	1.13
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	9	1.13
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	9	1.13
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	11	1.13
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	5	1.13
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	4	1.13
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	4	1.13
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	4	1.13
(1,1134)	1:59:B:GLU:H	1:60:B:PHE:H	17	1.13
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	14	1.13
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	14	1.13
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	14	1.13
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	18	1.13
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	18	1.13
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	6	1.13
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	7	1.13
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	9	1.12
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	20	1.12
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	7	1.12
(1,4061)	1:253:A:GLY:H	1:254:A:SER:H	9	1.12
(1,3810)	1:197:B:LEU:HA	1:204:B:ALA:HA	4	1.12
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	4	1.12
(1,3769)	1:193:B:TYR:HD2	1:211:B:ASP:HA	1	1.12
(1,3725)	1:190:B:LEU:HD11	1:212:B:TYR:HA	3	1.12
(1,3725)	1:190:B:LEU:HD12	1:212:B:TYR:HA	3	1.12
(1,3725)	1:190:B:LEU:HD13	1:212:B:TYR:HA	3	1.12
(1,3612)	1:177:B:GLY:HA2	1:192:B:ALA:H	11	1.12
(1,3612)	1:177:B:GLY:HA3	1:192:B:ALA:H	11	1.12
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	10	1.12
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	10	1.12
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG21	1	1.12
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG22	1	1.12
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG23	1	1.12
(1,3542)	1:170:B:PHE:HD2	1:171:B:ARG:HD2	11	1.12
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	10	1.12
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	10	1.12
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	10	1.12
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	10	1.12
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	10	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	10	1.12
(1,3256)	1:143:B:ALA:HA	1:155:B:ALA:H	2	1.12
(1,3082)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	13	1.12
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	8	1.12
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	6	1.12
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	5	1.12
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	9	1.12
(1,2345)	1:180:A:LYS:HB2	1:189:A:ALA:H	16	1.12
(1,2345)	1:180:A:LYS:HB3	1:189:A:ALA:H	16	1.12
(1,1467)	1:98:A:THR:HA	1:101:A:LYS:H	19	1.12
(1,1338)	1:36:A:ALA:HA	1:36:B:ALA:HA	11	1.12
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	11	1.12
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	11	1.12
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	15	1.12
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	15	1.12
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	15	1.12
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	15	1.12
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	9	1.12
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	14	1.12
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	14	1.12
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	13	1.12
(1,1165)	1:62:B:GLY:H	1:64:B:HIS:H	14	1.12
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	2	1.12
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	2	1.12
(1,836)	1:20:B:VAL:HA	1:30:B:ALA:HA	2	1.12
(1,529)	1:59:A:GLU:HA	1:64:A:HIS:HA	14	1.12
(1,3367)	1:152:B:TYR:HD1	1:183:B:GLN:HG3	16	1.11
(1,3252)	1:143:B:ALA:H	1:155:B:ALA:HA	4	1.11
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	7	1.11
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	4	1.11
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	19	1.11
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	19	1.11
(1,1519)	1:103:A:GLU:HA	1:107:A:MET:H	15	1.11
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	11	1.11
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	2	1.11
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	10	1.11
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	7	1.11
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	10	1.11
(1,623)	1:4:B:SER:H	1:7:B:GLU:H	14	1.11
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	14	1.1
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	13	1.1
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	3	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3832)	1:200:B:GLU:HA	1:203:B:ASN:H	16	1.1
(1,2948)	1:113:B:MET:HE1	1:142:B:ARG:HA	10	1.1
(1,2948)	1:113:B:MET:HE2	1:142:B:ARG:HA	10	1.1
(1,2948)	1:113:B:MET:HE3	1:142:B:ARG:HA	10	1.1
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	2	1.1
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	2	1.1
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	13	1.1
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	13	1.1
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	1	1.1
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	1	1.1
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	1	1.1
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	1	1.1
(1,1248)	1:9:A:ALA:H	1:16:B:PHE:HZ	19	1.1
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE1	3	1.1
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE2	3	1.1
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	19	1.1
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	19	1.1
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	19	1.1
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	19	1.1
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD11	12	1.1
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD12	12	1.1
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD13	12	1.1
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD11	12	1.1
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD12	12	1.1
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD13	12	1.1
(1,1213)	1:71:B:SER:H	1:72:B:ALA:H	20	1.1
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	5	1.1
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	5	1.1
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	5	1.1
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	3	1.1
(1,886)	1:27:B:GLU:HA	1:31:B:ASP:H	12	1.1
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	8	1.1
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	14	1.1
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	14	1.1
(1,726)	1:13:B:VAL:HA	1:17:B:SER:H	3	1.1
(1,624)	1:4:B:SER:H	1:8:B:ILE:H	10	1.1
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	18	1.1
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	18	1.1
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	4	1.1
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	14	1.1
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	15	1.09
(1,3749)	1:193:B:TYR:H	1:212:B:TYR:HA	4	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3666)	1:181:B:TYR:HA	1:189:B:ALA:HB1	11	1.09
(1,3666)	1:181:B:TYR:HA	1:189:B:ALA:HB2	11	1.09
(1,3666)	1:181:B:TYR:HA	1:189:B:ALA:HB3	11	1.09
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	20	1.09
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	11	1.09
(1,3074)	1:125:B:TYR:HB2	1:142:B:ARG:H	13	1.09
(1,3074)	1:125:B:TYR:HB3	1:142:B:ARG:H	13	1.09
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	7	1.09
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	2	1.09
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	2	1.09
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	2	1.09
(1,2343)	1:180:A:LYS:HB2	1:188:A:GLU:H	16	1.09
(1,2343)	1:180:A:LYS:HB3	1:188:A:GLU:H	16	1.09
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	5	1.09
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	17	1.09
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	1	1.09
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	1	1.09
(1,1300)	1:16:A:PHE:HE1	1:44:B:PHE:HE2	17	1.09
(1,1300)	1:16:A:PHE:HE2	1:44:B:PHE:HE2	17	1.09
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	4	1.09
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	4	1.09
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	10	1.09
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	10	1.09
(1,635)	1:5:B:LYS:HA	1:9:B:ALA:H	6	1.09
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	10	1.09
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	10	1.09
(1,3536)	1:170:B:PHE:HE1	1:171:B:ARG:H	1	1.08
(1,3536)	1:170:B:PHE:HE2	1:171:B:ARG:H	1	1.08
(1,3082)	1:125:B:TYR:HD1	1:141:B:ASN:HB3	1	1.08
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	9	1.08
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	9	1.08
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	8	1.08
(1,2697)	1:221:A:GLN:HA	1:224:A:ASN:H	3	1.08
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB2	4	1.08
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	4	1.08
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB2	4	1.08
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB3	4	1.08
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	19	1.08
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	17	1.08
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	3	1.08
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	3	1.08
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	6	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	11	1.08
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	11	1.08
(1,1321)	1:32:A:SER:HB2	1:43:B:ALA:H	16	1.08
(1,1321)	1:32:A:SER:HB3	1:43:B:ALA:H	16	1.08
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	2	1.08
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	2	1.08
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	12	1.08
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	19	1.08
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	19	1.08
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	19	1.08
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	10	1.08
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	10	1.08
(1,627)	1:4:B:SER:HA	1:6:B:GLU:H	6	1.08
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	17	1.08
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	1	1.07
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	4	1.07
(1,3297)	1:146:B:HIS:HA	1:151:B:GLU:H	8	1.07
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	17	1.07
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	17	1.07
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	17	1.07
(1,2941)	1:113:B:MET:HA	1:118:B:TYR:HA	11	1.07
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB2	3	1.07
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB3	3	1.07
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	9	1.07
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	9	1.07
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	9	1.07
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	20	1.07
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	10	1.07
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	19	1.07
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	19	1.07
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	10	1.07
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	19	1.07
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	17	1.07
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	19	1.07
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	19	1.07
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	2	1.07
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	9	1.07
(1,507)	1:55:A:LEU:HD21	1:71:A:SER:HA	2	1.07
(1,507)	1:55:A:LEU:HD22	1:71:A:SER:HA	2	1.07
(1,507)	1:55:A:LEU:HD23	1:71:A:SER:HA	2	1.07
(1,225)	1:20:A:VAL:HA	1:23:A:LYS:HA	17	1.07
(1,3898)	1:208:B:MET:HA	1:211:B:ASP:H	6	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3828)	1:199:B:ILE:HA	1:201:B:GLY:H	6	1.06
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	6	1.06
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	10	1.06
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	10	1.06
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	10	1.06
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	10	1.06
(1,3599)	1:176:B:LEU:HA	1:180:B:LYS:H	12	1.06
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	18	1.06
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	18	1.06
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE1	11	1.06
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	3	1.06
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG11	7	1.06
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG12	7	1.06
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG13	7	1.06
(1,2746)	1:95:B:ASP:H	1:96:B:ALA:H	5	1.06
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	11	1.06
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	11	1.06
(1,2526)	1:200:A:GLU:HA	1:203:A:ASN:H	14	1.06
(1,1855)	1:135:A:ASN:HB2	1:138:A:TYR:HE1	14	1.06
(1,1855)	1:135:A:ASN:HB2	1:138:A:TYR:HE2	14	1.06
(1,1855)	1:135:A:ASN:HB3	1:138:A:TYR:HE1	14	1.06
(1,1855)	1:135:A:ASN:HB3	1:138:A:TYR:HE2	14	1.06
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	3	1.06
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	3	1.06
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	13	1.06
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	13	1.06
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	13	1.06
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	13	1.06
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	20	1.06
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	20	1.06
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE1	10	1.06
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE2	10	1.06
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE3	10	1.06
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	9	1.06
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	9	1.06
(1,4027)	1:225:B:LEU:H	1:226:B:GLU:H	17	1.05
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	3	1.05
(1,3816)	1:197:B:LEU:HD21	1:209:B:LYS:HA	17	1.05
(1,3816)	1:197:B:LEU:HD22	1:209:B:LYS:HA	17	1.05
(1,3816)	1:197:B:LEU:HD23	1:209:B:LYS:HA	17	1.05
(1,3651)	1:180:B:LYS:HB2	1:189:B:ALA:H	3	1.05
(1,3651)	1:180:B:LYS:HB3	1:189:B:ALA:H	3	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3649)	1:180:B:LYS:HB2	1:188:B:GLU:H	11	1.05
(1,3649)	1:180:B:LYS:HB3	1:188:B:GLU:H	11	1.05
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	18	1.05
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	18	1.05
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	18	1.05
(1,1431)	1:93:A:GLU:HA	1:95:A:ASP:H	2	1.05
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	15	1.05
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	9	1.05
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	9	1.05
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	7	1.05
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	7	1.05
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	7	1.05
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	7	1.05
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	13	1.05
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	2	1.05
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	3	1.05
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	2	1.04
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	2	1.04
(1,3810)	1:197:B:LEU:HA	1:204:B:ALA:HA	11	1.04
(1,3655)	1:181:B:TYR:H	1:186:B:PRO:HA	8	1.04
(1,3357)	1:152:B:TYR:HA	1:156:B:VAL:H	4	1.04
(1,3145)	1:132:B:LEU:HD11	1:134:B:THR:H	17	1.04
(1,3145)	1:132:B:LEU:HD12	1:134:B:THR:H	17	1.04
(1,3145)	1:132:B:LEU:HD13	1:134:B:THR:H	17	1.04
(1,3044)	1:122:B:ILE:HD11	1:146:B:HIS:HA	6	1.04
(1,3044)	1:122:B:ILE:HD12	1:146:B:HIS:HA	6	1.04
(1,3044)	1:122:B:ILE:HD13	1:146:B:HIS:HA	6	1.04
(1,2464)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	7	1.04
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	18	1.04
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	18	1.04
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	18	1.04
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	18	1.04
(1,1338)	1:36:A:ALA:HA	1:36:B:ALA:HA	19	1.04
(1,1336)	1:36:A:ALA:H	1:36:B:ALA:HA	11	1.04
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	5	1.04
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	5	1.04
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	5	1.04
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	8	1.04
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	8	1.04
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	4	1.04
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	20	1.04
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	20	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG21	12	1.04
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG22	12	1.04
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG23	12	1.04
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	13	1.04
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	12	1.04
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	3	1.04
(1,953)	1:35:B:VAL:HA	1:38:B:ASP:HA	3	1.04
(1,803)	1:17:B:SER:H	1:37:B:MET:HE1	3	1.04
(1,803)	1:17:B:SER:H	1:37:B:MET:HE2	3	1.04
(1,803)	1:17:B:SER:H	1:37:B:MET:HE3	3	1.04
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	8	1.04
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	8	1.04
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	11	1.04
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	11	1.04
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	11	1.03
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	10	1.03
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	15	1.03
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	18	1.03
(1,3843)	1:202:B:ASP:H	1:204:B:ALA:H	4	1.03
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	8	1.03
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	8	1.03
(1,3756)	1:193:B:TYR:HA	1:197:B:LEU:H	17	1.03
(1,3725)	1:190:B:LEU:HD11	1:212:B:TYR:HA	9	1.03
(1,3725)	1:190:B:LEU:HD12	1:212:B:TYR:HA	9	1.03
(1,3725)	1:190:B:LEU:HD13	1:212:B:TYR:HA	9	1.03
(1,3145)	1:132:B:LEU:HD11	1:134:B:THR:H	14	1.03
(1,3145)	1:132:B:LEU:HD12	1:134:B:THR:H	14	1.03
(1,3145)	1:132:B:LEU:HD13	1:134:B:THR:H	14	1.03
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	15	1.03
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	15	1.03
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	6	1.03
(1,2146)	1:161:A:SER:HA	1:165:A:ILE:H	12	1.03
(1,1474)	1:99:A:LYS:HA	1:102:A:ALA:H	15	1.03
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	20	1.03
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	19	1.03
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB2	16	1.03
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB3	16	1.03
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	12	1.03
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	12	1.03
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	16	1.03
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	16	1.03
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	18	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	18	1.03
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	18	1.03
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	18	1.03
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	9	1.03
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	9	1.03
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	3	1.03
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	3	1.03
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	3	1.03
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	3	1.03
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	8	1.03
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	8	1.03
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	8	1.03
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	8	1.03
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	1	1.03
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	1	1.03
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	8	1.03
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	8	1.03
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	8	1.03
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	8	1.03
(1,544)	1:60:A:PHE:HB2	1:63:A:GLN:HG2	2	1.03
(1,544)	1:60:A:PHE:HB2	1:63:A:GLN:HG3	2	1.03
(1,544)	1:60:A:PHE:HB3	1:63:A:GLN:HG2	2	1.03
(1,544)	1:60:A:PHE:HB3	1:63:A:GLN:HG3	2	1.03
(1,537)	1:60:A:PHE:HA	1:63:A:GLN:H	1	1.03
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	5	1.02
(1,4048)	1:238:A:VAL:H	1:239:A:ASP:H	14	1.02
(1,3848)	1:203:B:ASN:H	1:204:B:ALA:H	4	1.02
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG21	11	1.02
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG22	11	1.02
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG23	11	1.02
(1,3551)	1:171:B:ARG:HA	1:175:B:ARG:H	17	1.02
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	11	1.02
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	3	1.02
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	18	1.02
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	9	1.02
(1,2004)	1:147:A:SER:HA	1:150:A:LYS:HA	7	1.02
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	1	1.02
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	8	1.02
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	1	1.02
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	1	1.02
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	6	1.02
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	14	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	14	1.02
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	20	1.02
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD11	20	1.02
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD12	20	1.02
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD13	20	1.02
(1,4021)	1:224:B:ASN:H	1:225:B:LEU:H	17	1.01
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	20	1.01
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	20	1.01
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	20	1.01
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	18	1.01
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	7	1.01
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE1	2	1.01
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE2	2	1.01
(1,3856)	1:204:B:ALA:HA	1:208:B:MET:HE3	2	1.01
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	10	1.01
(1,2973)	1:116:B:LYS:HA	1:118:B:TYR:HA	20	1.01
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	19	1.01
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	7	1.01
(1,2746)	1:95:B:ASP:H	1:96:B:ALA:H	2	1.01
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	20	1.01
(1,2262)	1:173:A:TYR:HA	1:192:A:ALA:HB1	8	1.01
(1,2262)	1:173:A:TYR:HA	1:192:A:ALA:HB2	8	1.01
(1,2262)	1:173:A:TYR:HA	1:192:A:ALA:HB3	8	1.01
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG21	9	1.01
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG22	9	1.01
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG23	9	1.01
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG21	9	1.01
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG22	9	1.01
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG23	9	1.01
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD2	12	1.01
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD3	12	1.01
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	3	1.01
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	3	1.01
(1,1535)	1:105:A:LEU:HA	1:108:A:GLN:H	19	1.01
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	19	1.01
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	19	1.01
(1,1313)	1:29:A:GLY:H	1:43:B:ALA:HA	13	1.01
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	19	1.01
(1,1202)	1:69:B:LEU:H	1:70:B:ASN:H	17	1.01
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	18	1.01
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	13	1.0
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	4	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	4	1.0
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	8	1.0
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	8	1.0
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	7	1.0
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	11	1.0
(1,3946)	1:214:B:SER:HA	1:217:B:LYS:H	5	1.0
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	9	1.0
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	15	1.0
(1,3532)	1:170:B:PHE:HD1	1:171:B:ARG:HD2	10	1.0
(1,3532)	1:170:B:PHE:HD1	1:171:B:ARG:HD3	10	1.0
(1,3532)	1:170:B:PHE:HD2	1:171:B:ARG:HD2	10	1.0
(1,3532)	1:170:B:PHE:HD2	1:171:B:ARG:HD3	10	1.0
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	2	1.0
(1,3147)	1:134:B:THR:H	1:135:B:ASN:H	1	1.0
(1,2919)	1:112:B:ALA:HA	1:117:B:ASP:H	7	1.0
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	7	1.0
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	5	1.0
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB2	11	1.0
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB3	11	1.0
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	10	1.0
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	14	1.0
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	14	1.0
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	14	1.0
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	10	1.0
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	1	1.0
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	1	1.0
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	4	1.0
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	4	1.0
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	13	1.0
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	13	1.0
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	13	1.0
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	13	1.0
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	17	1.0
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	17	1.0
(1,1145)	1:60:B:PHE:HA	1:62:B:GLY:H	18	1.0
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	12	1.0
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	19	1.0
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	19	1.0
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	3	0.99
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	3	0.99
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	5	0.99
(1,3912)	1:210:B:ARG:HA	1:213:B:GLU:H	18	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	18	0.99
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	18	0.99
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	15	0.99
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	15	0.99
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	15	0.99
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	15	0.99
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	15	0.99
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	15	0.99
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	11	0.99
(1,3396)	1:156:B:VAL:HA	1:176:B:LEU:HA	16	0.99
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	9	0.99
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG21	6	0.99
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG22	6	0.99
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG23	6	0.99
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG21	6	0.99
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG22	6	0.99
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG23	6	0.99
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG21	6	0.99
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG22	6	0.99
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG23	6	0.99
(1,2351)	1:181:A:TYR:H	1:189:A:ALA:HA	7	0.99
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	11	0.99
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	10	0.99
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	6	0.99
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	6	0.99
(1,1391)	1:44:A:PHE:HE1	1:19:B:ILE:HG12	12	0.99
(1,1391)	1:44:A:PHE:HE1	1:19:B:ILE:HG13	12	0.99
(1,1391)	1:44:A:PHE:HE2	1:19:B:ILE:HG12	12	0.99
(1,1391)	1:44:A:PHE:HE2	1:19:B:ILE:HG13	12	0.99
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	7	0.99
(1,1274)	1:15:A:TYR:HH	1:5:B:LYS:HA	5	0.99
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	10	0.99
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	12	0.99
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	12	0.99
(1,4077)	1:305:A:GLY:H	1:307:A:GLY:H	1	0.98
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	20	0.98
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	6	0.98
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	6	0.98
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	1	0.98
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	1	0.98
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	1	0.98
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	1	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3649)	1:180:B:LYS:HB2	1:188:B:GLU:H	9	0.98
(1,3649)	1:180:B:LYS:HB3	1:188:B:GLU:H	9	0.98
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD11	1	0.98
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD12	1	0.98
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD13	1	0.98
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	20	0.98
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	10	0.98
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	10	0.98
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	10	0.98
(1,2942)	1:113:B:MET:HA	1:121:B:ALA:H	9	0.98
(1,2892)	1:109:B:GLY:HA2	1:113:B:MET:H	13	0.98
(1,2892)	1:109:B:GLY:HA3	1:113:B:MET:H	13	0.98
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	9	0.98
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	9	0.98
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	15	0.98
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG21	8	0.98
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG22	8	0.98
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG23	8	0.98
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE1	18	0.98
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE2	18	0.98
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE1	18	0.98
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE2	18	0.98
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE1	18	0.98
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE2	18	0.98
(1,1839)	1:132:A:LEU:HD11	1:134:A:THR:H	20	0.98
(1,1839)	1:132:A:LEU:HD12	1:134:A:THR:H	20	0.98
(1,1839)	1:132:A:LEU:HD13	1:134:A:THR:H	20	0.98
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	10	0.98
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	10	0.98
(1,1431)	1:93:A:GLU:HA	1:95:A:ASP:H	18	0.98
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	13	0.98
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	13	0.98
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	12	0.98
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	9	0.98
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	9	0.98
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	16	0.98
(1,685)	1:10:B:ALA:HA	1:48:B:ARG:HA	16	0.98
(1,627)	1:4:B:SER:HA	1:6:B:GLU:H	5	0.98
(1,625)	1:4:B:SER:HA	1:5:B:LYS:H	6	0.98
(1,344)	1:35:A:VAL:HA	1:38:A:ASP:HA	3	0.98
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	8	0.97
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	13	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3809)	1:197:B:LEU:HA	1:201:B:GLY:H	10	0.97
(1,3800)	1:196:B:VAL:HG11	1:208:B:MET:HA	7	0.97
(1,3800)	1:196:B:VAL:HG12	1:208:B:MET:HA	7	0.97
(1,3800)	1:196:B:VAL:HG13	1:208:B:MET:HA	7	0.97
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	2	0.97
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	2	0.97
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	2	0.97
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	2	0.97
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	6	0.97
(1,2746)	1:95:B:ASP:H	1:96:B:ALA:H	8	0.97
(1,2351)	1:181:A:TYR:H	1:189:A:ALA:HA	2	0.97
(1,2345)	1:180:A:LYS:HB2	1:189:A:ALA:H	1	0.97
(1,2345)	1:180:A:LYS:HB3	1:189:A:ALA:H	1	0.97
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG21	20	0.97
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG22	20	0.97
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG23	20	0.97
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG21	20	0.97
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG22	20	0.97
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG23	20	0.97
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	7	0.97
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	14	0.97
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	11	0.97
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB2	15	0.97
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB3	15	0.97
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB2	15	0.97
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB3	15	0.97
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB2	15	0.97
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB3	15	0.97
(1,1288)	1:16:A:PHE:HE1	1:12:B:ILE:HD11	14	0.97
(1,1288)	1:16:A:PHE:HE2	1:12:B:ILE:HD11	14	0.97
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	8	0.97
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	11	0.97
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	5	0.97
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	8	0.97
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	8	0.97
(1,4061)	1:253:A:GLY:H	1:254:A:SER:H	6	0.96
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	18	0.96
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	18	0.96
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	11	0.96
(1,3815)	1:197:B:LEU:HD21	1:209:B:LYS:H	4	0.96
(1,3815)	1:197:B:LEU:HD22	1:209:B:LYS:H	4	0.96
(1,3815)	1:197:B:LEU:HD23	1:209:B:LYS:H	4	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG2	8	0.96
(1,3195)	1:138:B:TYR:HA	1:141:B:ASN:H	7	0.96
(1,3145)	1:132:B:LEU:HD11	1:134:B:THR:H	16	0.96
(1,3145)	1:132:B:LEU:HD12	1:134:B:THR:H	16	0.96
(1,3145)	1:132:B:LEU:HD13	1:134:B:THR:H	16	0.96
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	13	0.96
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	13	0.96
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	13	0.96
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	10	0.96
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG11	19	0.96
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG12	19	0.96
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG13	19	0.96
(1,2769)	1:98:B:THR:H	1:101:B:LYS:H	11	0.96
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	2	0.96
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	2	0.96
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	2	0.96
(1,2416)	1:190:A:LEU:HA	1:212:A:TYR:HA	6	0.96
(1,1973)	1:144:A:ALA:HB1	1:175:A:ARG:HE	3	0.96
(1,1973)	1:144:A:ALA:HB2	1:175:A:ARG:HE	3	0.96
(1,1973)	1:144:A:ALA:HB3	1:175:A:ARG:HE	3	0.96
(1,1431)	1:93:A:GLU:HA	1:95:A:ASP:H	17	0.96
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG12	2	0.96
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG13	2	0.96
(1,1337)	1:36:A:ALA:HA	1:36:B:ALA:H	11	0.96
(1,1289)	1:16:A:PHE:HE1	1:12:B:ILE:HD12	17	0.96
(1,1289)	1:16:A:PHE:HE2	1:12:B:ILE:HD12	17	0.96
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	18	0.96
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	18	0.96
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	18	0.96
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	18	0.96
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	10	0.96
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	12	0.96
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	12	0.96
(1,885)	1:27:B:GLU:HA	1:30:B:ALA:HA	20	0.96
(1,835)	1:20:B:VAL:HA	1:24:B:GLU:H	18	0.96
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	15	0.96
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	15	0.96
(1,452)	1:47:A:GLU:HB2	1:49:A:GLU:H	16	0.96
(1,452)	1:47:A:GLU:HB3	1:49:A:GLU:H	16	0.96
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	12	0.96
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	12	0.96
(1,280)	1:28:A:ASP:H	1:31:A:ASP:H	4	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	19	0.95
(1,3858)	1:205:B:THR:H	1:208:B:MET:H	7	0.95
(1,3763)	1:193:B:TYR:HD1	1:211:B:ASP:HA	19	0.95
(1,3763)	1:193:B:TYR:HD2	1:211:B:ASP:HA	19	0.95
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	9	0.95
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	9	0.95
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	6	0.95
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	14	0.95
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	14	0.95
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	14	0.95
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD11	15	0.95
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD12	15	0.95
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD13	15	0.95
(1,2796)	1:101:B:LYS:HA	1:104:B:ASP:H	5	0.95
(1,2796)	1:101:B:LYS:HA	1:104:B:ASP:H	11	0.95
(1,2714)	1:223:A:LEU:HA	1:226:A:GLU:H	9	0.95
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	7	0.95
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	7	0.95
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	7	0.95
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	7	0.95
(1,1576)	1:109:A:GLY:H	1:121:A:ALA:HA	18	0.95
(1,1427)	1:69:A:LEU:HD11	1:2:B:SER:HG	13	0.95
(1,1427)	1:69:A:LEU:HD12	1:2:B:SER:HG	13	0.95
(1,1427)	1:69:A:LEU:HD13	1:2:B:SER:HG	13	0.95
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB2	13	0.95
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB3	13	0.95
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	3	0.95
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	2	0.95
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	2	0.95
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	5	0.95
(1,625)	1:4:B:SER:HA	1:5:B:LYS:H	17	0.95
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	8	0.95
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	18	0.95
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	18	0.95
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	3	0.95
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	19	0.94
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE1	7	0.94
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE2	7	0.94
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE3	7	0.94
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG21	11	0.94
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG22	11	0.94
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG23	11	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3651)	1:180:B:LYS:HB2	1:189:B:ALA:H	9	0.94
(1,3651)	1:180:B:LYS:HB3	1:189:B:ALA:H	9	0.94
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	15	0.94
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	15	0.94
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	15	0.94
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	9	0.94
(1,3361)	1:152:B:TYR:HB2	1:183:B:GLN:H	17	0.94
(1,3361)	1:152:B:TYR:HB3	1:183:B:GLN:H	17	0.94
(1,3339)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	7	0.94
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE1	18	0.94
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE2	18	0.94
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE1	18	0.94
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE2	18	0.94
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	8	0.94
(1,2714)	1:223:A:LEU:HA	1:226:A:GLU:H	10	0.94
(1,2232)	1:170:A:PHE:HE1	1:171:A:ARG:HD2	3	0.94
(1,2232)	1:170:A:PHE:HE1	1:171:A:ARG:HD3	3	0.94
(1,2232)	1:170:A:PHE:HE2	1:171:A:ARG:HD2	3	0.94
(1,2232)	1:170:A:PHE:HE2	1:171:A:ARG:HD3	3	0.94
(1,2076)	1:154:A:GLN:HA	1:158:A:ASP:H	3	0.94
(1,2004)	1:147:A:SER:HA	1:150:A:LYS:HA	1	0.94
(1,1900)	1:139:A:TYR:HA	1:158:A:ASP:HA	7	0.94
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	4	0.93
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	1	0.93
(1,4032)	1:226:B:GLU:HA	1:227:B:LYS:H	17	0.93
(1,4027)	1:225:B:LEU:H	1:226:B:GLU:H	5	0.93
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	12	0.93
(1,3870)	1:206:B:GLU:H	1:207:B:ALA:H	8	0.93
(1,3599)	1:176:B:LEU:HA	1:180:B:LYS:H	5	0.93
(1,3521)	1:170:B:PHE:HA	1:174:B:SER:H	17	0.93
(1,3298)	1:146:B:HIS:HB2	1:151:B:GLU:HB2	8	0.93
(1,3298)	1:146:B:HIS:HB2	1:151:B:GLU:HB3	8	0.93
(1,3298)	1:146:B:HIS:HB3	1:151:B:GLU:HB2	8	0.93
(1,3298)	1:146:B:HIS:HB3	1:151:B:GLU:HB3	8	0.93
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE1	7	0.93
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	19	0.93
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	19	0.93
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	19	0.93
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	7	0.93
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	7	0.93
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	7	0.93
(1,2817)	1:102:B:ALA:HB1	1:132:B:LEU:HD21	9	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2817)	1:102:B:ALA:HB1	1:132:B:LEU:HD22	9	0.93
(1,2817)	1:102:B:ALA:HB1	1:132:B:LEU:HD23	9	0.93
(1,2817)	1:102:B:ALA:HB2	1:132:B:LEU:HD21	9	0.93
(1,2817)	1:102:B:ALA:HB2	1:132:B:LEU:HD22	9	0.93
(1,2817)	1:102:B:ALA:HB2	1:132:B:LEU:HD23	9	0.93
(1,2817)	1:102:B:ALA:HB3	1:132:B:LEU:HD21	9	0.93
(1,2817)	1:102:B:ALA:HB3	1:132:B:LEU:HD22	9	0.93
(1,2817)	1:102:B:ALA:HB3	1:132:B:LEU:HD23	9	0.93
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	1	0.93
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	15	0.93
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	19	0.93
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	19	0.93
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	19	0.93
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	19	0.93
(1,2349)	1:181:A:TYR:H	1:186:A:PRO:HA	10	0.93
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	3	0.93
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	3	0.93
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	12	0.93
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	11	0.93
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	11	0.93
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	20	0.93
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	20	0.93
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	20	0.93
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB2	5	0.93
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB3	5	0.93
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB2	5	0.93
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB3	5	0.93
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB2	5	0.93
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB3	5	0.93
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	13	0.93
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	5	0.93
(1,452)	1:47:A:GLU:HB2	1:49:A:GLU:H	3	0.93
(1,452)	1:47:A:GLU:HB3	1:49:A:GLU:H	3	0.93
(1,4208)	1:345:B:LYS:H	1:346:B:GLN:H	4	0.92
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	5	0.92
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	8	0.92
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	5	0.92
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	7	0.92
(1,3832)	1:200:B:GLU:HA	1:203:B:ASN:H	2	0.92
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	8	0.92
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	10	0.92
(1,3366)	1:152:B:TYR:HD1	1:182:B:ALA:HB3	13	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3256)	1:143:B:ALA:HA	1:155:B:ALA:H	4	0.92
(1,3147)	1:134:B:THR:H	1:135:B:ASN:H	7	0.92
(1,2995)	1:118:B:TYR:HA	1:145:B:ALA:HA	5	0.92
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	11	0.92
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	6	0.92
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	6	0.92
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	15	0.92
(1,2813)	1:102:B:ALA:HB1	1:128:B:ALA:HA	12	0.92
(1,2813)	1:102:B:ALA:HB2	1:128:B:ALA:HA	12	0.92
(1,2813)	1:102:B:ALA:HB3	1:128:B:ALA:HA	12	0.92
(1,2805)	1:102:B:ALA:HA	1:105:B:LEU:H	19	0.92
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD11	14	0.92
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD12	14	0.92
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD13	14	0.92
(1,1537)	1:105:A:LEU:HA	1:124:A:LYS:HA	14	0.92
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	14	0.92
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	14	0.92
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	11	0.92
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	11	0.92
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	7	0.92
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	7	0.92
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	7	0.92
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	7	0.92
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD11	20	0.92
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD12	20	0.92
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD13	20	0.92
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	12	0.92
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	13	0.92
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	19	0.92
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	19	0.92
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	11	0.92
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	14	0.92
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	14	0.92
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	20	0.92
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	20	0.92
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	12	0.91
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	9	0.91
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	16	0.91
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	18	0.91
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	15	0.91
(1,3188)	1:137:B:ILE:HA	1:141:B:ASN:H	17	0.91
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG11	9	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG12	9	0.91
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG13	9	0.91
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	8	0.91
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	8	0.91
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	8	0.91
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	8	0.91
(1,2263)	1:173:A:TYR:HB2	1:195:A:LYS:H	11	0.91
(1,2263)	1:173:A:TYR:HB3	1:195:A:LYS:H	11	0.91
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	14	0.91
(1,1431)	1:93:A:GLU:HA	1:95:A:ASP:H	13	0.91
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	9	0.91
(1,1114)	1:55:B:LEU:HD11	1:71:B:SER:HA	20	0.91
(1,1114)	1:55:B:LEU:HD12	1:71:B:SER:HA	20	0.91
(1,1114)	1:55:B:LEU:HD13	1:71:B:SER:HA	20	0.91
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	12	0.91
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	12	0.91
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	5	0.91
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	5	0.91
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD11	19	0.91
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD12	19	0.91
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD13	19	0.91
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	13	0.91
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	13	0.91
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	2	0.91
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	18	0.91
(1,3921)	1:211:B:ASP:HA	1:215:B:ALA:H	20	0.9
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	9	0.9
(1,3656)	1:181:B:TYR:H	1:189:B:ALA:H	10	0.9
(1,3536)	1:170:B:PHE:HE1	1:171:B:ARG:H	6	0.9
(1,3536)	1:170:B:PHE:HE2	1:171:B:ARG:H	6	0.9
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	12	0.9
(1,3382)	1:154:B:GLN:HA	1:158:B:ASP:H	8	0.9
(1,3145)	1:132:B:LEU:HD11	1:134:B:THR:H	4	0.9
(1,3145)	1:132:B:LEU:HD12	1:134:B:THR:H	4	0.9
(1,3145)	1:132:B:LEU:HD13	1:134:B:THR:H	4	0.9
(1,3074)	1:125:B:TYR:HB2	1:142:B:ARG:H	18	0.9
(1,3074)	1:125:B:TYR:HB3	1:142:B:ARG:H	18	0.9
(1,3002)	1:118:B:TYR:HB2	1:148:B:SER:HB2	1	0.9
(1,3002)	1:118:B:TYR:HB2	1:148:B:SER:HB3	1	0.9
(1,3002)	1:118:B:TYR:HB3	1:148:B:SER:HB2	1	0.9
(1,3002)	1:118:B:TYR:HB3	1:148:B:SER:HB3	1	0.9
(1,2995)	1:118:B:TYR:HA	1:145:B:ALA:HA	18	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2939)	1:113:B:MET:HA	1:116:B:LYS:HA	1	0.9
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	5	0.9
(1,2583)	1:207:A:ALA:HA	1:211:A:ASP:H	1	0.9
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	3	0.9
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	3	0.9
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	3	0.9
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	3	0.9
(1,2245)	1:171:A:ARG:HA	1:175:A:ARG:H	9	0.9
(1,2244)	1:171:A:ARG:HA	1:174:A:SER:HA	11	0.9
(1,2004)	1:147:A:SER:HA	1:150:A:LYS:HA	17	0.9
(1,1951)	1:143:A:ALA:HA	1:155:A:ALA:HA	8	0.9
(1,1572)	1:108:A:GLN:HA	1:111:A:LYS:H	18	0.9
(1,1522)	1:104:A:ASP:H	1:107:A:MET:H	1	0.9
(1,1391)	1:44:A:PHE:HE1	1:19:B:ILE:HG12	9	0.9
(1,1391)	1:44:A:PHE:HE1	1:19:B:ILE:HG13	9	0.9
(1,1391)	1:44:A:PHE:HE2	1:19:B:ILE:HG12	9	0.9
(1,1391)	1:44:A:PHE:HE2	1:19:B:ILE:HG13	9	0.9
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	6	0.9
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	6	0.9
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	3	0.9
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	3	0.9
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	3	0.9
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	6	0.9
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	6	0.9
(1,1106)	1:54:B:ILE:HA	1:57:B:LYS:HG2	1	0.9
(1,1106)	1:54:B:ILE:HA	1:57:B:LYS:HG3	1	0.9
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE1	10	0.9
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE2	10	0.9
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE3	10	0.9
(1,634)	1:5:B:LYS:HA	1:8:B:ILE:H	6	0.9
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD11	12	0.9
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD12	12	0.9
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD13	12	0.9
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD11	12	0.9
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD12	12	0.9
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD13	12	0.9
(1,172)	1:16:A:PHE:HA	1:18:A:SER:HB2	19	0.9
(1,172)	1:16:A:PHE:HA	1:18:A:SER:HB3	19	0.9
(1,4088)	1:321:A:ARG:H	1:322:A:ASN:H	3	0.89
(1,4048)	1:238:A:VAL:H	1:239:A:ASP:H	7	0.89
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	2	0.89
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	2	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4032)	1:226:B:GLU:HA	1:227:B:LYS:H	14	0.89
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	12	0.89
(1,3921)	1:211:B:ASP:HA	1:215:B:ALA:H	16	0.89
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	3	0.89
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG21	12	0.89
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG22	12	0.89
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG23	12	0.89
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	1	0.89
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB1	2	0.89
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB2	2	0.89
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB3	2	0.89
(1,3434)	1:159:B:ALA:HB1	1:176:B:LEU:HD11	9	0.89
(1,3434)	1:159:B:ALA:HB1	1:176:B:LEU:HD12	9	0.89
(1,3434)	1:159:B:ALA:HB1	1:176:B:LEU:HD13	9	0.89
(1,3434)	1:159:B:ALA:HB2	1:176:B:LEU:HD11	9	0.89
(1,3434)	1:159:B:ALA:HB2	1:176:B:LEU:HD12	9	0.89
(1,3434)	1:159:B:ALA:HB2	1:176:B:LEU:HD13	9	0.89
(1,3434)	1:159:B:ALA:HB3	1:176:B:LEU:HD11	9	0.89
(1,3434)	1:159:B:ALA:HB3	1:176:B:LEU:HD12	9	0.89
(1,3434)	1:159:B:ALA:HB3	1:176:B:LEU:HD13	9	0.89
(1,3335)	1:150:B:LYS:HA	1:152:B:TYR:HA	10	0.89
(1,3299)	1:146:B:HIS:HB2	1:154:B:GLN:HB2	8	0.89
(1,3299)	1:146:B:HIS:HB2	1:154:B:GLN:HB3	8	0.89
(1,3299)	1:146:B:HIS:HB3	1:154:B:GLN:HB2	8	0.89
(1,3299)	1:146:B:HIS:HB3	1:154:B:GLN:HB3	8	0.89
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	7	0.89
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	10	0.89
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	13	0.89
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	13	0.89
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	13	0.89
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	13	0.89
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	10	0.89
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	10	0.89
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE1	10	0.89
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE2	10	0.89
(1,2741)	1:94:B:ASP:H	1:95:B:ASP:H	15	0.89
(1,2713)	1:223:A:LEU:HA	1:225:A:LEU:H	17	0.89
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	14	0.89
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	14	0.89
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	14	0.89
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	9	0.89
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	17	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	17	0.89
(1,2453)	1:193:A:TYR:HB2	1:212:A:TYR:HA	15	0.89
(1,2453)	1:193:A:TYR:HB3	1:212:A:TYR:HA	15	0.89
(1,2033)	1:150:A:LYS:HB2	1:152:A:TYR:HE2	2	0.89
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	5	0.89
(1,1011)	1:41:B:SER:HA	1:46:B:PHE:H	16	0.89
(1,878)	1:27:B:GLU:H	1:28:B:ASP:H	20	0.89
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	18	0.89
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	18	0.89
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD21	12	0.89
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD22	12	0.89
(1,3878)	1:206:B:GLU:HA	1:210:B:ARG:H	7	0.88
(1,3791)	1:195:B:LYS:HA	1:199:B:ILE:H	18	0.88
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	3	0.88
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	19	0.88
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	19	0.88
(1,3313)	1:147:B:SER:HA	1:152:B:TYR:HA	8	0.88
(1,3145)	1:132:B:LEU:HD11	1:134:B:THR:H	20	0.88
(1,3145)	1:132:B:LEU:HD12	1:134:B:THR:H	20	0.88
(1,3145)	1:132:B:LEU:HD13	1:134:B:THR:H	20	0.88
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	7	0.88
(1,2895)	1:110:B:ASN:H	1:125:B:TYR:HE1	3	0.88
(1,2895)	1:110:B:ASN:H	1:125:B:TYR:HE2	3	0.88
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	11	0.88
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	11	0.88
(1,2872)	1:107:B:MET:HA	1:111:B:LYS:H	3	0.88
(1,2846)	1:105:B:LEU:HD11	1:128:B:ALA:HA	14	0.88
(1,2846)	1:105:B:LEU:HD12	1:128:B:ALA:HA	14	0.88
(1,2846)	1:105:B:LEU:HD13	1:128:B:ALA:HA	14	0.88
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	6	0.88
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	1	0.88
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	14	0.88
(1,2664)	1:217:A:LYS:HA	1:220:A:GLU:H	18	0.88
(1,2615)	1:211:A:ASP:HA	1:215:A:ALA:H	18	0.88
(1,2342)	1:180:A:LYS:HB2	1:185:A:LYS:H	3	0.88
(1,2342)	1:180:A:LYS:HB3	1:185:A:LYS:H	3	0.88
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	8	0.88
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	2	0.88
(1,1527)	1:104:A:ASP:HA	1:107:A:MET:H	19	0.88
(1,1411)	1:67:A:ASP:HA	1:62:B:GLY:H	19	0.88
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	2	0.88
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	2	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	19	0.88
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	20	0.88
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	13	0.88
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	20	0.88
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	7	0.88
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	7	0.88
(1,1114)	1:55:B:LEU:HD11	1:71:B:SER:HA	14	0.88
(1,1114)	1:55:B:LEU:HD12	1:71:B:SER:HA	14	0.88
(1,1114)	1:55:B:LEU:HD13	1:71:B:SER:HA	14	0.88
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	8	0.88
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	8	0.88
(1,634)	1:5:B:LYS:HA	1:8:B:ILE:H	17	0.88
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	3	0.88
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	3	0.88
(1,172)	1:16:A:PHE:HA	1:18:A:SER:HB2	18	0.88
(1,172)	1:16:A:PHE:HA	1:18:A:SER:HB3	18	0.88
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	1	0.87
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	13	0.87
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	14	0.87
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	14	0.87
(1,3673)	1:181:B:TYR:HE1	1:218:B:LYS:HE2	9	0.87
(1,3673)	1:181:B:TYR:HE1	1:218:B:LYS:HE3	9	0.87
(1,3673)	1:181:B:TYR:HE2	1:218:B:LYS:HE2	9	0.87
(1,3673)	1:181:B:TYR:HE2	1:218:B:LYS:HE3	9	0.87
(1,3593)	1:175:B:ARG:HA	1:178:B:PHE:H	7	0.87
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	2	0.87
(1,2871)	1:107:B:MET:HA	1:110:B:ASN:H	7	0.87
(1,2828)	1:104:B:ASP:H	1:107:B:MET:H	6	0.87
(1,2828)	1:104:B:ASP:H	1:107:B:MET:H	7	0.87
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	13	0.87
(1,2719)	1:224:A:ASN:HA	1:226:A:GLU:H	1	0.87
(1,2719)	1:224:A:ASN:HA	1:226:A:GLU:H	17	0.87
(1,2469)	1:194:A:LYS:H	1:212:A:TYR:HA	6	0.87
(1,2279)	1:174:A:SER:HA	1:193:A:TYR:HA	12	0.87
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	4	0.87
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD2	2	0.87
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD3	2	0.87
(1,1626)	1:113:A:MET:H	1:121:A:ALA:H	18	0.87
(1,1518)	1:103:A:GLU:HA	1:106:A:LYS:H	5	0.87
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB1	15	0.87
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB2	15	0.87
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB3	15	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	13	0.87
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	13	0.87
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	13	0.87
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	3	0.87
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	3	0.87
(1,1325)	1:33:A:LEU:HA	1:40:B:ILE:HA	16	0.87
(1,1278)	1:16:A:PHE:HA	1:44:B:PHE:HZ	4	0.87
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	15	0.87
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	15	0.87
(1,1010)	1:41:B:SER:HA	1:45:B:GLY:H	3	0.87
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	7	0.87
(1,835)	1:20:B:VAL:HA	1:24:B:GLU:H	3	0.87
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	7	0.87
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	7	0.87
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD11	11	0.87
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD12	11	0.87
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD13	11	0.87
(1,96)	1:11:A:LEU:HD11	1:12:A:ILE:HA	16	0.87
(1,96)	1:11:A:LEU:HD12	1:12:A:ILE:HA	16	0.87
(1,96)	1:11:A:LEU:HD13	1:12:A:ILE:HA	16	0.87
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	13	0.86
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	8	0.86
(1,4048)	1:238:A:VAL:H	1:239:A:ASP:H	9	0.86
(1,3931)	1:212:B:TYR:HD1	1:213:B:GLU:HA	17	0.86
(1,3931)	1:212:B:TYR:HD2	1:213:B:GLU:HA	17	0.86
(1,3846)	1:202:B:ASP:HA	1:204:B:ALA:H	4	0.86
(1,3839)	1:201:B:GLY:H	1:203:B:ASN:H	16	0.86
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	8	0.86
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	2	0.86
(1,3291)	1:146:B:HIS:H	1:155:B:ALA:HA	11	0.86
(1,3147)	1:134:B:THR:H	1:135:B:ASN:H	18	0.86
(1,3075)	1:125:B:TYR:HB2	1:142:B:ARG:HA	18	0.86
(1,3075)	1:125:B:TYR:HB3	1:142:B:ARG:HA	18	0.86
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	15	0.86
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	15	0.86
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	15	0.86
(1,2697)	1:221:A:GLN:HA	1:224:A:ASN:H	13	0.86
(1,2669)	1:218:A:LYS:H	1:221:A:GLN:H	10	0.86
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	7	0.86
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	20	0.86
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	1	0.86
(1,1519)	1:103:A:GLU:HA	1:107:A:MET:H	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	6	0.86
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	9	0.86
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	19	0.86
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	8	0.86
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	8	0.86
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	4	0.86
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	4	0.86
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	4	0.86
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	4	0.86
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	18	0.86
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	6	0.86
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	6	0.86
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	9	0.86
(1,1075)	1:50:B:ALA:H	1:51:B:VAL:H	1	0.86
(1,1011)	1:41:B:SER:HA	1:46:B:PHE:H	3	0.86
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	15	0.86
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	5	0.86
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	5	0.86
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	6	0.86
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	11	0.86
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	11	0.86
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	18	0.86
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	2	0.86
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	2	0.86
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	18	0.85
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	18	0.85
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	18	0.85
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	12	0.85
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	5	0.85
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	15	0.85
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	10	0.85
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	8	0.85
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	10	0.85
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	9	0.85
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	9	0.85
(1,4032)	1:226:B:GLU:HA	1:227:B:LYS:H	7	0.85
(1,4027)	1:225:B:LEU:H	1:226:B:GLU:H	20	0.85
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	5	0.85
(1,3646)	1:180:B:LYS:HA	1:185:B:LYS:H	7	0.85
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG2	10	0.85
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG3	10	0.85
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG2	10	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG3	10	0.85
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	6	0.85
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB2	17	0.85
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB3	17	0.85
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	7	0.85
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	7	0.85
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	5	0.85
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	5	0.85
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	5	0.85
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	15	0.85
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	15	0.85
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	17	0.85
(1,2824)	1:103:B:GLU:HA	1:106:B:LYS:H	17	0.85
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD11	17	0.85
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD12	17	0.85
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD13	17	0.85
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB1	9	0.85
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB2	9	0.85
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB3	9	0.85
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	13	0.85
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	13	0.85
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	13	0.85
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	13	0.85
(1,2423)	1:190:A:LEU:HD21	1:216:A:LYS:HA	16	0.85
(1,2423)	1:190:A:LEU:HD22	1:216:A:LYS:HA	16	0.85
(1,2423)	1:190:A:LEU:HD23	1:216:A:LYS:HA	16	0.85
(1,2421)	1:190:A:LEU:HD11	1:216:A:LYS:H	14	0.85
(1,2421)	1:190:A:LEU:HD12	1:216:A:LYS:H	14	0.85
(1,2421)	1:190:A:LEU:HD13	1:216:A:LYS:H	14	0.85
(1,1946)	1:143:A:ALA:H	1:155:A:ALA:HA	8	0.85
(1,1761)	1:125:A:TYR:HA	1:129:A:ILE:H	3	0.85
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB2	4	0.85
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB3	4	0.85
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	15	0.85
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	17	0.85
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	17	0.85
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	17	0.85
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	17	0.85
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	17	0.85
(1,1265)	1:15:A:TYR:HE1	1:2:B:SER:HB2	10	0.85
(1,1265)	1:15:A:TYR:HE1	1:2:B:SER:HB3	10	0.85
(1,1265)	1:15:A:TYR:HE2	1:2:B:SER:HB2	10	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:15:A:TYR:HE2	1:2:B:SER:HB3	10	0.85
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	18	0.85
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD11	17	0.85
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD12	17	0.85
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD13	17	0.85
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	5	0.85
(1,1062)	1:48:B:ARG:H	1:49:B:GLU:H	1	0.85
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	9	0.85
(1,878)	1:27:B:GLU:H	1:28:B:ASP:H	11	0.85
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	14	0.85
(1,445)	1:47:A:GLU:H	1:50:A:ALA:H	4	0.85
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD21	17	0.85
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD22	17	0.85
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	13	0.84
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	3	0.84
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	18	0.84
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	18	0.84
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	18	0.84
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	7	0.84
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE1	11	0.84
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE2	11	0.84
(1,3837)	1:200:B:GLU:HB2	1:208:B:MET:HE3	11	0.84
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE1	11	0.84
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE2	11	0.84
(1,3837)	1:200:B:GLU:HB3	1:208:B:MET:HE3	11	0.84
(1,3810)	1:197:B:LEU:HA	1:204:B:ALA:HA	3	0.84
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	6	0.84
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	6	0.84
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	6	0.84
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	6	0.84
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	3	0.84
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	3	0.84
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	3	0.84
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	3	0.84
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	3	0.84
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	3	0.84
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD11	17	0.84
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD12	17	0.84
(1,3495)	1:169:B:TYR:H	1:199:B:ILE:HD13	17	0.84
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG2	14	0.84
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE2	19	0.84
(1,2788)	1:101:B:LYS:H	1:102:B:ALA:H	12	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	11	0.84
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	11	0.84
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	11	0.84
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	13	0.84
(1,2464)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	9	0.84
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG21	7	0.84
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG22	7	0.84
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG23	7	0.84
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	8	0.84
(1,2067)	1:153:A:ASP:HA	1:156:A:VAL:H	11	0.84
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	7	0.84
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	7	0.84
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	11	0.84
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	14	0.84
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	14	0.84
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	14	0.84
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	8	0.84
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	16	0.84
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	16	0.84
(1,1393)	1:44:A:PHE:HE1	1:25:B:ILE:HD11	2	0.84
(1,1393)	1:44:A:PHE:HE2	1:25:B:ILE:HD11	2	0.84
(1,1314)	1:29:A:GLY:HA2	1:43:B:ALA:H	11	0.84
(1,1314)	1:29:A:GLY:HA3	1:43:B:ALA:H	11	0.84
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	19	0.84
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	19	0.84
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	19	0.84
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	19	0.84
(1,1266)	1:15:A:TYR:HE1	1:5:B:LYS:H	10	0.84
(1,1266)	1:15:A:TYR:HE2	1:5:B:LYS:H	10	0.84
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	17	0.84
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	12	0.84
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	7	0.84
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	20	0.84
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	1	0.84
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	1	0.84
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB1	2	0.84
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB2	2	0.84
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB3	2	0.84
(1,452)	1:47:A:GLU:HB2	1:49:A:GLU:H	17	0.84
(1,452)	1:47:A:GLU:HB3	1:49:A:GLU:H	17	0.84
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	3	0.84
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	3	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4019)	1:223:B:LEU:HA	1:225:B:LEU:H	13	0.83
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	11	0.83
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	7	0.83
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	7	0.83
(1,3599)	1:176:B:LEU:HA	1:180:B:LYS:H	13	0.83
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	1	0.83
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	1	0.83
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	1	0.83
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	1	0.83
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	1	0.83
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	1	0.83
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	7	0.83
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	7	0.83
(1,3081)	1:125:B:TYR:HE1	1:142:B:ARG:HA	20	0.83
(1,3081)	1:125:B:TYR:HE2	1:142:B:ARG:HA	20	0.83
(1,2992)	1:118:B:TYR:HA	1:121:B:ALA:H	7	0.83
(1,2779)	1:99:B:LYS:HA	1:101:B:LYS:H	12	0.83
(1,2737)	1:93:B:GLU:HA	1:95:B:ASP:H	2	0.83
(1,2714)	1:223:A:LEU:HA	1:226:A:GLU:H	4	0.83
(1,2645)	1:215:A:ALA:H	1:218:A:LYS:H	9	0.83
(1,2555)	1:205:A:THR:H	1:209:A:LYS:H	12	0.83
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	11	0.83
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	11	0.83
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	11	0.83
(1,1536)	1:105:A:LEU:HA	1:109:A:GLY:H	20	0.83
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	11	0.83
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	11	0.83
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	11	0.83
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB2	12	0.83
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB3	12	0.83
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	10	0.83
(1,1431)	1:93:A:GLU:HA	1:95:A:ASP:H	14	0.83
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	2	0.83
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	2	0.83
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	9	0.83
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	9	0.83
(1,1282)	1:16:A:PHE:HE1	1:9:B:ALA:HB2	8	0.83
(1,1282)	1:16:A:PHE:HE2	1:9:B:ALA:HB2	8	0.83
(1,1274)	1:15:A:TYR:HH	1:5:B:LYS:HA	19	0.83
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	1	0.83
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	13	0.83
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD11	10	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD12	10	0.83
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD13	10	0.83
(1,1133)	1:58:B:SER:HB2	1:60:B:PHE:H	12	0.83
(1,1133)	1:58:B:SER:HB3	1:60:B:PHE:H	12	0.83
(1,1114)	1:55:B:LEU:HD11	1:71:B:SER:HA	15	0.83
(1,1114)	1:55:B:LEU:HD12	1:71:B:SER:HA	15	0.83
(1,1114)	1:55:B:LEU:HD13	1:71:B:SER:HA	15	0.83
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD11	10	0.83
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD12	10	0.83
(1,668)	1:9:B:ALA:HA	1:12:B:ILE:HD13	10	0.83
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	19	0.83
(1,458)	1:48:A:ARG:HA	1:50:A:ALA:H	4	0.83
(1,4105)	1:338:A:GLU:H	1:339:A:THR:H	2	0.82
(1,3998)	1:221:B:GLN:H	1:222:B:SER:H	9	0.82
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	16	0.82
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG21	8	0.82
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG22	8	0.82
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG23	8	0.82
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	10	0.82
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	10	0.82
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	17	0.82
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	18	0.82
(1,2941)	1:113:B:MET:HA	1:118:B:TYR:HA	2	0.82
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	9	0.82
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	10	0.82
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	13	0.82
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	13	0.82
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	13	0.82
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	9	0.82
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	12	0.82
(1,2526)	1:200:A:GLU:HA	1:203:A:ASN:H	9	0.82
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	16	0.82
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	4	0.82
(1,1536)	1:105:A:LEU:HA	1:109:A:GLY:H	13	0.82
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	5	0.82
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	5	0.82
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	20	0.82
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	6	0.82
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	18	0.82
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	12	0.82
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	12	0.82
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	20	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	20	0.82
(1,1135)	1:59:B:GLU:H	1:60:B:PHE:HA	17	0.82
(1,1128)	1:58:B:SER:HA	1:59:B:GLU:H	5	0.82
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	6	0.82
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	6	0.82
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	6	0.82
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	6	0.82
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	15	0.82
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	15	0.82
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	20	0.82
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE2	9	0.82
(1,498)	1:54:A:ILE:HA	1:57:A:LYS:HE3	9	0.82
(1,225)	1:20:A:VAL:HA	1:23:A:LYS:HA	14	0.82
(1,143)	1:14:A:ASN:HA	1:18:A:SER:H	10	0.82
(1,41)	1:7:A:GLU:HA	1:55:A:LEU:HD21	3	0.82
(1,41)	1:7:A:GLU:HA	1:55:A:LEU:HD22	3	0.82
(1,41)	1:7:A:GLU:HA	1:55:A:LEU:HD23	3	0.82
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	8	0.81
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	12	0.81
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	19	0.81
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	19	0.81
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB2	19	0.81
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	19	0.81
(1,3648)	1:180:B:LYS:HB2	1:185:B:LYS:H	9	0.81
(1,3648)	1:180:B:LYS:HB3	1:185:B:LYS:H	9	0.81
(1,3641)	1:180:B:LYS:H	1:189:B:ALA:HA	2	0.81
(1,3452)	1:161:B:SER:HA	1:165:B:ILE:H	3	0.81
(1,3399)	1:156:B:VAL:HG11	1:157:B:LYS:HA	13	0.81
(1,3399)	1:156:B:VAL:HG12	1:157:B:LYS:HA	13	0.81
(1,3399)	1:156:B:VAL:HG13	1:157:B:LYS:HA	13	0.81
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD11	9	0.81
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD12	9	0.81
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD13	9	0.81
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB1	13	0.81
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB2	13	0.81
(1,3365)	1:152:B:TYR:HE1	1:182:B:ALA:HB3	13	0.81
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB1	13	0.81
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB2	13	0.81
(1,3365)	1:152:B:TYR:HE2	1:182:B:ALA:HB3	13	0.81
(1,3147)	1:134:B:THR:H	1:135:B:ASN:H	6	0.81
(1,3082)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	18	0.81
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	5	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	5	0.81
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	5	0.81
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	5	0.81
(1,2833)	1:104:B:ASP:HA	1:107:B:MET:H	19	0.81
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE1	18	0.81
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE2	18	0.81
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE3	18	0.81
(1,2783)	1:100:B:ALA:H	1:102:B:ALA:H	12	0.81
(1,2215)	1:170:A:PHE:HA	1:174:A:SER:H	9	0.81
(1,1813)	1:129:A:ILE:HA	1:133:A:PRO:HA	11	0.81
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD2	4	0.81
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD3	4	0.81
(1,1474)	1:99:A:LYS:HA	1:102:A:ALA:H	17	0.81
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	7	0.81
(1,1393)	1:44:A:PHE:HE1	1:25:B:ILE:HD11	12	0.81
(1,1393)	1:44:A:PHE:HE2	1:25:B:ILE:HD11	12	0.81
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	1	0.81
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	1	0.81
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	12	0.81
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	20	0.81
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	20	0.81
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	1	0.81
(1,1150)	1:60:B:PHE:HB2	1:63:B:GLN:H	4	0.81
(1,1150)	1:60:B:PHE:HB3	1:63:B:GLN:H	4	0.81
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	4	0.81
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	4	0.81
(1,892)	1:28:B:ASP:HA	1:31:B:ASP:H	10	0.81
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	11	0.81
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	17	0.81
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	1	0.81
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	14	0.81
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB2	19	0.81
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB3	19	0.81
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	4	0.81
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	4	0.81
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	20	0.8
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	16	0.8
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	2	0.8
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	17	0.8
(1,3878)	1:206:B:GLU:HA	1:210:B:ARG:H	16	0.8
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	7	0.8
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	7	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3832)	1:200:B:GLU:HA	1:203:B:ASN:H	6	0.8
(1,3798)	1:196:B:VAL:HG11	1:197:B:LEU:HA	11	0.8
(1,3798)	1:196:B:VAL:HG12	1:197:B:LEU:HA	11	0.8
(1,3798)	1:196:B:VAL:HG13	1:197:B:LEU:HA	11	0.8
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG21	11	0.8
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG22	11	0.8
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG23	11	0.8
(1,3654)	1:181:B:TYR:H	1:185:B:LYS:H	7	0.8
(1,3206)	1:139:B:TYR:HA	1:158:B:ASP:HA	2	0.8
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	5	0.8
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	12	0.8
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	12	0.8
(1,2973)	1:116:B:LYS:HA	1:118:B:TYR:HA	3	0.8
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	7	0.8
(1,2763)	1:97:B:GLU:H	1:99:B:LYS:H	15	0.8
(1,2714)	1:223:A:LEU:HA	1:226:A:GLU:H	5	0.8
(1,2583)	1:207:A:ALA:HA	1:211:A:ASP:H	7	0.8
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	18	0.8
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	18	0.8
(1,2009)	1:147:A:SER:HA	1:179:A:ALA:HA	15	0.8
(1,1767)	1:125:A:TYR:HB2	1:139:A:TYR:H	11	0.8
(1,1767)	1:125:A:TYR:HB3	1:139:A:TYR:H	11	0.8
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	17	0.8
(1,1386)	1:44:A:PHE:HE1	1:16:B:PHE:HD1	3	0.8
(1,1386)	1:44:A:PHE:HE2	1:16:B:PHE:HD1	3	0.8
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG12	9	0.8
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG13	9	0.8
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	14	0.8
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	14	0.8
(1,1313)	1:29:A:GLY:H	1:43:B:ALA:HA	15	0.8
(1,1308)	1:25:A:ILE:HD11	1:43:B:ALA:HA	5	0.8
(1,1308)	1:25:A:ILE:HD12	1:43:B:ALA:HA	5	0.8
(1,1308)	1:25:A:ILE:HD13	1:43:B:ALA:HA	5	0.8
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	5	0.8
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	5	0.8
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	5	0.8
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	5	0.8
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	3	0.8
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	3	0.8
(1,1281)	1:16:A:PHE:HE1	1:9:B:ALA:HB1	7	0.8
(1,1281)	1:16:A:PHE:HE2	1:9:B:ALA:HB1	7	0.8
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	19	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	12	0.8
(1,1106)	1:54:B:ILE:HA	1:57:B:LYS:HG2	17	0.8
(1,1106)	1:54:B:ILE:HA	1:57:B:LYS:HG3	17	0.8
(1,945)	1:34:B:ASN:HA	1:38:B:ASP:H	3	0.8
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	20	0.8
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	20	0.8
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	20	0.8
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	20	0.8
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD21	17	0.8
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD22	17	0.8
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD23	17	0.8
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	6	0.8
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	1	0.8
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	1	0.8
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	5	0.8
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	5	0.8
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	7	0.79
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	7	0.79
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	7	0.79
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	18	0.79
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	11	0.79
(1,4105)	1:338:A:GLU:H	1:339:A:THR:H	6	0.79
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	1	0.79
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	1	0.79
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	8	0.79
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	8	0.79
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	4	0.79
(1,3147)	1:134:B:THR:H	1:135:B:ASN:H	15	0.79
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	18	0.79
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	15	0.79
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	15	0.79
(1,2948)	1:113:B:MET:HE1	1:142:B:ARG:HA	6	0.79
(1,2948)	1:113:B:MET:HE2	1:142:B:ARG:HA	6	0.79
(1,2948)	1:113:B:MET:HE3	1:142:B:ARG:HA	6	0.79
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD21	20	0.79
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD22	20	0.79
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD23	20	0.79
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	9	0.79
(1,2779)	1:99:B:LYS:HA	1:101:B:LYS:H	5	0.79
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	6	0.79
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	6	0.79
(1,2419)	1:190:A:LEU:HD11	1:212:A:TYR:HA	14	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2419)	1:190:A:LEU:HD12	1:212:A:TYR:HA	14	0.79
(1,2419)	1:190:A:LEU:HD13	1:212:A:TYR:HA	14	0.79
(1,2205)	1:169:A:TYR:HD1	1:171:A:ARG:H	14	0.79
(1,1431)	1:93:A:GLU:HA	1:95:A:ASP:H	4	0.79
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB2	16	0.79
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB3	16	0.79
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB2	16	0.79
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB3	16	0.79
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB2	16	0.79
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB3	16	0.79
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	7	0.79
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	7	0.79
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	7	0.79
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	7	0.79
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	7	0.79
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	7	0.79
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB2	14	0.79
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB3	14	0.79
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	6	0.79
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	19	0.79
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	5	0.79
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD11	4	0.79
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD12	4	0.79
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD13	4	0.79
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	9	0.79
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	1	0.79
(1,529)	1:59:A:GLU:HA	1:64:A:HIS:HA	11	0.79
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	19	0.78
(1,3840)	1:201:B:GLY:H	1:204:B:ALA:H	4	0.78
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	1	0.78
(1,3808)	1:197:B:LEU:HA	1:200:B:GLU:H	8	0.78
(1,3626)	1:178:B:PHE:HA	1:182:B:ALA:H	17	0.78
(1,3543)	1:170:B:PHE:HE2	1:208:B:MET:HE1	11	0.78
(1,3357)	1:152:B:TYR:HA	1:156:B:VAL:H	8	0.78
(1,3278)	1:144:B:ALA:HB1	1:175:B:ARG:HD2	13	0.78
(1,3278)	1:144:B:ALA:HB1	1:175:B:ARG:HD3	13	0.78
(1,3278)	1:144:B:ALA:HB2	1:175:B:ARG:HD2	13	0.78
(1,3278)	1:144:B:ALA:HB2	1:175:B:ARG:HD3	13	0.78
(1,3278)	1:144:B:ALA:HB3	1:175:B:ARG:HD2	13	0.78
(1,3278)	1:144:B:ALA:HB3	1:175:B:ARG:HD3	13	0.78
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	3	0.78
(1,3041)	1:122:B:ILE:HA	1:126:B:THR:H	12	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2995)	1:118:B:TYR:HA	1:145:B:ALA:HA	1	0.78
(1,2933)	1:113:B:MET:H	1:121:B:ALA:HA	12	0.78
(1,2820)	1:103:B:GLU:H	1:106:B:LYS:H	7	0.78
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	19	0.78
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	6	0.78
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	6	0.78
(1,2572)	1:206:A:GLU:HA	1:210:A:ARG:H	12	0.78
(1,2463)	1:193:A:TYR:HD2	1:211:A:ASP:HA	8	0.78
(1,2349)	1:181:A:TYR:H	1:186:A:PRO:HA	14	0.78
(1,1946)	1:143:A:ALA:H	1:155:A:ALA:HA	7	0.78
(1,1900)	1:139:A:TYR:HA	1:158:A:ASP:HA	8	0.78
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	8	0.78
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE1	19	0.78
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE2	19	0.78
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE3	19	0.78
(1,1507)	1:102:A:ALA:HB1	1:128:A:ALA:HA	6	0.78
(1,1507)	1:102:A:ALA:HB2	1:128:A:ALA:HA	6	0.78
(1,1507)	1:102:A:ALA:HB3	1:128:A:ALA:HA	6	0.78
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	3	0.78
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	3	0.78
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	3	0.78
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	1	0.78
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	6	0.78
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	19	0.78
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	19	0.78
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	13	0.78
(1,1321)	1:32:A:SER:HB2	1:43:B:ALA:H	11	0.78
(1,1321)	1:32:A:SER:HB3	1:43:B:ALA:H	11	0.78
(1,1268)	1:15:A:TYR:HE1	1:5:B:LYS:HB2	6	0.78
(1,1268)	1:15:A:TYR:HE1	1:5:B:LYS:HB3	6	0.78
(1,1268)	1:15:A:TYR:HE2	1:5:B:LYS:HB2	6	0.78
(1,1268)	1:15:A:TYR:HE2	1:5:B:LYS:HB3	6	0.78
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	13	0.78
(1,1140)	1:59:B:GLU:HB2	1:64:B:HIS:HA	12	0.78
(1,1140)	1:59:B:GLU:HB3	1:64:B:HIS:HA	12	0.78
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD11	12	0.78
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD12	12	0.78
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD13	12	0.78
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	13	0.78
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	6	0.77
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	6	0.77
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	6	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	12	0.77
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	10	0.77
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	3	0.77
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	19	0.77
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	3	0.77
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	3	0.77
(1,3982)	1:219:B:VAL:H	1:220:B:GLU:H	3	0.77
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	15	0.77
(1,3834)	1:200:B:GLU:HB2	1:204:B:ALA:H	12	0.77
(1,3834)	1:200:B:GLU:HB3	1:204:B:ALA:H	12	0.77
(1,3749)	1:193:B:TYR:H	1:212:B:TYR:HA	10	0.77
(1,3496)	1:169:B:TYR:HA	1:170:B:PHE:H	19	0.77
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	7	0.77
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	7	0.77
(1,2850)	1:105:B:LEU:HD21	1:124:B:LYS:HA	20	0.77
(1,2850)	1:105:B:LEU:HD22	1:124:B:LYS:HA	20	0.77
(1,2850)	1:105:B:LEU:HD23	1:124:B:LYS:HA	20	0.77
(1,2469)	1:194:A:LYS:H	1:212:A:TYR:HA	13	0.77
(1,2419)	1:190:A:LEU:HD11	1:212:A:TYR:HA	13	0.77
(1,2419)	1:190:A:LEU:HD12	1:212:A:TYR:HA	13	0.77
(1,2419)	1:190:A:LEU:HD13	1:212:A:TYR:HA	13	0.77
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	12	0.77
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	13	0.77
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	13	0.77
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	13	0.77
(1,1412)	1:67:A:ASP:HB2	1:60:B:PHE:HB2	18	0.77
(1,1412)	1:67:A:ASP:HB2	1:60:B:PHE:HB3	18	0.77
(1,1412)	1:67:A:ASP:HB3	1:60:B:PHE:HB2	18	0.77
(1,1412)	1:67:A:ASP:HB3	1:60:B:PHE:HB3	18	0.77
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	7	0.77
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD11	10	0.77
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD12	10	0.77
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD13	10	0.77
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	9	0.77
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	9	0.77
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	7	0.77
(1,1117)	1:56:B:GLY:H	1:57:B:LYS:H	17	0.77
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	19	0.77
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	13	0.77
(1,834)	1:20:B:VAL:HA	1:23:B:LYS:HA	7	0.77
(1,772)	1:15:B:TYR:HD1	1:18:B:SER:HB2	4	0.77
(1,772)	1:15:B:TYR:HD1	1:18:B:SER:HB3	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:15:B:TYR:HD2	1:18:B:SER:HB2	4	0.77
(1,772)	1:15:B:TYR:HD2	1:18:B:SER:HB3	4	0.77
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	12	0.77
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	8	0.77
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	12	0.77
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	12	0.77
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	1	0.76
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	2	0.76
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	15	0.76
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	18	0.76
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	16	0.76
(1,3913)	1:210:B:ARG:HA	1:214:B:SER:H	6	0.76
(1,3729)	1:190:B:LEU:HD21	1:216:B:LYS:HA	6	0.76
(1,3729)	1:190:B:LEU:HD22	1:216:B:LYS:HA	6	0.76
(1,3729)	1:190:B:LEU:HD23	1:216:B:LYS:HA	6	0.76
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	8	0.76
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE1	7	0.76
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE2	7	0.76
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE3	7	0.76
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE1	7	0.76
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE2	7	0.76
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE3	7	0.76
(1,3339)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	8	0.76
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	15	0.76
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	15	0.76
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	3	0.76
(1,2697)	1:221:A:GLN:HA	1:224:A:ASN:H	6	0.76
(1,2450)	1:193:A:TYR:HA	1:197:A:LEU:H	15	0.76
(1,2349)	1:181:A:TYR:H	1:186:A:PRO:HA	16	0.76
(1,2216)	1:170:A:PHE:HA	1:196:A:VAL:HA	8	0.76
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	8	0.76
(1,1946)	1:143:A:ALA:H	1:155:A:ALA:HA	9	0.76
(1,1645)	1:113:A:MET:HE1	1:145:A:ALA:H	3	0.76
(1,1645)	1:113:A:MET:HE2	1:145:A:ALA:H	3	0.76
(1,1645)	1:113:A:MET:HE3	1:145:A:ALA:H	3	0.76
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	9	0.76
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	20	0.76
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	20	0.76
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	20	0.76
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	20	0.76
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	3	0.76
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB2	19	0.76
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB3	19	0.76
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB2	19	0.76
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB3	19	0.76
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB2	19	0.76
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB3	19	0.76
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	11	0.76
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	11	0.76
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	14	0.76
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	14	0.76
(1,857)	1:23:B:LYS:H	1:25:B:ILE:H	20	0.76
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	16	0.76
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	3	0.76
(1,3913)	1:210:B:ARG:HA	1:214:B:SER:H	16	0.75
(1,3898)	1:208:B:MET:HA	1:211:B:ASP:H	8	0.75
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	4	0.75
(1,3725)	1:190:B:LEU:HD11	1:212:B:TYR:HA	14	0.75
(1,3725)	1:190:B:LEU:HD12	1:212:B:TYR:HA	14	0.75
(1,3725)	1:190:B:LEU:HD13	1:212:B:TYR:HA	14	0.75
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG21	3	0.75
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG22	3	0.75
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG23	3	0.75
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	18	0.75
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	18	0.75
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	18	0.75
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	18	0.75
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB1	11	0.75
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB2	11	0.75
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB3	11	0.75
(1,3550)	1:171:B:ARG:HA	1:174:B:SER:HA	3	0.75
(1,3204)	1:139:B:TYR:HA	1:142:B:ARG:H	13	0.75
(1,3159)	1:135:B:ASN:HB2	1:138:B:TYR:H	5	0.75
(1,3159)	1:135:B:ASN:HB3	1:138:B:TYR:H	5	0.75
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	19	0.75
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	19	0.75
(1,2942)	1:113:B:MET:HA	1:121:B:ALA:H	12	0.75
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG11	10	0.75
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG12	10	0.75
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG13	10	0.75
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	18	0.75
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	1	0.75
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	8	0.75
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	8	0.75
(1,2640)	1:214:A:SER:HA	1:217:A:LYS:H	5	0.75
(1,2625)	1:212:A:TYR:HD1	1:213:A:GLU:HA	15	0.75
(1,2625)	1:212:A:TYR:HD2	1:213:A:GLU:HA	15	0.75
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	14	0.75
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	14	0.75
(1,2345)	1:180:A:LYS:HB2	1:189:A:ALA:H	10	0.75
(1,2345)	1:180:A:LYS:HB3	1:189:A:ALA:H	10	0.75
(1,1919)	1:140:A:ALA:H	1:162:A:ALA:HA	10	0.75
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD1	13	0.75
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD2	13	0.75
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD1	13	0.75
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD2	13	0.75
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	9	0.75
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	4	0.75
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	4	0.75
(1,1633)	1:113:A:MET:HA	1:116:A:LYS:HA	20	0.75
(1,1544)	1:105:A:LEU:HD21	1:124:A:LYS:HA	13	0.75
(1,1544)	1:105:A:LEU:HD22	1:124:A:LYS:HA	13	0.75
(1,1544)	1:105:A:LEU:HD23	1:124:A:LYS:HA	13	0.75
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	2	0.75
(1,1419)	1:68:A:ILE:HG21	1:8:B:ILE:HD11	10	0.75
(1,1419)	1:68:A:ILE:HG21	1:8:B:ILE:HD12	10	0.75
(1,1419)	1:68:A:ILE:HG21	1:8:B:ILE:HD13	10	0.75
(1,1419)	1:68:A:ILE:HG22	1:8:B:ILE:HD11	10	0.75
(1,1419)	1:68:A:ILE:HG22	1:8:B:ILE:HD12	10	0.75
(1,1419)	1:68:A:ILE:HG22	1:8:B:ILE:HD13	10	0.75
(1,1419)	1:68:A:ILE:HG23	1:8:B:ILE:HD11	10	0.75
(1,1419)	1:68:A:ILE:HG23	1:8:B:ILE:HD12	10	0.75
(1,1419)	1:68:A:ILE:HG23	1:8:B:ILE:HD13	10	0.75
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	14	0.75
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	14	0.75
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	9	0.75
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	9	0.75
(1,1293)	1:16:A:PHE:HE1	1:40:B:ILE:HG21	5	0.75
(1,1293)	1:16:A:PHE:HE2	1:40:B:ILE:HG21	5	0.75
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	6	0.75
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	20	0.75
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	20	0.75
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG2	16	0.75
(1,1047)	1:46:B:PHE:HA	1:47:B:GLU:HG3	16	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	16	0.75
(1,4159)	1:253:B:GLY:H	1:254:B:SER:H	8	0.74
(1,4145)	1:237:B:ASP:H	1:238:B:VAL:H	17	0.74
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	7	0.74
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	19	0.74
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	19	0.74
(1,3878)	1:206:B:GLU:HA	1:210:B:ARG:H	5	0.74
(1,3738)	1:191:B:GLU:HA	1:195:B:LYS:H	2	0.74
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	8	0.74
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	9	0.74
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	9	0.74
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	17	0.74
(1,3158)	1:135:B:ASN:HA	1:138:B:TYR:H	5	0.74
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	1	0.74
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	11	0.74
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	11	0.74
(1,2800)	1:102:B:ALA:H	1:105:B:LEU:H	5	0.74
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	11	0.74
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	11	0.74
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	11	0.74
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	8	0.74
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	5	0.74
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	5	0.74
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	5	0.74
(1,2669)	1:218:A:LYS:H	1:221:A:GLN:H	9	0.74
(1,2526)	1:200:A:GLU:HA	1:203:A:ASN:H	2	0.74
(1,2343)	1:180:A:LYS:HB2	1:188:A:GLU:H	1	0.74
(1,2343)	1:180:A:LYS:HB3	1:188:A:GLU:H	1	0.74
(1,2261)	1:173:A:TYR:HA	1:192:A:ALA:HA	19	0.74
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB2	7	0.74
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	7	0.74
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB2	7	0.74
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB3	7	0.74
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	16	0.74
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	13	0.74
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG2	11	0.74
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG3	11	0.74
(1,1544)	1:105:A:LEU:HD21	1:124:A:LYS:HA	9	0.74
(1,1544)	1:105:A:LEU:HD22	1:124:A:LYS:HA	9	0.74
(1,1544)	1:105:A:LEU:HD23	1:124:A:LYS:HA	9	0.74
(1,1540)	1:105:A:LEU:HD11	1:128:A:ALA:HA	20	0.74
(1,1540)	1:105:A:LEU:HD12	1:128:A:ALA:HA	20	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1540)	1:105:A:LEU:HD13	1:128:A:ALA:HA	20	0.74
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	17	0.74
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	8	0.74
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	14	0.74
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	14	0.74
(1,1350)	1:39:A:CYS:HB2	1:32:B:SER:HA	11	0.74
(1,1350)	1:39:A:CYS:HB3	1:32:B:SER:HA	11	0.74
(1,1228)	1:2:A:SER:HB2	1:68:B:ILE:HA	19	0.74
(1,1228)	1:2:A:SER:HB3	1:68:B:ILE:HA	19	0.74
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	12	0.74
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	5	0.74
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	18	0.74
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	11	0.74
(1,627)	1:4:B:SER:HA	1:6:B:GLU:H	17	0.74
(1,529)	1:59:A:GLU:HA	1:64:A:HIS:HA	16	0.74
(1,280)	1:28:A:ASP:H	1:31:A:ASP:H	6	0.74
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB2	1	0.74
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB3	1	0.74
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	13	0.74
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	13	0.74
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	14	0.73
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	3	0.73
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	6	0.73
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	6	0.73
(1,3668)	1:181:B:TYR:HD1	1:218:B:LYS:HB2	14	0.73
(1,3668)	1:181:B:TYR:HD1	1:218:B:LYS:HB3	14	0.73
(1,3668)	1:181:B:TYR:HD2	1:218:B:LYS:HB2	14	0.73
(1,3668)	1:181:B:TYR:HD2	1:218:B:LYS:HB3	14	0.73
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD11	8	0.73
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD12	8	0.73
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD13	8	0.73
(1,3313)	1:147:B:SER:HA	1:152:B:TYR:HA	15	0.73
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	6	0.73
(1,2833)	1:104:B:ASP:HA	1:107:B:MET:H	6	0.73
(1,2769)	1:98:B:THR:H	1:101:B:LYS:H	3	0.73
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	5	0.73
(1,2719)	1:224:A:ASN:HA	1:226:A:GLU:H	14	0.73
(1,2664)	1:217:A:LYS:HA	1:220:A:GLU:H	10	0.73
(1,2264)	1:173:A:TYR:HB2	1:195:A:LYS:HB2	11	0.73
(1,2264)	1:173:A:TYR:HB2	1:195:A:LYS:HB3	11	0.73
(1,2264)	1:173:A:TYR:HB3	1:195:A:LYS:HB2	11	0.73
(1,2264)	1:173:A:TYR:HB3	1:195:A:LYS:HB3	11	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1853)	1:135:A:ASN:HB2	1:138:A:TYR:H	3	0.73
(1,1853)	1:135:A:ASN:HB3	1:138:A:TYR:H	3	0.73
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	15	0.73
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	3	0.73
(1,1431)	1:93:A:GLU:HA	1:95:A:ASP:H	3	0.73
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	1	0.73
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	1	0.73
(1,1364)	1:40:A:ILE:HG12	1:36:B:ALA:HA	16	0.73
(1,1364)	1:40:A:ILE:HG13	1:36:B:ALA:HA	16	0.73
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	7	0.73
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	7	0.73
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	7	0.73
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	13	0.73
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	19	0.73
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	13	0.73
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	13	0.73
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	13	0.73
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	13	0.73
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	10	0.73
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	10	0.73
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	8	0.73
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	8	0.73
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	8	0.73
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	1	0.73
(1,1064)	1:48:B:ARG:H	1:50:B:ALA:H	1	0.73
(1,892)	1:28:B:ASP:HA	1:31:B:ASP:H	8	0.73
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD11	10	0.73
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD12	10	0.73
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD13	10	0.73
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	2	0.73
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	2	0.73
(1,3848)	1:203:B:ASN:H	1:204:B:ALA:H	16	0.72
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	11	0.72
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG21	20	0.72
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG22	20	0.72
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG23	20	0.72
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD2	19	0.72
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD3	19	0.72
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	19	0.72
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD3	19	0.72
(1,3310)	1:147:B:SER:HA	1:150:B:LYS:HA	8	0.72
(1,3068)	1:125:B:TYR:HA	1:138:B:TYR:HA	18	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2859)	1:106:B:LYS:HA	1:109:B:GLY:H	11	0.72
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	13	0.72
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	15	0.72
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	20	0.72
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	18	0.72
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	18	0.72
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	2	0.72
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	2	0.72
(1,1951)	1:143:A:ALA:HA	1:155:A:ALA:HA	9	0.72
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	12	0.72
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	20	0.72
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	20	0.72
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	8	0.72
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	8	0.72
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	8	0.72
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	8	0.72
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	19	0.72
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	4	0.72
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	4	0.72
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	8	0.72
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	8	0.72
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	10	0.72
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	10	0.72
(1,764)	1:15:B:TYR:HA	1:19:B:ILE:H	7	0.72
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	9	0.72
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	9	0.72
(1,162)	1:15:A:TYR:HB2	1:70:A:ASN:HD21	18	0.72
(1,162)	1:15:A:TYR:HB2	1:70:A:ASN:HD22	18	0.72
(1,162)	1:15:A:TYR:HB3	1:70:A:ASN:HD21	18	0.72
(1,162)	1:15:A:TYR:HB3	1:70:A:ASN:HD22	18	0.72
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	10	0.71
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	10	0.71
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	5	0.71
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	11	0.71
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	11	0.71
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	20	0.71
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	5	0.71
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	12	0.71
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	12	0.71
(1,3834)	1:200:B:GLU:HB2	1:204:B:ALA:H	7	0.71
(1,3834)	1:200:B:GLU:HB3	1:204:B:ALA:H	7	0.71
(1,3738)	1:191:B:GLU:HA	1:195:B:LYS:H	8	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	5	0.71
(1,3549)	1:171:B:ARG:HA	1:174:B:SER:H	3	0.71
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD2	13	0.71
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD3	13	0.71
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	13	0.71
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD3	13	0.71
(1,3536)	1:170:B:PHE:HE1	1:171:B:ARG:H	11	0.71
(1,3536)	1:170:B:PHE:HE2	1:171:B:ARG:H	11	0.71
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	5	0.71
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	3	0.71
(1,3339)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	9	0.71
(1,3225)	1:140:B:ALA:H	1:162:B:ALA:HA	17	0.71
(1,3074)	1:125:B:TYR:HB2	1:142:B:ARG:H	17	0.71
(1,3074)	1:125:B:TYR:HB3	1:142:B:ARG:H	17	0.71
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	6	0.71
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	11	0.71
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	11	0.71
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	11	0.71
(1,2820)	1:103:B:GLU:H	1:106:B:LYS:H	19	0.71
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG11	9	0.71
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG12	9	0.71
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG13	9	0.71
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	17	0.71
(1,2657)	1:216:A:LYS:HA	1:219:A:VAL:HG21	3	0.71
(1,2657)	1:216:A:LYS:HA	1:219:A:VAL:HG22	3	0.71
(1,2657)	1:216:A:LYS:HA	1:219:A:VAL:HG23	3	0.71
(1,2563)	1:205:A:THR:HG21	1:208:A:MET:HE1	14	0.71
(1,2563)	1:205:A:THR:HG21	1:208:A:MET:HE2	14	0.71
(1,2563)	1:205:A:THR:HG21	1:208:A:MET:HE3	14	0.71
(1,2563)	1:205:A:THR:HG22	1:208:A:MET:HE1	14	0.71
(1,2563)	1:205:A:THR:HG22	1:208:A:MET:HE2	14	0.71
(1,2563)	1:205:A:THR:HG22	1:208:A:MET:HE3	14	0.71
(1,2563)	1:205:A:THR:HG23	1:208:A:MET:HE1	14	0.71
(1,2563)	1:205:A:THR:HG23	1:208:A:MET:HE2	14	0.71
(1,2563)	1:205:A:THR:HG23	1:208:A:MET:HE3	14	0.71
(1,1499)	1:102:A:ALA:HA	1:105:A:LEU:H	11	0.71
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	10	0.71
(1,1490)	1:101:A:LYS:HA	1:104:A:ASP:H	1	0.71
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	14	0.71
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	6	0.71
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	6	0.71
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	6	0.71
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	17	0.71
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	17	0.71
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	16	0.71
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	16	0.71
(1,1281)	1:16:A:PHE:HE1	1:9:B:ALA:HB1	10	0.71
(1,1281)	1:16:A:PHE:HE2	1:9:B:ALA:HB1	10	0.71
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB2	12	0.71
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB3	12	0.71
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	12	0.71
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	12	0.71
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	10	0.71
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	1	0.71
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	7	0.71
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	7	0.71
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	19	0.71
(1,1054)	1:47:B:GLU:H	1:50:B:ALA:H	14	0.71
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD11	12	0.71
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD12	12	0.71
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD13	12	0.71
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD11	12	0.71
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD12	12	0.71
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD13	12	0.71
(1,763)	1:15:B:TYR:HA	1:18:B:SER:HB2	3	0.71
(1,763)	1:15:B:TYR:HA	1:18:B:SER:HB3	3	0.71
(1,625)	1:4:B:SER:HA	1:5:B:LYS:H	8	0.71
(1,541)	1:60:A:PHE:HB2	1:63:A:GLN:H	1	0.71
(1,541)	1:60:A:PHE:HB3	1:63:A:GLN:H	1	0.71
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	12	0.71
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	17	0.71
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	17	0.71
(1,155)	1:15:A:TYR:HA	1:19:A:ILE:H	10	0.71
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	4	0.7
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	6	0.7
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	20	0.7
(1,4016)	1:223:B:LEU:H	1:225:B:LEU:H	13	0.7
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	2	0.7
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	2	0.7
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	2	0.7
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	2	0.7
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	4	0.7
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	4	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	4	0.7
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	4	0.7
(1,3646)	1:180:B:LYS:HA	1:185:B:LYS:H	2	0.7
(1,3629)	1:178:B:PHE:HB2	1:179:B:ALA:H	20	0.7
(1,3629)	1:178:B:PHE:HB3	1:179:B:ALA:H	20	0.7
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	14	0.7
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	14	0.7
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	11	0.7
(1,3074)	1:125:B:TYR:HB2	1:142:B:ARG:H	7	0.7
(1,3074)	1:125:B:TYR:HB3	1:142:B:ARG:H	7	0.7
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB1	17	0.7
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB2	17	0.7
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB3	17	0.7
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB1	17	0.7
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB2	17	0.7
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB3	17	0.7
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB1	17	0.7
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB2	17	0.7
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB3	17	0.7
(1,2824)	1:103:B:GLU:HA	1:106:B:LYS:H	7	0.7
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB1	18	0.7
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB2	18	0.7
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB3	18	0.7
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	12	0.7
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	12	0.7
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	12	0.7
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	15	0.7
(1,2423)	1:190:A:LEU:HD21	1:216:A:LYS:HA	12	0.7
(1,2423)	1:190:A:LEU:HD22	1:216:A:LYS:HA	12	0.7
(1,2423)	1:190:A:LEU:HD23	1:216:A:LYS:HA	12	0.7
(1,1864)	1:136:A:ALA:HA	1:165:A:ILE:HD11	3	0.7
(1,1864)	1:136:A:ALA:HA	1:165:A:ILE:HD12	3	0.7
(1,1864)	1:136:A:ALA:HA	1:165:A:ILE:HD13	3	0.7
(1,1852)	1:135:A:ASN:HA	1:138:A:TYR:H	3	0.7
(1,1814)	1:129:A:ILE:HA	1:135:A:ASN:H	14	0.7
(1,1776)	1:125:A:TYR:HD2	1:141:A:ASN:HB3	4	0.7
(1,1776)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	8	0.7
(1,1587)	1:109:A:GLY:HA2	1:121:A:ALA:H	18	0.7
(1,1587)	1:109:A:GLY:HA3	1:121:A:ALA:H	18	0.7
(1,1474)	1:99:A:LYS:HA	1:102:A:ALA:H	8	0.7
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	2	0.7
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	2	0.7
(1,1463)	1:98:A:THR:H	1:101:A:LYS:H	10	0.7
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	20	0.7
(1,1309)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	9	0.7
(1,1309)	1:25:A:ILE:HD11	1:43:B:ALA:HB2	9	0.7
(1,1309)	1:25:A:ILE:HD11	1:43:B:ALA:HB3	9	0.7
(1,1309)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	9	0.7
(1,1309)	1:25:A:ILE:HD12	1:43:B:ALA:HB2	9	0.7
(1,1309)	1:25:A:ILE:HD12	1:43:B:ALA:HB3	9	0.7
(1,1309)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	9	0.7
(1,1309)	1:25:A:ILE:HD13	1:43:B:ALA:HB2	9	0.7
(1,1309)	1:25:A:ILE:HD13	1:43:B:ALA:HB3	9	0.7
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	14	0.7
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	20	0.7
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	7	0.7
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	10	0.7
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	17	0.7
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	8	0.7
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	8	0.7
(1,1029)	1:43:B:ALA:HB1	1:45:B:GLY:H	16	0.7
(1,1029)	1:43:B:ALA:HB2	1:45:B:GLY:H	16	0.7
(1,1029)	1:43:B:ALA:HB3	1:45:B:GLY:H	16	0.7
(1,506)	1:55:A:LEU:HD11	1:72:A:ALA:HA	9	0.7
(1,506)	1:55:A:LEU:HD12	1:72:A:ALA:HA	9	0.7
(1,506)	1:55:A:LEU:HD13	1:72:A:ALA:HA	9	0.7
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	16	0.7
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	11	0.69
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	17	0.69
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	7	0.69
(1,4105)	1:338:A:GLU:H	1:339:A:THR:H	5	0.69
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	9	0.69
(1,4072)	1:301:A:GLY:H	1:302:A:PHE:H	9	0.69
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	7	0.69
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	7	0.69
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	20	0.69
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	1	0.69
(1,3913)	1:210:B:ARG:HA	1:214:B:SER:H	7	0.69
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	18	0.69
(1,3629)	1:178:B:PHE:HB2	1:179:B:ALA:H	5	0.69
(1,3629)	1:178:B:PHE:HB3	1:179:B:ALA:H	5	0.69
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	12	0.69
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	14	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	9	0.69
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	7	0.69
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	7	0.69
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	12	0.69
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	9	0.69
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	10	0.69
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	10	0.69
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	10	0.69
(1,2750)	1:95:B:ASP:HA	1:97:B:GLU:H	5	0.69
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	6	0.69
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	6	0.69
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	16	0.69
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	16	0.69
(1,2367)	1:181:A:TYR:HE1	1:218:A:LYS:HE2	9	0.69
(1,2367)	1:181:A:TYR:HE1	1:218:A:LYS:HE3	9	0.69
(1,2367)	1:181:A:TYR:HE2	1:218:A:LYS:HE2	9	0.69
(1,2367)	1:181:A:TYR:HE2	1:218:A:LYS:HE3	9	0.69
(1,2266)	1:173:A:TYR:HB2	1:196:A:VAL:H	11	0.69
(1,2266)	1:173:A:TYR:HB3	1:196:A:VAL:H	11	0.69
(1,2227)	1:170:A:PHE:HD1	1:196:A:VAL:HA	8	0.69
(1,2227)	1:170:A:PHE:HD2	1:196:A:VAL:HA	8	0.69
(1,2163)	1:163:A:ILE:HA	1:167:A:PRO:HA	9	0.69
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	8	0.69
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	8	0.69
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	8	0.69
(1,1447)	1:95:A:ASP:HA	1:99:A:LYS:H	2	0.69
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	14	0.69
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	20	0.69
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	12	0.69
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	12	0.69
(1,1354)	1:39:A:CYS:HB2	1:36:B:ALA:HA	3	0.69
(1,1354)	1:39:A:CYS:HB3	1:36:B:ALA:HA	3	0.69
(1,1278)	1:16:A:PHE:HA	1:44:B:PHE:HZ	5	0.69
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD11	7	0.69
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD12	7	0.69
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD13	7	0.69
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD11	7	0.69
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD12	7	0.69
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD13	7	0.69
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG21	2	0.69
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG22	2	0.69
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG23	2	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	20	0.69
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	18	0.69
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	10	0.69
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	8	0.69
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	8	0.69
(1,1117)	1:56:B:GLY:H	1:57:B:LYS:H	1	0.69
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	14	0.69
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	6	0.69
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	12	0.69
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	20	0.69
(1,781)	1:16:B:PHE:HA	1:18:B:SER:HB2	3	0.69
(1,781)	1:16:B:PHE:HA	1:18:B:SER:HB3	3	0.69
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	11	0.69
(1,560)	1:63:A:GLN:HA	1:65:A:LEU:H	17	0.69
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	14	0.69
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	14	0.69
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	19	0.69
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	19	0.69
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB2	7	0.69
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB3	7	0.69
(1,226)	1:20:A:VAL:HA	1:24:A:GLU:H	17	0.69
(1,4202)	1:337:B:ASP:H	1:338:B:GLU:H	4	0.68
(1,4088)	1:321:A:ARG:H	1:322:A:ASN:H	12	0.68
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	13	0.68
(1,3791)	1:195:B:LYS:HA	1:199:B:ILE:H	17	0.68
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG21	20	0.68
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG22	20	0.68
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG23	20	0.68
(1,3657)	1:181:B:TYR:H	1:189:B:ALA:HA	3	0.68
(1,3420)	1:158:B:ASP:HA	1:162:B:ALA:H	11	0.68
(1,3310)	1:147:B:SER:HA	1:150:B:LYS:HA	4	0.68
(1,3252)	1:143:B:ALA:H	1:155:B:ALA:HA	11	0.68
(1,3195)	1:138:B:TYR:HA	1:141:B:ASN:H	13	0.68
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE1	1	0.68
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE2	1	0.68
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE3	1	0.68
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	1	0.68
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG21	9	0.68
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG22	9	0.68
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG23	9	0.68
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG21	9	0.68
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG22	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG23	9	0.68
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG21	9	0.68
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG22	9	0.68
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG23	9	0.68
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG11	9	0.68
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG12	9	0.68
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG13	9	0.68
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	20	0.68
(1,2713)	1:223:A:LEU:HA	1:225:A:LEU:H	3	0.68
(1,2682)	1:219:A:VAL:HG11	1:220:A:GLU:HA	13	0.68
(1,2682)	1:219:A:VAL:HG12	1:220:A:GLU:HA	13	0.68
(1,2682)	1:219:A:VAL:HG13	1:220:A:GLU:HA	13	0.68
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	8	0.68
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	8	0.68
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	13	0.68
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	13	0.68
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG21	3	0.68
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG22	3	0.68
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG23	3	0.68
(1,2386)	1:187:A:GLU:H	1:219:A:VAL:HG21	13	0.68
(1,2386)	1:187:A:GLU:H	1:219:A:VAL:HG22	13	0.68
(1,2386)	1:187:A:GLU:H	1:219:A:VAL:HG23	13	0.68
(1,2146)	1:161:A:SER:HA	1:165:A:ILE:H	16	0.68
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE1	11	0.68
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE2	11	0.68
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE1	11	0.68
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE2	11	0.68
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE1	11	0.68
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE2	11	0.68
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	8	0.68
(1,1919)	1:140:A:ALA:H	1:162:A:ALA:HA	16	0.68
(1,1767)	1:125:A:TYR:HB2	1:139:A:TYR:H	14	0.68
(1,1767)	1:125:A:TYR:HB3	1:139:A:TYR:H	14	0.68
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	19	0.68
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	19	0.68
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	10	0.68
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	10	0.68
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD11	6	0.68
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD12	6	0.68
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD13	6	0.68
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	16	0.68
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	4	0.68
(1,1110)	1:55:B:LEU:H	1:57:B:LYS:H	5	0.68
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	8	0.68
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	8	0.68
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE2	12	0.68
(1,1107)	1:54:B:ILE:HA	1:57:B:LYS:HE3	12	0.68
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	11	0.68
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	11	0.68
(1,642)	1:6:B:GLU:HA	1:10:B:ALA:H	13	0.68
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	11	0.68
(1,561)	1:63:A:GLN:HA	1:67:A:ASP:H	17	0.68
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG2	14	0.68
(1,438)	1:46:A:PHE:HA	1:47:A:GLU:HG3	14	0.68
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	19	0.67
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	17	0.67
(1,4156)	1:248:B:GLY:H	1:249:B:LEU:H	13	0.67
(1,4051)	1:241:A:SER:H	1:242:A:GLN:H	10	0.67
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	9	0.67
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	9	0.67
(1,3869)	1:205:B:THR:HG21	1:208:B:MET:HE1	19	0.67
(1,3869)	1:205:B:THR:HG21	1:208:B:MET:HE2	19	0.67
(1,3869)	1:205:B:THR:HG21	1:208:B:MET:HE3	19	0.67
(1,3869)	1:205:B:THR:HG22	1:208:B:MET:HE1	19	0.67
(1,3869)	1:205:B:THR:HG22	1:208:B:MET:HE2	19	0.67
(1,3869)	1:205:B:THR:HG22	1:208:B:MET:HE3	19	0.67
(1,3869)	1:205:B:THR:HG23	1:208:B:MET:HE1	19	0.67
(1,3869)	1:205:B:THR:HG23	1:208:B:MET:HE2	19	0.67
(1,3869)	1:205:B:THR:HG23	1:208:B:MET:HE3	19	0.67
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	7	0.67
(1,3648)	1:180:B:LYS:HB2	1:185:B:LYS:H	14	0.67
(1,3648)	1:180:B:LYS:HB3	1:185:B:LYS:H	14	0.67
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	9	0.67
(1,3511)	1:169:B:TYR:HD2	1:171:B:ARG:H	8	0.67
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	8	0.67
(1,3366)	1:152:B:TYR:HD2	1:182:B:ALA:HB1	3	0.67
(1,3310)	1:147:B:SER:HA	1:150:B:LYS:HA	10	0.67
(1,3119)	1:129:B:ILE:HA	1:133:B:PRO:HA	15	0.67
(1,3075)	1:125:B:TYR:HB2	1:142:B:ARG:HA	13	0.67
(1,3075)	1:125:B:TYR:HB3	1:142:B:ARG:HA	13	0.67
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	4	0.67
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	4	0.67
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	11	0.67
(1,2819)	1:103:B:GLU:H	1:105:B:LEU:H	11	0.67
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	15	0.67
(1,2755)	1:96:B:ALA:H	1:97:B:GLU:H	9	0.67
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	11	0.67
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	11	0.67
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	6	0.67
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	6	0.67
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	6	0.67
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	6	0.67
(1,2205)	1:169:A:TYR:HD1	1:171:A:ARG:H	13	0.67
(1,1882)	1:137:A:ILE:HA	1:141:A:ASN:H	20	0.67
(1,1865)	1:136:A:ALA:HA	1:166:A:ASP:H	9	0.67
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	1	0.67
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	19	0.67
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	17	0.67
(1,1537)	1:105:A:LEU:HA	1:124:A:LYS:HA	18	0.67
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	17	0.67
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	17	0.67
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	16	0.67
(1,1374)	1:43:A:ALA:HA	1:32:B:SER:H	18	0.67
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	19	0.67
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	1	0.67
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	1	0.67
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	1	0.67
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	1	0.67
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	9	0.67
(1,1307)	1:25:A:ILE:HG12	1:44:B:PHE:HA	4	0.67
(1,1307)	1:25:A:ILE:HG13	1:44:B:PHE:HA	4	0.67
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	3	0.67
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	3	0.67
(1,1266)	1:15:A:TYR:HE1	1:5:B:LYS:H	6	0.67
(1,1266)	1:15:A:TYR:HE2	1:5:B:LYS:H	6	0.67
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	18	0.67
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	11	0.67
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	1	0.67
(1,758)	1:15:B:TYR:H	1:18:B:SER:H	7	0.67
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	9	0.67
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	5	0.67
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	5	0.67
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	18	0.67
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	18	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4205)	1:342:B:ASN:H	1:343:B:GLU:H	19	0.66
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	19	0.66
(1,3769)	1:193:B:TYR:HE2	1:211:B:ASP:HA	19	0.66
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	17	0.66
(1,3361)	1:152:B:TYR:HB2	1:183:B:GLN:H	18	0.66
(1,3361)	1:152:B:TYR:HB3	1:183:B:GLN:H	18	0.66
(1,3334)	1:150:B:LYS:HA	1:152:B:TYR:H	8	0.66
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	11	0.66
(1,2464)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	6	0.66
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	10	0.66
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	10	0.66
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	10	0.66
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	10	0.66
(1,2390)	1:187:A:GLU:HA	1:190:A:LEU:H	3	0.66
(1,2003)	1:147:A:SER:HA	1:150:A:LYS:H	17	0.66
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	19	0.66
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	13	0.66
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	18	0.66
(1,1374)	1:43:A:ALA:HA	1:32:B:SER:H	1	0.66
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	4	0.66
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	4	0.66
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	7	0.66
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD11	7	0.66
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD12	7	0.66
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD13	7	0.66
(1,1134)	1:59:B:GLU:H	1:60:B:PHE:H	5	0.66
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	2	0.66
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	2	0.66
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	16	0.66
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	16	0.66
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB1	4	0.66
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB2	4	0.66
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB3	4	0.66
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	9	0.65
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	16	0.65
(1,3828)	1:199:B:ILE:HA	1:201:B:GLY:H	18	0.65
(1,3791)	1:195:B:LYS:HA	1:199:B:ILE:H	9	0.65
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	15	0.65
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	15	0.65
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	15	0.65
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	15	0.65
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3686)	1:185:B:LYS:H	1:186:B:PRO:HA	1	0.65
(1,3543)	1:170:B:PHE:HD2	1:208:B:MET:HE3	9	0.65
(1,3543)	1:170:B:PHE:HE2	1:208:B:MET:HE3	19	0.65
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	15	0.65
(1,3367)	1:152:B:TYR:HD1	1:183:B:GLN:HG2	10	0.65
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	19	0.65
(1,3195)	1:138:B:TYR:HA	1:141:B:ASN:H	3	0.65
(1,3091)	1:126:B:THR:HA	1:130:B:LYS:H	20	0.65
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	18	0.65
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	18	0.65
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	18	0.65
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	18	0.65
(1,2805)	1:102:B:ALA:HA	1:105:B:LEU:H	15	0.65
(1,2800)	1:102:B:ALA:H	1:105:B:LEU:H	11	0.65
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	7	0.65
(1,2580)	1:207:A:ALA:HA	1:210:A:ARG:H	7	0.65
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	9	0.65
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	9	0.65
(1,2230)	1:170:A:PHE:HE1	1:171:A:ARG:H	9	0.65
(1,2230)	1:170:A:PHE:HE2	1:171:A:ARG:H	9	0.65
(1,1973)	1:144:A:ALA:HB1	1:175:A:ARG:HE	15	0.65
(1,1973)	1:144:A:ALA:HB2	1:175:A:ARG:HE	15	0.65
(1,1973)	1:144:A:ALA:HB3	1:175:A:ARG:HE	15	0.65
(1,1951)	1:143:A:ALA:HA	1:155:A:ALA:HA	7	0.65
(1,1820)	1:129:A:ILE:HD11	1:139:A:TYR:HA	2	0.65
(1,1820)	1:129:A:ILE:HD12	1:139:A:TYR:HA	2	0.65
(1,1820)	1:129:A:ILE:HD13	1:139:A:TYR:HA	2	0.65
(1,1785)	1:126:A:THR:HA	1:130:A:LYS:H	14	0.65
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	8	0.65
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD11	20	0.65
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD12	20	0.65
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD13	20	0.65
(1,1417)	1:68:A:ILE:HA	1:2:B:SER:HB2	3	0.65
(1,1417)	1:68:A:ILE:HA	1:2:B:SER:HB3	3	0.65
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	12	0.65
(1,1387)	1:44:A:PHE:HE1	1:16:B:PHE:HE1	3	0.65
(1,1387)	1:44:A:PHE:HE2	1:16:B:PHE:HE1	3	0.65
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	10	0.65
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	10	0.65
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	10	0.65
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	10	0.65
(1,1177)	1:65:B:LEU:HA	1:66:B:ALA:H	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1177)	1:65:B:LEU:HA	1:66:B:ALA:H	19	0.65
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	2	0.65
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	2	0.65
(1,685)	1:10:B:ALA:HA	1:48:B:ARG:HA	9	0.65
(1,452)	1:47:A:GLU:HB2	1:49:A:GLU:H	20	0.65
(1,452)	1:47:A:GLU:HB3	1:49:A:GLU:H	20	0.65
(1,284)	1:28:A:ASP:HA	1:32:A:SER:H	1	0.65
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	1	0.64
(1,4149)	1:241:B:SER:H	1:242:B:GLN:H	18	0.64
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	13	0.64
(1,4000)	1:221:B:GLN:H	1:224:B:ASN:H	1	0.64
(1,3951)	1:215:B:ALA:H	1:218:B:LYS:H	14	0.64
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	16	0.64
(1,3722)	1:190:B:LEU:HA	1:212:B:TYR:HA	16	0.64
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	20	0.64
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	20	0.64
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	20	0.64
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	20	0.64
(1,3649)	1:180:B:LYS:HB2	1:188:B:GLU:H	10	0.64
(1,3649)	1:180:B:LYS:HB3	1:188:B:GLU:H	10	0.64
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	20	0.64
(1,3452)	1:161:B:SER:HA	1:165:B:ILE:H	7	0.64
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	12	0.64
(1,3374)	1:153:B:ASP:HA	1:156:B:VAL:HG21	6	0.64
(1,3374)	1:153:B:ASP:HA	1:156:B:VAL:HG22	6	0.64
(1,3374)	1:153:B:ASP:HA	1:156:B:VAL:HG23	6	0.64
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	5	0.64
(1,3291)	1:146:B:HIS:H	1:155:B:ALA:HA	4	0.64
(1,3199)	1:139:B:TYR:H	1:142:B:ARG:H	13	0.64
(1,2984)	1:117:B:ASP:HA	1:120:B:LEU:H	15	0.64
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	7	0.64
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	7	0.64
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB1	19	0.64
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB2	19	0.64
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB3	19	0.64
(1,2750)	1:95:B:ASP:HA	1:97:B:GLU:H	7	0.64
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	1	0.64
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG21	17	0.64
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG22	17	0.64
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG23	17	0.64
(1,2351)	1:181:A:TYR:H	1:189:A:ALA:HA	10	0.64
(1,2350)	1:181:A:TYR:H	1:189:A:ALA:H	16	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2231)	1:170:A:PHE:HE1	1:171:A:ARG:HA	19	0.64
(1,2231)	1:170:A:PHE:HE2	1:171:A:ARG:HA	19	0.64
(1,2226)	1:170:A:PHE:HD1	1:171:A:ARG:HD2	3	0.64
(1,2226)	1:170:A:PHE:HD1	1:171:A:ARG:HD3	3	0.64
(1,2226)	1:170:A:PHE:HD2	1:171:A:ARG:HD2	3	0.64
(1,2226)	1:170:A:PHE:HD2	1:171:A:ARG:HD3	3	0.64
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	12	0.64
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	16	0.64
(1,1586)	1:109:A:GLY:HA2	1:113:A:MET:H	18	0.64
(1,1586)	1:109:A:GLY:HA3	1:113:A:MET:H	18	0.64
(1,1499)	1:102:A:ALA:HA	1:105:A:LEU:H	6	0.64
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	6	0.64
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	6	0.64
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	6	0.64
(1,1398)	1:44:A:PHE:HE1	1:33:B:LEU:HD11	12	0.64
(1,1398)	1:44:A:PHE:HE2	1:33:B:LEU:HD11	12	0.64
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	4	0.64
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	4	0.64
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	4	0.64
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	4	0.64
(1,1336)	1:36:A:ALA:H	1:36:B:ALA:HA	16	0.64
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB2	19	0.64
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB3	19	0.64
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	18	0.64
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	18	0.64
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	9	0.64
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	9	0.64
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	18	0.64
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	18	0.64
(1,1140)	1:59:B:GLU:HB2	1:64:B:HIS:HA	14	0.64
(1,1140)	1:59:B:GLU:HB3	1:64:B:HIS:HA	14	0.64
(1,1114)	1:55:B:LEU:HD11	1:71:B:SER:HA	8	0.64
(1,1114)	1:55:B:LEU:HD12	1:71:B:SER:HA	8	0.64
(1,1114)	1:55:B:LEU:HD13	1:71:B:SER:HA	8	0.64
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	11	0.64
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	11	0.64
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	19	0.63
(1,4207)	1:344:B:ASN:H	1:345:B:LYS:H	18	0.63
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	16	0.63
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	17	0.63
(1,4169)	1:300:B:GLU:H	1:301:B:GLY:H	1	0.63
(1,4159)	1:253:B:GLY:H	1:254:B:SER:H	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	6	0.63
(1,4050)	1:240:A:ALA:H	1:241:A:SER:H	18	0.63
(1,3808)	1:197:B:LEU:HA	1:200:B:GLU:H	1	0.63
(1,3781)	1:194:B:LYS:HA	1:198:B:ASP:H	4	0.63
(1,3584)	1:174:B:SER:HA	1:178:B:PHE:H	6	0.63
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	10	0.63
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	14	0.63
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE1	10	0.63
(1,2952)	1:113:B:MET:HE1	1:145:B:ALA:HA	13	0.63
(1,2952)	1:113:B:MET:HE2	1:145:B:ALA:HA	13	0.63
(1,2952)	1:113:B:MET:HE3	1:145:B:ALA:HA	13	0.63
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE1	10	0.63
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE2	10	0.63
(1,2900)	1:110:B:ASN:HA	1:113:B:MET:HE3	10	0.63
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	17	0.63
(1,2664)	1:217:A:LYS:HA	1:220:A:GLU:H	1	0.63
(1,2243)	1:171:A:ARG:HA	1:174:A:SER:H	11	0.63
(1,2090)	1:156:A:VAL:HA	1:176:A:LEU:HA	3	0.63
(1,1950)	1:143:A:ALA:HA	1:155:A:ALA:H	7	0.63
(1,1950)	1:143:A:ALA:HA	1:155:A:ALA:H	8	0.63
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD1	10	0.63
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD2	10	0.63
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD1	10	0.63
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD2	10	0.63
(1,1689)	1:118:A:TYR:HA	1:145:A:ALA:HA	4	0.63
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	11	0.63
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	11	0.63
(1,1424)	1:69:A:LEU:HD11	1:2:B:SER:H	7	0.63
(1,1424)	1:69:A:LEU:HD12	1:2:B:SER:H	7	0.63
(1,1424)	1:69:A:LEU:HD13	1:2:B:SER:H	7	0.63
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB2	9	0.63
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB3	9	0.63
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB2	9	0.63
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB3	9	0.63
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB2	9	0.63
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB3	9	0.63
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	15	0.63
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	7	0.63
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	9	0.63
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	17	0.63
(1,776)	1:16:B:PHE:H	1:18:B:SER:H	7	0.63
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:15:A:TYR:HD1	1:18:A:SER:HB2	1	0.63
(1,163)	1:15:A:TYR:HD1	1:18:A:SER:HB3	1	0.63
(1,163)	1:15:A:TYR:HD2	1:18:A:SER:HB2	1	0.63
(1,163)	1:15:A:TYR:HD2	1:18:A:SER:HB3	1	0.63
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	15	0.62
(1,4167)	1:294:B:SER:H	1:295:B:ILE:H	10	0.62
(1,4158)	1:252:B:LEU:H	1:253:B:GLY:H	13	0.62
(1,4072)	1:301:A:GLY:H	1:302:A:PHE:H	19	0.62
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	16	0.62
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	16	0.62
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	16	0.62
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	16	0.62
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	15	0.62
(1,3569)	1:173:B:TYR:HB2	1:195:B:LYS:H	10	0.62
(1,3569)	1:173:B:TYR:HB3	1:195:B:LYS:H	10	0.62
(1,3361)	1:152:B:TYR:HB2	1:183:B:GLN:H	12	0.62
(1,3361)	1:152:B:TYR:HB3	1:183:B:GLN:H	12	0.62
(1,3108)	1:128:B:ALA:HA	1:132:B:LEU:H	2	0.62
(1,3091)	1:126:B:THR:HA	1:130:B:LYS:H	9	0.62
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	10	0.62
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	10	0.62
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	7	0.62
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	17	0.62
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	2	0.62
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	2	0.62
(1,2842)	1:105:B:LEU:HA	1:109:B:GLY:H	2	0.62
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	17	0.62
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	17	0.62
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	17	0.62
(1,2615)	1:211:A:ASP:HA	1:215:A:ALA:H	19	0.62
(1,2463)	1:193:A:TYR:HE2	1:211:A:ASP:HA	3	0.62
(1,2287)	1:175:A:ARG:HA	1:178:A:PHE:H	6	0.62
(1,2182)	1:166:A:ASP:HA	1:169:A:TYR:H	18	0.62
(1,1696)	1:118:A:TYR:HB2	1:148:A:SER:HB2	3	0.62
(1,1696)	1:118:A:TYR:HB2	1:148:A:SER:HB3	3	0.62
(1,1696)	1:118:A:TYR:HB3	1:148:A:SER:HB2	3	0.62
(1,1696)	1:118:A:TYR:HB3	1:148:A:SER:HB3	3	0.62
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	1	0.62
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	1	0.62
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	8	0.62
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	8	0.62
(1,1666)	1:116:A:LYS:HA	1:118:A:TYR:H	15	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	5	0.62
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG2	19	0.62
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG3	19	0.62
(1,1424)	1:69:A:LEU:HD11	1:2:B:SER:H	19	0.62
(1,1424)	1:69:A:LEU:HD12	1:2:B:SER:H	19	0.62
(1,1424)	1:69:A:LEU:HD13	1:2:B:SER:H	19	0.62
(1,1372)	1:43:A:ALA:HA	1:25:B:ILE:HD11	3	0.62
(1,1372)	1:43:A:ALA:HA	1:25:B:ILE:HD12	3	0.62
(1,1372)	1:43:A:ALA:HA	1:25:B:ILE:HD13	3	0.62
(1,1337)	1:36:A:ALA:HA	1:36:B:ALA:H	19	0.62
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	14	0.62
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	14	0.62
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	14	0.62
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	3	0.62
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	3	0.62
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	17	0.62
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB2	5	0.62
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB3	5	0.62
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	5	0.62
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	1	0.62
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	2	0.62
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	19	0.62
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	19	0.62
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	19	0.62
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	19	0.62
(1,623)	1:4:B:SER:H	1:7:B:GLU:H	15	0.62
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	8	0.62
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	8	0.62
(1,452)	1:47:A:GLU:HB2	1:49:A:GLU:H	8	0.62
(1,452)	1:47:A:GLU:HB3	1:49:A:GLU:H	8	0.62
(1,76)	1:10:A:ALA:HA	1:48:A:ARG:HA	9	0.62
(1,4206)	1:343:B:GLU:H	1:344:B:ASN:H	18	0.61
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	14	0.61
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	10	0.61
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	15	0.61
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	20	0.61
(1,4105)	1:338:A:GLU:H	1:339:A:THR:H	19	0.61
(1,4088)	1:321:A:ARG:H	1:322:A:ASN:H	19	0.61
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	6	0.61
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	6	0.61
(1,3946)	1:214:B:SER:HA	1:217:B:LYS:H	14	0.61
(1,3629)	1:178:B:PHE:HB2	1:179:B:ALA:H	6	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3629)	1:178:B:PHE:HB3	1:179:B:ALA:H	6	0.61
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	5	0.61
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	5	0.61
(1,3572)	1:173:B:TYR:HB2	1:196:B:VAL:H	1	0.61
(1,3572)	1:173:B:TYR:HB3	1:196:B:VAL:H	1	0.61
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE1	9	0.61
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE2	9	0.61
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE3	9	0.61
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE1	9	0.61
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE2	9	0.61
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE3	9	0.61
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	2	0.61
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD11	12	0.61
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD12	12	0.61
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD13	12	0.61
(1,2892)	1:109:B:GLY:HA2	1:113:B:MET:H	12	0.61
(1,2892)	1:109:B:GLY:HA3	1:113:B:MET:H	12	0.61
(1,2813)	1:102:B:ALA:HB1	1:128:B:ALA:HA	15	0.61
(1,2813)	1:102:B:ALA:HB2	1:128:B:ALA:HA	15	0.61
(1,2813)	1:102:B:ALA:HB3	1:128:B:ALA:HA	15	0.61
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	6	0.61
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	6	0.61
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	9	0.61
(1,2750)	1:95:B:ASP:HA	1:97:B:GLU:H	11	0.61
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	2	0.61
(1,2628)	1:213:A:GLU:H	1:216:A:LYS:H	8	0.61
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	11	0.61
(1,1784)	1:126:A:THR:HA	1:129:A:ILE:HD11	2	0.61
(1,1784)	1:126:A:THR:HA	1:129:A:ILE:HD12	2	0.61
(1,1784)	1:126:A:THR:HA	1:129:A:ILE:HD13	2	0.61
(1,1761)	1:125:A:TYR:HA	1:129:A:ILE:H	14	0.61
(1,1641)	1:113:A:MET:HE1	1:141:A:ASN:HA	3	0.61
(1,1641)	1:113:A:MET:HE2	1:141:A:ASN:HA	3	0.61
(1,1641)	1:113:A:MET:HE3	1:141:A:ASN:HA	3	0.61
(1,1542)	1:105:A:LEU:HD11	1:131:A:VAL:H	20	0.61
(1,1542)	1:105:A:LEU:HD12	1:131:A:VAL:H	20	0.61
(1,1542)	1:105:A:LEU:HD13	1:131:A:VAL:H	20	0.61
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	14	0.61
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	18	0.61
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	18	0.61
(1,1353)	1:39:A:CYS:HB2	1:36:B:ALA:H	16	0.61
(1,1353)	1:39:A:CYS:HB3	1:36:B:ALA:H	16	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	11	0.61
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	11	0.61
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	15	0.61
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	15	0.61
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	4	0.61
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	4	0.61
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG21	13	0.61
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG22	13	0.61
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG23	13	0.61
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD11	11	0.61
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD12	11	0.61
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD13	11	0.61
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	6	0.61
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD11	10	0.61
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD12	10	0.61
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD13	10	0.61
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	10	0.61
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	10	0.61
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	1	0.61
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	1	0.61
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	6	0.61
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	6	0.61
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	4	0.61
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	8	0.61
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	8	0.61
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	20	0.61
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	20	0.61
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	18	0.61
(1,77)	1:10:A:ALA:HA	1:51:A:VAL:HA	5	0.61
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	2	0.6
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	16	0.6
(1,4077)	1:305:A:GLY:H	1:307:A:GLY:H	2	0.6
(1,3729)	1:190:B:LEU:HD21	1:216:B:LYS:HA	7	0.6
(1,3729)	1:190:B:LEU:HD22	1:216:B:LYS:HA	7	0.6
(1,3729)	1:190:B:LEU:HD23	1:216:B:LYS:HA	7	0.6
(1,3724)	1:190:B:LEU:HA	1:216:B:LYS:H	17	0.6
(1,3722)	1:190:B:LEU:HA	1:212:B:TYR:HA	5	0.6
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG21	9	0.6
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG22	9	0.6
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG23	9	0.6
(1,3599)	1:176:B:LEU:HA	1:180:B:LYS:H	18	0.6
(1,3575)	1:173:B:TYR:HE2	1:199:B:ILE:HD13	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	19	0.6
(1,3461)	1:162:B:ALA:HB1	1:172:B:GLY:H	4	0.6
(1,3461)	1:162:B:ALA:HB2	1:172:B:GLY:H	4	0.6
(1,3461)	1:162:B:ALA:HB3	1:172:B:GLY:H	4	0.6
(1,3444)	1:160:B:GLU:HA	1:164:B:SER:H	7	0.6
(1,3357)	1:152:B:TYR:HA	1:156:B:VAL:H	13	0.6
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	4	0.6
(1,3241)	1:141:B:ASN:HA	1:145:B:ALA:H	13	0.6
(1,3098)	1:127:B:GLU:HA	1:130:B:LYS:H	10	0.6
(1,2939)	1:113:B:MET:HA	1:116:B:LYS:HA	9	0.6
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE1	18	0.6
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE2	18	0.6
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	2	0.6
(1,2805)	1:102:B:ALA:HA	1:105:B:LEU:H	11	0.6
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	7	0.6
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	4	0.6
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	4	0.6
(1,2572)	1:206:A:GLU:HA	1:210:A:ARG:H	18	0.6
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	1	0.6
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	1	0.6
(1,2504)	1:197:A:LEU:HA	1:204:A:ALA:HA	9	0.6
(1,2473)	1:194:A:LYS:HA	1:197:A:LEU:H	13	0.6
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	2	0.6
(1,2141)	1:161:A:SER:H	1:164:A:SER:H	12	0.6
(1,1950)	1:143:A:ALA:HA	1:155:A:ALA:H	9	0.6
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	15	0.6
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	15	0.6
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	9	0.6
(1,1499)	1:102:A:ALA:HA	1:105:A:LEU:H	14	0.6
(1,1439)	1:94:A:ASP:HA	1:96:A:ALA:H	17	0.6
(1,1336)	1:36:A:ALA:H	1:36:B:ALA:HA	19	0.6
(1,1321)	1:32:A:SER:HB2	1:43:B:ALA:H	9	0.6
(1,1321)	1:32:A:SER:HB3	1:43:B:ALA:H	9	0.6
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD11	20	0.6
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD12	20	0.6
(1,1194)	1:67:B:ASP:HA	1:69:B:LEU:HD13	20	0.6
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	9	0.6
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	1	0.6
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	1	0.6
(1,1154)	1:60:B:PHE:HB2	1:63:B:GLN:HE21	6	0.6
(1,1154)	1:60:B:PHE:HB2	1:63:B:GLN:HE22	6	0.6
(1,1154)	1:60:B:PHE:HB3	1:63:B:GLN:HE21	6	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:60:B:PHE:HB3	1:63:B:GLN:HE22	6	0.6
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	14	0.6
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	14	0.6
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	14	0.6
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	14	0.6
(1,1121)	1:56:B:GLY:HA2	1:58:B:SER:H	3	0.6
(1,1121)	1:56:B:GLY:HA3	1:58:B:SER:H	3	0.6
(1,1096)	1:53:B:GLY:H	1:56:B:GLY:H	17	0.6
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	14	0.6
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	5	0.6
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	8	0.6
(1,861)	1:24:B:GLU:H	1:25:B:ILE:H	20	0.6
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	13	0.6
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	13	0.6
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	13	0.6
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	13	0.6
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	20	0.6
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	20	0.6
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	4	0.6
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	4	0.6
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	17	0.6
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB2	18	0.6
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB3	18	0.6
(1,76)	1:10:A:ALA:HA	1:48:A:ARG:HA	18	0.6
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	18	0.59
(1,4202)	1:337:B:ASP:H	1:338:B:GLU:H	3	0.59
(1,4072)	1:301:A:GLY:H	1:302:A:PHE:H	13	0.59
(1,4048)	1:238:A:VAL:H	1:239:A:ASP:H	18	0.59
(1,4027)	1:225:B:LEU:H	1:226:B:GLU:H	12	0.59
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	12	0.59
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	4	0.59
(1,3876)	1:206:B:GLU:HA	1:209:B:LYS:H	8	0.59
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	6	0.59
(1,3727)	1:190:B:LEU:HD11	1:216:B:LYS:H	9	0.59
(1,3727)	1:190:B:LEU:HD12	1:216:B:LYS:H	9	0.59
(1,3727)	1:190:B:LEU:HD13	1:216:B:LYS:H	9	0.59
(1,3724)	1:190:B:LEU:HA	1:216:B:LYS:H	10	0.59
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	3	0.59
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	3	0.59
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	3	0.59
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	3	0.59
(1,3656)	1:181:B:TYR:H	1:189:B:ALA:H	9	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	18	0.59
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	17	0.59
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	9	0.59
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	9	0.59
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	16	0.59
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	16	0.59
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	16	0.59
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	15	0.59
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	19	0.59
(1,2432)	1:191:A:GLU:HA	1:195:A:LYS:H	15	0.59
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	20	0.59
(1,2265)	1:173:A:TYR:HB2	1:195:A:LYS:HG2	6	0.59
(1,2265)	1:173:A:TYR:HB2	1:195:A:LYS:HG3	6	0.59
(1,2265)	1:173:A:TYR:HB3	1:195:A:LYS:HG2	6	0.59
(1,2265)	1:173:A:TYR:HB3	1:195:A:LYS:HG3	6	0.59
(1,2164)	1:163:A:ILE:HA	1:169:A:TYR:H	16	0.59
(1,2036)	1:150:A:LYS:HD2	1:152:A:TYR:HE1	17	0.59
(1,2036)	1:150:A:LYS:HD2	1:152:A:TYR:HE2	17	0.59
(1,2036)	1:150:A:LYS:HD3	1:152:A:TYR:HE1	17	0.59
(1,2036)	1:150:A:LYS:HD3	1:152:A:TYR:HE2	17	0.59
(1,1839)	1:132:A:LEU:HD11	1:134:A:THR:H	7	0.59
(1,1839)	1:132:A:LEU:HD12	1:134:A:THR:H	7	0.59
(1,1839)	1:132:A:LEU:HD13	1:134:A:THR:H	7	0.59
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE1	2	0.59
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE2	2	0.59
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE1	9	0.59
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE2	9	0.59
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE3	9	0.59
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	3	0.59
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	15	0.59
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	10	0.59
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	10	0.59
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG12	7	0.59
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG13	7	0.59
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	8	0.59
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	15	0.59
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	15	0.59
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	15	0.59
(1,1293)	1:16:A:PHE:HE1	1:40:B:ILE:HG21	2	0.59
(1,1293)	1:16:A:PHE:HE2	1:40:B:ILE:HG21	2	0.59
(1,1282)	1:16:A:PHE:HE1	1:9:B:ALA:HB2	20	0.59
(1,1282)	1:16:A:PHE:HE2	1:9:B:ALA:HB2	20	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	6	0.59
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	1	0.59
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	3	0.59
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	1	0.59
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	1	0.59
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	1	0.59
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	15	0.59
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	15	0.59
(1,1052)	1:46:B:PHE:HD1	1:54:B:ILE:HD12	10	0.59
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	3	0.59
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	6	0.59
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	8	0.59
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	8	0.59
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	11	0.59
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	5	0.59
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	3	0.59
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	3	0.59
(1,4208)	1:345:B:LYS:H	1:346:B:GLN:H	16	0.58
(1,4169)	1:300:B:GLU:H	1:301:B:GLY:H	4	0.58
(1,4138)	1:228:B:THR:H	1:229:B:VAL:H	12	0.58
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	4	0.58
(1,3970)	1:217:B:LYS:HA	1:220:B:GLU:H	7	0.58
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	1	0.58
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	12	0.58
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	12	0.58
(1,3600)	1:176:B:LEU:HD11	1:180:B:LYS:H	15	0.58
(1,3600)	1:176:B:LEU:HD12	1:180:B:LYS:H	15	0.58
(1,3600)	1:176:B:LEU:HD13	1:180:B:LYS:H	15	0.58
(1,3527)	1:170:B:PHE:HB2	1:196:B:VAL:HA	11	0.58
(1,3527)	1:170:B:PHE:HB3	1:196:B:VAL:HA	11	0.58
(1,3514)	1:170:B:PHE:H	1:171:B:ARG:H	19	0.58
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	19	0.58
(1,3382)	1:154:B:GLN:HA	1:158:B:ASP:H	20	0.58
(1,3279)	1:144:B:ALA:HB1	1:175:B:ARG:HE	16	0.58
(1,3279)	1:144:B:ALA:HB2	1:175:B:ARG:HE	16	0.58
(1,3279)	1:144:B:ALA:HB3	1:175:B:ARG:HE	16	0.58
(1,3082)	1:125:B:TYR:HD1	1:141:B:ASN:HB3	16	0.58
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	2	0.58
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	2	0.58
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	19	0.58
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	19	0.58
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	19	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG21	17	0.58
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG22	17	0.58
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG23	17	0.58
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	17	0.58
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	4	0.58
(1,2583)	1:207:A:ALA:HA	1:211:A:ASP:H	5	0.58
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	12	0.58
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	12	0.58
(1,2300)	1:177:A:GLY:H	1:189:A:ALA:HA	8	0.58
(1,2076)	1:154:A:GLN:HA	1:158:A:ASP:H	9	0.58
(1,1900)	1:139:A:TYR:HA	1:158:A:ASP:HA	13	0.58
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB2	8	0.58
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	8	0.58
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB2	8	0.58
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB3	8	0.58
(1,1632)	1:113:A:MET:HA	1:116:A:LYS:H	20	0.58
(1,1569)	1:108:A:GLN:H	1:111:A:LYS:H	18	0.58
(1,1544)	1:105:A:LEU:HD21	1:124:A:LYS:HA	20	0.58
(1,1544)	1:105:A:LEU:HD22	1:124:A:LYS:HA	20	0.58
(1,1544)	1:105:A:LEU:HD23	1:124:A:LYS:HA	20	0.58
(1,1519)	1:103:A:GLU:HA	1:107:A:MET:H	18	0.58
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	20	0.58
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	6	0.58
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	2	0.58
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	2	0.58
(1,1350)	1:39:A:CYS:HB2	1:32:B:SER:HA	3	0.58
(1,1350)	1:39:A:CYS:HB3	1:32:B:SER:HA	3	0.58
(1,1336)	1:36:A:ALA:H	1:36:B:ALA:HA	3	0.58
(1,1293)	1:16:A:PHE:HE1	1:40:B:ILE:HG21	13	0.58
(1,1293)	1:16:A:PHE:HE2	1:40:B:ILE:HG21	13	0.58
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	10	0.58
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	10	0.58
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	10	0.58
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	10	0.58
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	10	0.58
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	13	0.58
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD11	20	0.58
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD12	20	0.58
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD13	20	0.58
(1,1133)	1:58:B:SER:HB2	1:60:B:PHE:H	15	0.58
(1,1133)	1:58:B:SER:HB3	1:60:B:PHE:H	15	0.58
(1,1118)	1:56:B:GLY:H	1:58:B:SER:H	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	16	0.58
(1,1096)	1:53:B:GLY:H	1:56:B:GLY:H	10	0.58
(1,948)	1:35:B:VAL:H	1:38:B:ASP:H	3	0.58
(1,892)	1:28:B:ASP:HA	1:31:B:ASP:H	11	0.58
(1,889)	1:28:B:ASP:H	1:31:B:ASP:H	12	0.58
(1,857)	1:23:B:LYS:H	1:25:B:ILE:H	3	0.58
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	8	0.58
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD11	7	0.58
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD12	7	0.58
(1,591)	1:68:A:ILE:HA	1:69:A:LEU:HD13	7	0.58
(1,344)	1:35:A:VAL:HA	1:38:A:ASP:HA	19	0.58
(1,284)	1:28:A:ASP:HA	1:32:A:SER:H	10	0.58
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	1	0.58
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	13	0.58
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	10	0.57
(1,4171)	1:302:B:PHE:H	1:303:B:ALA:H	14	0.57
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	17	0.57
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	17	0.57
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	15	0.57
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	15	0.57
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	8	0.57
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	12	0.57
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	8	0.57
(1,3801)	1:196:B:VAL:HG11	1:208:B:MET:HB2	3	0.57
(1,3801)	1:196:B:VAL:HG11	1:208:B:MET:HB3	3	0.57
(1,3801)	1:196:B:VAL:HG12	1:208:B:MET:HB2	3	0.57
(1,3801)	1:196:B:VAL:HG12	1:208:B:MET:HB3	3	0.57
(1,3801)	1:196:B:VAL:HG13	1:208:B:MET:HB2	3	0.57
(1,3801)	1:196:B:VAL:HG13	1:208:B:MET:HB3	3	0.57
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	17	0.57
(1,3551)	1:171:B:ARG:HA	1:175:B:ARG:H	6	0.57
(1,3551)	1:171:B:ARG:HA	1:175:B:ARG:H	14	0.57
(1,3476)	1:163:B:ILE:HD11	1:176:B:LEU:HD21	12	0.57
(1,3476)	1:163:B:ILE:HD11	1:176:B:LEU:HD22	12	0.57
(1,3476)	1:163:B:ILE:HD11	1:176:B:LEU:HD23	12	0.57
(1,3476)	1:163:B:ILE:HD12	1:176:B:LEU:HD21	12	0.57
(1,3476)	1:163:B:ILE:HD12	1:176:B:LEU:HD22	12	0.57
(1,3476)	1:163:B:ILE:HD12	1:176:B:LEU:HD23	12	0.57
(1,3476)	1:163:B:ILE:HD13	1:176:B:LEU:HD21	12	0.57
(1,3476)	1:163:B:ILE:HD13	1:176:B:LEU:HD22	12	0.57
(1,3476)	1:163:B:ILE:HD13	1:176:B:LEU:HD23	12	0.57
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	15	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3298)	1:146:B:HIS:HB2	1:151:B:GLU:HB2	2	0.57
(1,3298)	1:146:B:HIS:HB2	1:151:B:GLU:HB3	2	0.57
(1,3298)	1:146:B:HIS:HB3	1:151:B:GLU:HB2	2	0.57
(1,3298)	1:146:B:HIS:HB3	1:151:B:GLU:HB3	2	0.57
(1,3147)	1:134:B:THR:H	1:135:B:ASN:H	19	0.57
(1,3082)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	17	0.57
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	3	0.57
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	3	0.57
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	3	0.57
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	3	0.57
(1,2846)	1:105:B:LEU:HD11	1:128:B:ALA:HA	6	0.57
(1,2846)	1:105:B:LEU:HD12	1:128:B:ALA:HA	6	0.57
(1,2846)	1:105:B:LEU:HD13	1:128:B:ALA:HA	6	0.57
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	19	0.57
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	19	0.57
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	19	0.57
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	19	0.57
(1,2357)	1:181:A:TYR:HA	1:185:A:LYS:H	11	0.57
(1,2350)	1:181:A:TYR:H	1:189:A:ALA:H	7	0.57
(1,2221)	1:170:A:PHE:HB2	1:196:A:VAL:HA	9	0.57
(1,2221)	1:170:A:PHE:HB3	1:196:A:VAL:HA	9	0.57
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	16	0.57
(1,2114)	1:158:A:ASP:HA	1:162:A:ALA:H	16	0.57
(1,1991)	1:146:A:HIS:HA	1:151:A:GLU:H	7	0.57
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB2	18	0.57
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	18	0.57
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB2	18	0.57
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB3	18	0.57
(1,1527)	1:104:A:ASP:HA	1:107:A:MET:H	1	0.57
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD11	5	0.57
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD12	5	0.57
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD13	5	0.57
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	20	0.57
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	20	0.57
(1,1439)	1:94:A:ASP:HA	1:96:A:ALA:H	3	0.57
(1,1279)	1:16:A:PHE:HE1	1:9:B:ALA:HA	9	0.57
(1,1279)	1:16:A:PHE:HE2	1:9:B:ALA:HA	9	0.57
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	17	0.57
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	17	0.57
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	17	0.57
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	17	0.57
(1,1208)	1:70:B:ASN:H	1:71:B:SER:H	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	15	0.57
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	7	0.57
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	7	0.57
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	12	0.57
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	12	0.57
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	1	0.57
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	1	0.57
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	10	0.57
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	10	0.57
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	20	0.57
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	8	0.57
(1,336)	1:34:A:ASN:HA	1:38:A:ASP:H	13	0.57
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	2	0.57
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	4	0.57
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	20	0.57
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	1	0.56
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	13	0.56
(1,4189)	1:324:B:ALA:H	1:325:B:GLY:H	20	0.56
(1,4184)	1:319:B:ALA:H	1:320:B:LEU:H	10	0.56
(1,4169)	1:300:B:GLU:H	1:301:B:GLY:H	3	0.56
(1,4163)	1:257:B:GLY:H	1:258:B:GLY:H	20	0.56
(1,4158)	1:252:B:LEU:H	1:253:B:GLY:H	5	0.56
(1,4108)	1:343:A:GLU:H	1:344:A:ASN:H	19	0.56
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	18	0.56
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	12	0.56
(1,3882)	1:207:B:ALA:H	1:210:B:ARG:H	5	0.56
(1,3770)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	11	0.56
(1,3729)	1:190:B:LEU:HD21	1:216:B:LYS:HA	17	0.56
(1,3729)	1:190:B:LEU:HD22	1:216:B:LYS:HA	17	0.56
(1,3729)	1:190:B:LEU:HD23	1:216:B:LYS:HA	17	0.56
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	20	0.56
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	20	0.56
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	20	0.56
(1,3533)	1:170:B:PHE:HD1	1:196:B:VAL:HA	10	0.56
(1,3533)	1:170:B:PHE:HD2	1:196:B:VAL:HA	10	0.56
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	7	0.56
(1,3470)	1:163:B:ILE:HA	1:169:B:TYR:H	7	0.56
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB2	4	0.56
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB3	4	0.56
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB2	4	0.56
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB3	4	0.56
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB2	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB3	4	0.56
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	7	0.56
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB2	1	0.56
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB3	1	0.56
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB2	1	0.56
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB3	1	0.56
(1,2978)	1:116:B:LYS:HB2	1:118:B:TYR:HE1	1	0.56
(1,2978)	1:116:B:LYS:HB2	1:118:B:TYR:HE2	1	0.56
(1,2978)	1:116:B:LYS:HB3	1:118:B:TYR:HE1	1	0.56
(1,2978)	1:116:B:LYS:HB3	1:118:B:TYR:HE2	1	0.56
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	11	0.56
(1,2881)	1:109:B:GLY:H	1:112:B:ALA:H	13	0.56
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE1	5	0.56
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE2	5	0.56
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE3	5	0.56
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	11	0.56
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	1	0.56
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	4	0.56
(1,2660)	1:217:A:LYS:H	1:220:A:GLU:H	11	0.56
(1,2279)	1:174:A:SER:HA	1:193:A:TYR:HA	6	0.56
(1,2232)	1:170:A:PHE:HE1	1:171:A:ARG:HD2	10	0.56
(1,2232)	1:170:A:PHE:HE1	1:171:A:ARG:HD3	10	0.56
(1,2232)	1:170:A:PHE:HE2	1:171:A:ARG:HD2	10	0.56
(1,2232)	1:170:A:PHE:HE2	1:171:A:ARG:HD3	10	0.56
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	7	0.56
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	8	0.56
(1,1735)	1:122:A:ILE:HA	1:126:A:THR:H	3	0.56
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	16	0.56
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	16	0.56
(1,1463)	1:98:A:THR:H	1:101:A:LYS:H	13	0.56
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	8	0.56
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	7	0.56
(1,1349)	1:39:A:CYS:HA	1:32:B:SER:HA	16	0.56
(1,1337)	1:36:A:ALA:HA	1:36:B:ALA:H	3	0.56
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	7	0.56
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	7	0.56
(1,1239)	1:8:A:ILE:HG21	1:12:B:ILE:HA	5	0.56
(1,1239)	1:8:A:ILE:HG22	1:12:B:ILE:HA	5	0.56
(1,1239)	1:8:A:ILE:HG23	1:12:B:ILE:HA	5	0.56
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	4	0.56
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	4	0.56
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	16	0.56
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	8	0.56
(1,635)	1:5:B:LYS:HA	1:9:B:ALA:H	1	0.56
(1,588)	1:68:A:ILE:H	1:69:A:LEU:HD11	7	0.56
(1,588)	1:68:A:ILE:H	1:69:A:LEU:HD12	7	0.56
(1,588)	1:68:A:ILE:H	1:69:A:LEU:HD13	7	0.56
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	13	0.56
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	5	0.55
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	11	0.55
(1,4189)	1:324:B:ALA:H	1:325:B:GLY:H	8	0.55
(1,4138)	1:228:B:THR:H	1:229:B:VAL:H	10	0.55
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	10	0.55
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	3	0.55
(1,3722)	1:190:B:LEU:HA	1:212:B:TYR:HA	17	0.55
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD21	7	0.55
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD22	7	0.55
(1,3697)	1:187:B:GLU:HA	1:190:B:LEU:HD23	7	0.55
(1,3641)	1:180:B:LYS:H	1:189:B:ALA:HA	3	0.55
(1,3542)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	2	0.55
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	8	0.55
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	8	0.55
(1,3382)	1:154:B:GLN:HA	1:158:B:ASP:H	4	0.55
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB2	3	0.55
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB3	3	0.55
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB2	3	0.55
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB3	3	0.55
(1,3206)	1:139:B:TYR:HA	1:158:B:ASP:HA	17	0.55
(1,3114)	1:129:B:ILE:H	1:138:B:TYR:HB2	17	0.55
(1,3114)	1:129:B:ILE:H	1:138:B:TYR:HB3	17	0.55
(1,3082)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	3	0.55
(1,2945)	1:113:B:MET:HB2	1:125:B:TYR:HE2	18	0.55
(1,2776)	1:99:B:LYS:H	1:101:B:LYS:H	9	0.55
(1,2756)	1:96:B:ALA:H	1:98:B:THR:H	12	0.55
(1,2694)	1:221:A:GLN:H	1:224:A:ASN:H	6	0.55
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	9	0.55
(1,2358)	1:181:A:TYR:HA	1:186:A:PRO:HA	10	0.55
(1,2358)	1:181:A:TYR:HA	1:186:A:PRO:HA	16	0.55
(1,2323)	1:178:A:PHE:HB2	1:179:A:ALA:H	16	0.55
(1,2323)	1:178:A:PHE:HB3	1:179:A:ALA:H	16	0.55
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	14	0.55
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	14	0.55
(1,1762)	1:125:A:TYR:HA	1:138:A:TYR:HA	14	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1645)	1:113:A:MET:HE1	1:145:A:ALA:H	7	0.55
(1,1645)	1:113:A:MET:HE2	1:145:A:ALA:H	7	0.55
(1,1645)	1:113:A:MET:HE3	1:145:A:ALA:H	7	0.55
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	14	0.55
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	7	0.55
(1,1439)	1:94:A:ASP:HA	1:96:A:ALA:H	2	0.55
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	15	0.55
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	15	0.55
(1,1411)	1:67:A:ASP:HA	1:62:B:GLY:H	3	0.55
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	8	0.55
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	8	0.55
(1,1325)	1:33:A:LEU:HA	1:40:B:ILE:HA	9	0.55
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	2	0.55
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB2	6	0.55
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB3	6	0.55
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB2	6	0.55
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB3	6	0.55
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB2	6	0.55
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB3	6	0.55
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	9	0.55
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	9	0.55
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	5	0.55
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	5	0.55
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	5	0.55
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	5	0.55
(1,1233)	1:5:A:LYS:HA	1:15:B:TYR:HE1	12	0.55
(1,1233)	1:5:A:LYS:HA	1:15:B:TYR:HE2	12	0.55
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	7	0.55
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	10	0.55
(1,1145)	1:60:B:PHE:HA	1:62:B:GLY:H	8	0.55
(1,1142)	1:60:B:PHE:HA	1:61:B:LYS:H	18	0.55
(1,1140)	1:59:B:GLU:HB2	1:64:B:HIS:HA	7	0.55
(1,1140)	1:59:B:GLU:HB3	1:64:B:HIS:HA	7	0.55
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	12	0.55
(1,1115)	1:55:B:LEU:HD11	1:72:B:ALA:HA	20	0.55
(1,1115)	1:55:B:LEU:HD12	1:72:B:ALA:HA	20	0.55
(1,1115)	1:55:B:LEU:HD13	1:72:B:ALA:HA	20	0.55
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	15	0.55
(1,1005)	1:41:B:SER:H	1:46:B:PHE:HE1	3	0.55
(1,945)	1:34:B:ASN:HA	1:38:B:ASP:H	18	0.55
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD21	12	0.55
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD22	12	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD23	12	0.55
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	3	0.55
(1,163)	1:15:A:TYR:HD1	1:18:A:SER:HB2	19	0.55
(1,163)	1:15:A:TYR:HD1	1:18:A:SER:HB3	19	0.55
(1,163)	1:15:A:TYR:HD2	1:18:A:SER:HB2	19	0.55
(1,163)	1:15:A:TYR:HD2	1:18:A:SER:HB3	19	0.55
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	15	0.55
(1,14)	1:4:A:SER:H	1:7:A:GLU:H	4	0.55
(1,4068)	1:260:A:LEU:H	1:261:A:GLY:H	18	0.54
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	2	0.54
(1,3825)	1:199:B:ILE:H	1:201:B:GLY:H	7	0.54
(1,3810)	1:197:B:LEU:HA	1:204:B:ALA:HA	14	0.54
(1,3791)	1:195:B:LYS:HA	1:199:B:ILE:H	4	0.54
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	4	0.54
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	19	0.54
(1,3721)	1:190:B:LEU:HA	1:194:B:LYS:H	8	0.54
(1,3686)	1:185:B:LYS:H	1:186:B:PRO:HA	13	0.54
(1,3527)	1:170:B:PHE:HB2	1:196:B:VAL:HA	6	0.54
(1,3527)	1:170:B:PHE:HB3	1:196:B:VAL:HA	6	0.54
(1,3312)	1:147:B:SER:HA	1:152:B:TYR:H	8	0.54
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB2	20	0.54
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB3	20	0.54
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB2	20	0.54
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB3	20	0.54
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	19	0.54
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	19	0.54
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	2	0.54
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	1	0.54
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	18	0.54
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	18	0.54
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	1	0.54
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	8	0.54
(1,2615)	1:211:A:ASP:HA	1:215:A:ALA:H	1	0.54
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	8	0.54
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	13	0.54
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	11	0.54
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	11	0.54
(1,2469)	1:194:A:LYS:H	1:212:A:TYR:HA	9	0.54
(1,2418)	1:190:A:LEU:HA	1:216:A:LYS:H	15	0.54
(1,2356)	1:181:A:TYR:HA	1:184:A:GLY:H	3	0.54
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	4	0.54
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	13	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	20	0.54
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	20	0.54
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	20	0.54
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	2	0.54
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	2	0.54
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	11	0.54
(1,1288)	1:16:A:PHE:HE1	1:12:B:ILE:HD11	11	0.54
(1,1288)	1:16:A:PHE:HE2	1:12:B:ILE:HD11	11	0.54
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	2	0.54
(1,1258)	1:12:A:ILE:HG12	1:12:B:ILE:HA	6	0.54
(1,1258)	1:12:A:ILE:HG13	1:12:B:ILE:HA	6	0.54
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD11	18	0.54
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD12	18	0.54
(1,1238)	1:5:A:LYS:HB2	1:19:B:ILE:HD13	18	0.54
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD11	18	0.54
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD12	18	0.54
(1,1238)	1:5:A:LYS:HB3	1:19:B:ILE:HD13	18	0.54
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG21	3	0.54
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG22	3	0.54
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG23	3	0.54
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	11	0.54
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	11	0.54
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	11	0.54
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	6	0.54
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	5	0.54
(1,762)	1:15:B:TYR:HA	1:18:B:SER:H	7	0.54
(1,624)	1:4:B:SER:H	1:8:B:ILE:H	3	0.54
(1,560)	1:63:A:GLN:HA	1:65:A:LEU:H	19	0.54
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB2	18	0.54
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB3	18	0.54
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	16	0.54
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	16	0.54
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	14	0.53
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	19	0.53
(1,4064)	1:256:A:LEU:H	1:257:A:GLY:H	6	0.53
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	17	0.53
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	4	0.53
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	4	0.53
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	16	0.53
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	16	0.53
(1,3689)	1:185:B:LYS:HA	1:188:B:GLU:H	1	0.53
(1,3663)	1:181:B:TYR:HA	1:185:B:LYS:H	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3656)	1:181:B:TYR:H	1:189:B:ALA:H	2	0.53
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	7	0.53
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	7	0.53
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	7	0.53
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	7	0.53
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	7	0.53
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	7	0.53
(1,3432)	1:159:B:ALA:HB1	1:176:B:LEU:H	9	0.53
(1,3432)	1:159:B:ALA:HB2	1:176:B:LEU:H	9	0.53
(1,3432)	1:159:B:ALA:HB3	1:176:B:LEU:H	9	0.53
(1,3382)	1:154:B:GLN:HA	1:158:B:ASP:H	12	0.53
(1,3310)	1:147:B:SER:HA	1:150:B:LYS:HA	6	0.53
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	12	0.53
(1,3168)	1:136:B:ALA:HA	1:162:B:ALA:HA	8	0.53
(1,2933)	1:113:B:MET:H	1:121:B:ALA:HA	7	0.53
(1,2807)	1:102:B:ALA:HA	1:128:B:ALA:HA	2	0.53
(1,2789)	1:101:B:LYS:H	1:103:B:GLU:H	12	0.53
(1,2714)	1:223:A:LEU:HA	1:226:A:GLU:H	3	0.53
(1,2570)	1:206:A:GLU:HA	1:209:A:LYS:H	13	0.53
(1,2555)	1:205:A:THR:H	1:209:A:LYS:H	3	0.53
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG21	9	0.53
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG22	9	0.53
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG23	9	0.53
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	9	0.53
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	9	0.53
(1,2216)	1:170:A:PHE:HA	1:196:A:VAL:HA	11	0.53
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	4	0.53
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	4	0.53
(1,2076)	1:154:A:GLN:HA	1:158:A:ASP:H	5	0.53
(1,2032)	1:150:A:LYS:HB2	1:152:A:TYR:HE1	2	0.53
(1,2032)	1:150:A:LYS:HB2	1:152:A:TYR:HE2	2	0.53
(1,2032)	1:150:A:LYS:HB3	1:152:A:TYR:HE1	2	0.53
(1,2032)	1:150:A:LYS:HB3	1:152:A:TYR:HE2	2	0.53
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	7	0.53
(1,1855)	1:135:A:ASN:HB2	1:138:A:TYR:HE1	10	0.53
(1,1855)	1:135:A:ASN:HB2	1:138:A:TYR:HE2	10	0.53
(1,1855)	1:135:A:ASN:HB3	1:138:A:TYR:HE1	10	0.53
(1,1855)	1:135:A:ASN:HB3	1:138:A:TYR:HE2	10	0.53
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	3	0.53
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	11	0.53
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB1	8	0.53
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB2	8	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB3	8	0.53
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	13	0.53
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	13	0.53
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	20	0.53
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	20	0.53
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	20	0.53
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	20	0.53
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG21	16	0.53
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG22	16	0.53
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG23	16	0.53
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG21	16	0.53
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG22	16	0.53
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG23	16	0.53
(1,1351)	1:39:A:CYS:HB2	1:33:B:LEU:HA	3	0.53
(1,1351)	1:39:A:CYS:HB3	1:33:B:LEU:HA	3	0.53
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	18	0.53
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	18	0.53
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	18	0.53
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD11	8	0.53
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD12	8	0.53
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD13	8	0.53
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD11	8	0.53
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD12	8	0.53
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD13	8	0.53
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	9	0.53
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	9	0.53
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	9	0.53
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	9	0.53
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	17	0.53
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	17	0.53
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	17	0.53
(1,1146)	1:60:B:PHE:HA	1:63:B:GLN:H	18	0.53
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	19	0.53
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	19	0.53
(1,988)	1:39:B:CYS:HA	1:42:B:GLU:H	3	0.53
(1,886)	1:27:B:GLU:HA	1:31:B:ASP:H	19	0.53
(1,852)	1:22:B:LYS:H	1:24:B:GLU:H	17	0.53
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG11	9	0.53
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG12	9	0.53
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG13	9	0.53
(1,625)	1:4:B:SER:HA	1:5:B:LYS:H	1	0.53
(1,578)	1:66:A:ALA:HA	1:68:A:ILE:H	20	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:65:A:LEU:HD21	1:71:A:SER:H	7	0.53
(1,573)	1:65:A:LEU:HD22	1:71:A:SER:H	7	0.53
(1,573)	1:65:A:LEU:HD23	1:71:A:SER:H	7	0.53
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	6	0.53
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	6	0.53
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB2	5	0.53
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB3	5	0.53
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB2	4	0.53
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB3	4	0.53
(1,40)	1:7:A:GLU:HA	1:10:A:ALA:H	17	0.53
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	13	0.52
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	13	0.52
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	13	0.52
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	2	0.52
(1,4159)	1:253:B:GLY:H	1:254:B:SER:H	2	0.52
(1,4156)	1:248:B:GLY:H	1:249:B:LEU:H	18	0.52
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	11	0.52
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	13	0.52
(1,4000)	1:221:B:GLN:H	1:224:B:ASN:H	3	0.52
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	17	0.52
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD11	18	0.52
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD12	18	0.52
(1,3780)	1:194:B:LYS:HA	1:197:B:LEU:HD13	18	0.52
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	3	0.52
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	3	0.52
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	3	0.52
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	3	0.52
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG21	17	0.52
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG22	17	0.52
(1,3692)	1:187:B:GLU:H	1:219:B:VAL:HG23	17	0.52
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	9	0.52
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	9	0.52
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	9	0.52
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	9	0.52
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	9	0.52
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	9	0.52
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	15	0.52
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	4	0.52
(1,3411)	1:157:B:LYS:HA	1:160:B:GLU:H	6	0.52
(1,3355)	1:152:B:TYR:HA	1:155:B:ALA:HA	8	0.52
(1,3206)	1:139:B:TYR:HA	1:158:B:ASP:HA	13	0.52
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	17	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	17	0.52
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	17	0.52
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	17	0.52
(1,3079)	1:125:B:TYR:HB2	1:142:B:ARG:HD2	12	0.52
(1,3079)	1:125:B:TYR:HB2	1:142:B:ARG:HD3	12	0.52
(1,3079)	1:125:B:TYR:HB3	1:142:B:ARG:HD2	12	0.52
(1,3079)	1:125:B:TYR:HB3	1:142:B:ARG:HD3	12	0.52
(1,3077)	1:125:B:TYR:HB2	1:138:B:TYR:HB2	10	0.52
(1,3077)	1:125:B:TYR:HB2	1:138:B:TYR:HB3	10	0.52
(1,3077)	1:125:B:TYR:HB3	1:138:B:TYR:HB2	10	0.52
(1,3077)	1:125:B:TYR:HB3	1:138:B:TYR:HB3	10	0.52
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	15	0.52
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	15	0.52
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE1	19	0.52
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE2	19	0.52
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	19	0.52
(1,2779)	1:99:B:LYS:HA	1:101:B:LYS:H	19	0.52
(1,2769)	1:98:B:THR:H	1:101:B:LYS:H	19	0.52
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	8	0.52
(1,2706)	1:222:A:SER:HA	1:224:A:ASN:H	3	0.52
(1,2555)	1:205:A:THR:H	1:209:A:LYS:H	17	0.52
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	8	0.52
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	17	0.52
(1,1890)	1:138:A:TYR:HA	1:142:A:ARG:H	3	0.52
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	1	0.52
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	9	0.52
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD21	10	0.52
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD22	10	0.52
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD23	10	0.52
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG2	7	0.52
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG3	7	0.52
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	6	0.52
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD11	11	0.52
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD12	11	0.52
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD13	11	0.52
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	2	0.52
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	10	0.52
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	10	0.52
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	10	0.52
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	10	0.52
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	17	0.52
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	17	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	17	0.52
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	5	0.52
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	1	0.52
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	1	0.52
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	7	0.52
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	7	0.52
(1,1314)	1:29:A:GLY:HA2	1:43:B:ALA:H	13	0.52
(1,1314)	1:29:A:GLY:HA3	1:43:B:ALA:H	13	0.52
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	19	0.52
(1,1118)	1:56:B:GLY:H	1:58:B:SER:H	7	0.52
(1,818)	1:18:B:SER:HA	1:21:B:GLU:H	8	0.52
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	8	0.52
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE21	4	0.52
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE22	4	0.52
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE21	4	0.52
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE22	4	0.52
(1,529)	1:59:A:GLU:HA	1:64:A:HIS:HA	9	0.52
(1,336)	1:34:A:ASN:HA	1:38:A:ASP:H	19	0.52
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	1	0.51
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	16	0.51
(1,4077)	1:305:A:GLY:H	1:307:A:GLY:H	4	0.51
(1,4073)	1:302:A:PHE:H	1:303:A:ALA:H	3	0.51
(1,4058)	1:248:A:GLY:H	1:249:A:LEU:H	14	0.51
(1,4051)	1:241:A:SER:H	1:242:A:GLN:H	3	0.51
(1,4050)	1:240:A:ALA:H	1:241:A:SER:H	7	0.51
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	7	0.51
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	14	0.51
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	5	0.51
(1,4003)	1:221:B:GLN:HA	1:224:B:ASN:H	1	0.51
(1,3858)	1:205:B:THR:H	1:208:B:MET:H	11	0.51
(1,3782)	1:194:B:LYS:HB2	1:212:B:TYR:HD1	10	0.51
(1,3782)	1:194:B:LYS:HB2	1:212:B:TYR:HD2	10	0.51
(1,3782)	1:194:B:LYS:HB3	1:212:B:TYR:HD1	10	0.51
(1,3782)	1:194:B:LYS:HB3	1:212:B:TYR:HD2	10	0.51
(1,3774)	1:194:B:LYS:H	1:197:B:LEU:H	4	0.51
(1,3763)	1:193:B:TYR:HD1	1:211:B:ASP:HA	1	0.51
(1,3763)	1:193:B:TYR:HD2	1:211:B:ASP:HA	1	0.51
(1,3651)	1:180:B:LYS:HB2	1:189:B:ALA:H	14	0.51
(1,3651)	1:180:B:LYS:HB3	1:189:B:ALA:H	14	0.51
(1,3595)	1:176:B:LEU:H	1:178:B:PHE:H	6	0.51
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	9	0.51
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB2	12	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB3	12	0.51
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB2	12	0.51
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB3	12	0.51
(1,3569)	1:173:B:TYR:HB2	1:195:B:LYS:H	12	0.51
(1,3569)	1:173:B:TYR:HB3	1:195:B:LYS:H	12	0.51
(1,3569)	1:173:B:TYR:HB2	1:195:B:LYS:H	20	0.51
(1,3569)	1:173:B:TYR:HB3	1:195:B:LYS:H	20	0.51
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	1	0.51
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	1	0.51
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	5	0.51
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD11	16	0.51
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD12	16	0.51
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD13	16	0.51
(1,3396)	1:156:B:VAL:HA	1:176:B:LEU:HA	4	0.51
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB2	13	0.51
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB3	13	0.51
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB2	13	0.51
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB3	13	0.51
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	4	0.51
(1,3119)	1:129:B:ILE:HA	1:133:B:PRO:HA	6	0.51
(1,3081)	1:125:B:TYR:HE1	1:142:B:ARG:HA	14	0.51
(1,3081)	1:125:B:TYR:HE2	1:142:B:ARG:HA	14	0.51
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	1	0.51
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE1	4	0.51
(1,2944)	1:113:B:MET:HB2	1:125:B:TYR:HE2	4	0.51
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE1	4	0.51
(1,2944)	1:113:B:MET:HB3	1:125:B:TYR:HE2	4	0.51
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE1	4	0.51
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE2	4	0.51
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG21	14	0.51
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG22	14	0.51
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG23	14	0.51
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG21	14	0.51
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG22	14	0.51
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG23	14	0.51
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG21	14	0.51
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG22	14	0.51
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG23	14	0.51
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	17	0.51
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	17	0.51
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	17	0.51
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	5	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	1	0.51
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	10	0.51
(1,2635)	1:214:A:SER:H	1:216:A:LYS:H	8	0.51
(1,2419)	1:190:A:LEU:HD11	1:212:A:TYR:HA	16	0.51
(1,2419)	1:190:A:LEU:HD12	1:212:A:TYR:HA	16	0.51
(1,2419)	1:190:A:LEU:HD13	1:212:A:TYR:HA	16	0.51
(1,2350)	1:181:A:TYR:H	1:189:A:ALA:H	10	0.51
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE1	3	0.51
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE2	3	0.51
(1,2230)	1:170:A:PHE:HE1	1:171:A:ARG:H	12	0.51
(1,2230)	1:170:A:PHE:HE2	1:171:A:ARG:H	12	0.51
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	2	0.51
(1,2003)	1:147:A:SER:HA	1:150:A:LYS:H	7	0.51
(1,1913)	1:139:A:TYR:HE1	1:161:A:SER:HB2	3	0.51
(1,1913)	1:139:A:TYR:HE1	1:161:A:SER:HB3	3	0.51
(1,1913)	1:139:A:TYR:HE2	1:161:A:SER:HB2	3	0.51
(1,1913)	1:139:A:TYR:HE2	1:161:A:SER:HB3	3	0.51
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	12	0.51
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	15	0.51
(1,1646)	1:113:A:MET:HE1	1:145:A:ALA:HA	19	0.51
(1,1646)	1:113:A:MET:HE2	1:145:A:ALA:HA	19	0.51
(1,1646)	1:113:A:MET:HE3	1:145:A:ALA:HA	19	0.51
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	6	0.51
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	14	0.51
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	6	0.51
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	6	0.51
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	6	0.51
(1,1439)	1:94:A:ASP:HA	1:96:A:ALA:H	4	0.51
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	5	0.51
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	2	0.51
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	12	0.51
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	12	0.51
(1,1383)	1:44:A:PHE:HA	1:25:B:ILE:HD11	12	0.51
(1,1383)	1:44:A:PHE:HA	1:25:B:ILE:HD12	12	0.51
(1,1383)	1:44:A:PHE:HA	1:25:B:ILE:HD13	12	0.51
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	1	0.51
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB2	17	0.51
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB3	17	0.51
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	8	0.51
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	8	0.51
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB2	3	0.51
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB3	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB2	3	0.51
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB3	3	0.51
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB2	3	0.51
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB3	3	0.51
(1,1281)	1:16:A:PHE:HE1	1:9:B:ALA:HB1	8	0.51
(1,1281)	1:16:A:PHE:HE2	1:9:B:ALA:HB1	8	0.51
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	15	0.51
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB2	2	0.51
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB3	2	0.51
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	4	0.51
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	18	0.51
(1,1204)	1:69:B:LEU:H	1:71:B:SER:H	4	0.51
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	6	0.51
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	6	0.51
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	15	0.51
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	15	0.51
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	15	0.51
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	15	0.51
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	15	0.51
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	15	0.51
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	5	0.51
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	5	0.51
(1,835)	1:20:B:VAL:HA	1:24:B:GLU:H	16	0.51
(1,795)	1:16:B:PHE:HB2	1:33:B:LEU:HA	3	0.51
(1,795)	1:16:B:PHE:HB3	1:33:B:LEU:HA	3	0.51
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	7	0.51
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	2	0.51
(1,77)	1:10:A:ALA:HA	1:51:A:VAL:HA	3	0.51
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	12	0.51
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	17	0.51
(1,4208)	1:345:B:LYS:H	1:346:B:GLN:H	12	0.5
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	1	0.5
(1,4110)	1:345:A:LYS:H	1:346:A:GLN:H	5	0.5
(1,4110)	1:345:A:LYS:H	1:346:A:GLN:H	20	0.5
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	20	0.5
(1,3782)	1:194:B:LYS:HB2	1:212:B:TYR:HD1	8	0.5
(1,3782)	1:194:B:LYS:HB2	1:212:B:TYR:HD2	8	0.5
(1,3782)	1:194:B:LYS:HB3	1:212:B:TYR:HD1	8	0.5
(1,3782)	1:194:B:LYS:HB3	1:212:B:TYR:HD2	8	0.5
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	3	0.5
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	20	0.5
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	2	0.5
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG21	1	0.5
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG22	1	0.5
(1,3560)	1:173:B:TYR:H	1:196:B:VAL:HG23	1	0.5
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	6	0.5
(1,3511)	1:169:B:TYR:HD2	1:171:B:ARG:H	13	0.5
(1,3357)	1:152:B:TYR:HA	1:156:B:VAL:H	9	0.5
(1,3303)	1:147:B:SER:H	1:151:B:GLU:H	2	0.5
(1,3135)	1:130:B:LYS:HA	1:132:B:LEU:H	1	0.5
(1,3077)	1:125:B:TYR:HB2	1:138:B:TYR:HB2	17	0.5
(1,3077)	1:125:B:TYR:HB2	1:138:B:TYR:HB3	17	0.5
(1,3077)	1:125:B:TYR:HB3	1:138:B:TYR:HB2	17	0.5
(1,3077)	1:125:B:TYR:HB3	1:138:B:TYR:HB3	17	0.5
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB2	10	0.5
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB3	10	0.5
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE1	2	0.5
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	17	0.5
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	5	0.5
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	16	0.5
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	14	0.5
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	14	0.5
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	9	0.5
(1,2583)	1:207:A:ALA:HA	1:211:A:ASP:H	15	0.5
(1,2343)	1:180:A:LYS:HB2	1:188:A:GLU:H	10	0.5
(1,2343)	1:180:A:LYS:HB3	1:188:A:GLU:H	10	0.5
(1,2342)	1:180:A:LYS:HB2	1:185:A:LYS:H	16	0.5
(1,2342)	1:180:A:LYS:HB3	1:185:A:LYS:H	16	0.5
(1,2055)	1:152:A:TYR:HB2	1:183:A:GLN:H	20	0.5
(1,2055)	1:152:A:TYR:HB3	1:183:A:GLN:H	20	0.5
(1,1991)	1:146:A:HIS:HA	1:151:A:GLU:H	9	0.5
(1,1913)	1:139:A:TYR:HE1	1:161:A:SER:HB2	20	0.5
(1,1913)	1:139:A:TYR:HE1	1:161:A:SER:HB3	20	0.5
(1,1913)	1:139:A:TYR:HE2	1:161:A:SER:HB2	20	0.5
(1,1913)	1:139:A:TYR:HE2	1:161:A:SER:HB3	20	0.5
(1,1899)	1:139:A:TYR:HA	1:143:A:ALA:H	3	0.5
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	13	0.5
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	5	0.5
(1,1518)	1:103:A:GLU:HA	1:106:A:LYS:H	15	0.5
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	10	0.5
(1,1494)	1:102:A:ALA:H	1:105:A:LEU:H	12	0.5
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB1	17	0.5
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB2	17	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1475)	1:99:A:LYS:HA	1:102:A:ALA:HB3	17	0.5
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	6	0.5
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	6	0.5
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	14	0.5
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	14	0.5
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	20	0.5
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	7	0.5
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	7	0.5
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	17	0.5
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	17	0.5
(1,1313)	1:29:A:GLY:H	1:43:B:ALA:HA	19	0.5
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	12	0.5
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG21	2	0.5
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG22	2	0.5
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG23	2	0.5
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG21	2	0.5
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG22	2	0.5
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG23	2	0.5
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG21	2	0.5
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG22	2	0.5
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG23	2	0.5
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	9	0.5
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	7	0.5
(1,1145)	1:60:B:PHE:HA	1:62:B:GLY:H	11	0.5
(1,1142)	1:60:B:PHE:HA	1:61:B:LYS:H	8	0.5
(1,1011)	1:41:B:SER:HA	1:46:B:PHE:H	11	0.5
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	7	0.5
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	9	0.5
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	9	0.5
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	11	0.5
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	11	0.5
(1,452)	1:47:A:GLU:HB2	1:49:A:GLU:H	15	0.5
(1,452)	1:47:A:GLU:HB3	1:49:A:GLU:H	15	0.5
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	12	0.5
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	7	0.5
(1,4207)	1:344:B:ASN:H	1:345:B:LYS:H	1	0.49
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	3	0.49
(1,4156)	1:248:B:GLY:H	1:249:B:LEU:H	8	0.49
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	15	0.49
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	2	0.49
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	16	0.49
(1,3913)	1:210:B:ARG:HA	1:214:B:SER:H	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3800)	1:196:B:VAL:HG11	1:208:B:MET:HA	19	0.49
(1,3800)	1:196:B:VAL:HG12	1:208:B:MET:HA	19	0.49
(1,3800)	1:196:B:VAL:HG13	1:208:B:MET:HA	19	0.49
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	8	0.49
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	8	0.49
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	8	0.49
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	8	0.49
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	8	0.49
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	8	0.49
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG21	3	0.49
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG22	3	0.49
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG23	3	0.49
(1,3650)	1:180:B:LYS:HB2	1:188:B:GLU:HB2	9	0.49
(1,3650)	1:180:B:LYS:HB2	1:188:B:GLU:HB3	9	0.49
(1,3650)	1:180:B:LYS:HB3	1:188:B:GLU:HB2	9	0.49
(1,3650)	1:180:B:LYS:HB3	1:188:B:GLU:HB3	9	0.49
(1,3600)	1:176:B:LEU:HD11	1:180:B:LYS:H	13	0.49
(1,3600)	1:176:B:LEU:HD12	1:180:B:LYS:H	13	0.49
(1,3600)	1:176:B:LEU:HD13	1:180:B:LYS:H	13	0.49
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB2	10	0.49
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB3	10	0.49
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB2	10	0.49
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB3	10	0.49
(1,3474)	1:163:B:ILE:HD11	1:176:B:LEU:H	3	0.49
(1,3474)	1:163:B:ILE:HD12	1:176:B:LEU:H	3	0.49
(1,3474)	1:163:B:ILE:HD13	1:176:B:LEU:H	3	0.49
(1,3396)	1:156:B:VAL:HA	1:176:B:LEU:HA	11	0.49
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	5	0.49
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	9	0.49
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	3	0.49
(1,3241)	1:141:B:ASN:HA	1:145:B:ALA:H	12	0.49
(1,3229)	1:140:B:ALA:HA	1:143:B:ALA:H	17	0.49
(1,3195)	1:138:B:TYR:HA	1:141:B:ASN:H	8	0.49
(1,3148)	1:134:B:THR:H	1:135:B:ASN:HA	7	0.49
(1,3147)	1:134:B:THR:H	1:135:B:ASN:H	3	0.49
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	6	0.49
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	6	0.49
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	2	0.49
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	2	0.49
(1,2984)	1:117:B:ASP:HA	1:120:B:LEU:H	3	0.49
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	10	0.49
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	18	0.49
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	18	0.49
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	18	0.49
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	17	0.49
(1,2358)	1:181:A:TYR:HA	1:186:A:PRO:HA	14	0.49
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	3	0.49
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	7	0.49
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	7	0.49
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	11	0.49
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	11	0.49
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	13	0.49
(1,1767)	1:125:A:TYR:HB2	1:139:A:TYR:H	6	0.49
(1,1767)	1:125:A:TYR:HB3	1:139:A:TYR:H	6	0.49
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD1	15	0.49
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD2	15	0.49
(1,1666)	1:116:A:LYS:HA	1:118:A:TYR:H	2	0.49
(1,1534)	1:105:A:LEU:HA	1:107:A:MET:H	19	0.49
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE1	9	0.49
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE2	9	0.49
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE3	9	0.49
(1,1477)	1:100:A:ALA:H	1:102:A:ALA:H	15	0.49
(1,1444)	1:95:A:ASP:HA	1:97:A:GLU:H	5	0.49
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB2	19	0.49
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB3	19	0.49
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB2	19	0.49
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB3	19	0.49
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB2	19	0.49
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB3	19	0.49
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	5	0.49
(1,1394)	1:44:A:PHE:HE1	1:25:B:ILE:HD12	2	0.49
(1,1394)	1:44:A:PHE:HE2	1:25:B:ILE:HD12	2	0.49
(1,1385)	1:44:A:PHE:HA	1:25:B:ILE:HD13	2	0.49
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB2	3	0.49
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB3	3	0.49
(1,1358)	1:40:A:ILE:HA	1:33:B:LEU:HA	16	0.49
(1,1353)	1:39:A:CYS:HB2	1:36:B:ALA:H	17	0.49
(1,1353)	1:39:A:CYS:HB3	1:36:B:ALA:H	17	0.49
(1,1349)	1:39:A:CYS:HA	1:32:B:SER:HA	7	0.49
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	4	0.49
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	12	0.49
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	12	0.49
(1,298)	1:30:A:ALA:HA	1:33:A:LEU:H	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:20:A:VAL:HA	1:30:A:ALA:HA	15	0.49
(1,172)	1:16:A:PHE:HA	1:18:A:SER:HB2	1	0.49
(1,172)	1:16:A:PHE:HA	1:18:A:SER:HB3	1	0.49
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB2	10	0.49
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB3	10	0.49
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	17	0.49
(1,4156)	1:248:B:GLY:H	1:249:B:LEU:H	15	0.48
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	12	0.48
(1,4109)	1:344:A:ASN:H	1:345:A:LYS:H	10	0.48
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	6	0.48
(1,4064)	1:256:A:LEU:H	1:257:A:GLY:H	4	0.48
(1,4060)	1:252:A:LEU:H	1:253:A:GLY:H	13	0.48
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	5	0.48
(1,3864)	1:205:B:THR:HA	1:207:B:ALA:H	8	0.48
(1,3834)	1:200:B:GLU:HB2	1:204:B:ALA:H	18	0.48
(1,3834)	1:200:B:GLU:HB3	1:204:B:ALA:H	18	0.48
(1,3382)	1:154:B:GLN:HA	1:158:B:ASP:H	5	0.48
(1,3291)	1:146:B:HIS:H	1:155:B:ALA:HA	3	0.48
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB1	7	0.48
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB2	7	0.48
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB3	7	0.48
(1,2833)	1:104:B:ASP:HA	1:107:B:MET:H	11	0.48
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	15	0.48
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	3	0.48
(1,2580)	1:207:A:ALA:HA	1:210:A:ARG:H	11	0.48
(1,2419)	1:190:A:LEU:HD11	1:212:A:TYR:HA	8	0.48
(1,2419)	1:190:A:LEU:HD12	1:212:A:TYR:HA	8	0.48
(1,2419)	1:190:A:LEU:HD13	1:212:A:TYR:HA	8	0.48
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE1	8	0.48
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE2	8	0.48
(1,2294)	1:176:A:LEU:HD11	1:180:A:LYS:H	7	0.48
(1,2294)	1:176:A:LEU:HD12	1:180:A:LYS:H	7	0.48
(1,2294)	1:176:A:LEU:HD13	1:180:A:LYS:H	7	0.48
(1,2279)	1:174:A:SER:HA	1:193:A:TYR:HA	4	0.48
(1,2236)	1:170:A:PHE:HE2	1:171:A:ARG:HD3	14	0.48
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	2	0.48
(1,1855)	1:135:A:ASN:HB2	1:138:A:TYR:HE1	13	0.48
(1,1855)	1:135:A:ASN:HB2	1:138:A:TYR:HE2	13	0.48
(1,1855)	1:135:A:ASN:HB3	1:138:A:TYR:HE1	13	0.48
(1,1855)	1:135:A:ASN:HB3	1:138:A:TYR:HE2	13	0.48
(1,1829)	1:130:A:LYS:HA	1:132:A:LEU:H	20	0.48
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	2	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	18	0.48
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	18	0.48
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	6	0.48
(1,1522)	1:104:A:ASP:H	1:107:A:MET:H	5	0.48
(1,1507)	1:102:A:ALA:HB1	1:128:A:ALA:HA	9	0.48
(1,1507)	1:102:A:ALA:HB2	1:128:A:ALA:HA	9	0.48
(1,1507)	1:102:A:ALA:HB3	1:128:A:ALA:HA	9	0.48
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB2	13	0.48
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB3	13	0.48
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB2	13	0.48
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB3	13	0.48
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB2	13	0.48
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB3	13	0.48
(1,1337)	1:36:A:ALA:HA	1:36:B:ALA:H	16	0.48
(1,1288)	1:16:A:PHE:HE1	1:12:B:ILE:HD11	12	0.48
(1,1288)	1:16:A:PHE:HE2	1:12:B:ILE:HD11	12	0.48
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	1	0.48
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB2	9	0.48
(1,1272)	1:15:A:TYR:HH	1:2:B:SER:HB3	9	0.48
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG21	15	0.48
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG22	15	0.48
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG23	15	0.48
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG21	15	0.48
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG22	15	0.48
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG23	15	0.48
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG21	15	0.48
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG22	15	0.48
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG23	15	0.48
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	20	0.48
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	9	0.48
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD11	9	0.48
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD12	9	0.48
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD13	9	0.48
(1,1145)	1:60:B:PHE:HA	1:62:B:GLY:H	10	0.48
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	6	0.48
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	6	0.48
(1,726)	1:13:B:VAL:HA	1:17:B:SER:H	17	0.48
(1,703)	1:11:B:LEU:HA	1:71:B:SER:HA	16	0.48
(1,624)	1:4:B:SER:H	1:8:B:ILE:H	8	0.48
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	13	0.48
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	19	0.48
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	19	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	10	0.48
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	16	0.48
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB1	2	0.47
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB2	2	0.47
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB3	2	0.47
(1,4187)	1:322:B:ASN:H	1:323:B:MET:H	14	0.47
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	6	0.47
(1,4163)	1:257:B:GLY:H	1:258:B:GLY:H	11	0.47
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	4	0.47
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	1	0.47
(1,4105)	1:338:A:GLU:H	1:339:A:THR:H	16	0.47
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	9	0.47
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	8	0.47
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	1	0.47
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	6	0.47
(1,3970)	1:217:B:LYS:HA	1:220:B:GLU:H	14	0.47
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	18	0.47
(1,3749)	1:193:B:TYR:H	1:212:B:TYR:HA	17	0.47
(1,3749)	1:193:B:TYR:H	1:212:B:TYR:HA	19	0.47
(1,3738)	1:191:B:GLU:HA	1:195:B:LYS:H	10	0.47
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB1	19	0.47
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB2	19	0.47
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB3	19	0.47
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	17	0.47
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	17	0.47
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	17	0.47
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	17	0.47
(1,3533)	1:170:B:PHE:HD1	1:196:B:VAL:HA	13	0.47
(1,3533)	1:170:B:PHE:HD2	1:196:B:VAL:HA	13	0.47
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	6	0.47
(1,3433)	1:159:B:ALA:HB1	1:176:B:LEU:HA	16	0.47
(1,3433)	1:159:B:ALA:HB2	1:176:B:LEU:HA	16	0.47
(1,3433)	1:159:B:ALA:HB3	1:176:B:LEU:HA	16	0.47
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	3	0.47
(1,3119)	1:129:B:ILE:HA	1:133:B:PRO:HA	19	0.47
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB2	18	0.47
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB3	18	0.47
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB2	18	0.47
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB3	18	0.47
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	3	0.47
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	3	0.47
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE1	18	0.47
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE2	18	0.47
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE3	18	0.47
(1,2805)	1:102:B:ALA:HA	1:105:B:LEU:H	17	0.47
(1,2534)	1:201:A:GLY:H	1:204:A:ALA:H	2	0.47
(1,2432)	1:191:A:GLU:HA	1:195:A:LYS:H	13	0.47
(1,2383)	1:185:A:LYS:HA	1:188:A:GLU:H	18	0.47
(1,2265)	1:173:A:TYR:HB2	1:195:A:LYS:HG2	8	0.47
(1,2265)	1:173:A:TYR:HB2	1:195:A:LYS:HG3	8	0.47
(1,2265)	1:173:A:TYR:HB3	1:195:A:LYS:HG2	8	0.47
(1,2265)	1:173:A:TYR:HB3	1:195:A:LYS:HG3	8	0.47
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	12	0.47
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	12	0.47
(1,1880)	1:137:A:ILE:HA	1:140:A:ALA:H	13	0.47
(1,1865)	1:136:A:ALA:HA	1:166:A:ASP:H	4	0.47
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD11	3	0.47
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD12	3	0.47
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD13	3	0.47
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB2	2	0.47
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB3	2	0.47
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB2	2	0.47
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB3	2	0.47
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB2	2	0.47
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB3	2	0.47
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	12	0.47
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	12	0.47
(1,1566)	1:107:A:MET:HA	1:111:A:LYS:H	18	0.47
(1,1553)	1:106:A:LYS:HA	1:109:A:GLY:H	4	0.47
(1,1553)	1:106:A:LYS:HA	1:109:A:GLY:H	17	0.47
(1,1494)	1:102:A:ALA:H	1:105:A:LEU:H	8	0.47
(1,1483)	1:101:A:LYS:H	1:103:A:GLU:H	11	0.47
(1,1439)	1:94:A:ASP:HA	1:96:A:ALA:H	18	0.47
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	10	0.47
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	20	0.47
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	20	0.47
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	10	0.47
(1,1403)	1:62:A:GLY:H	1:67:B:ASP:HA	18	0.47
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	1	0.47
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	13	0.47
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	13	0.47
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	1	0.47
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	11	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	11	0.47
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	2	0.47
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	2	0.47
(1,1112)	1:55:B:LEU:HA	1:57:B:LYS:H	17	0.47
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	19	0.47
(1,886)	1:27:B:GLU:HA	1:31:B:ASP:H	20	0.47
(1,861)	1:24:B:GLU:H	1:25:B:ILE:H	3	0.47
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	19	0.47
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	13	0.47
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	13	0.47
(1,764)	1:15:B:TYR:HA	1:19:B:ILE:H	4	0.47
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	16	0.47
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	15	0.47
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	15	0.47
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	9	0.47
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	9	0.47
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	20	0.47
(1,117)	1:13:A:VAL:HA	1:17:A:SER:H	10	0.47
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	12	0.47
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	1	0.46
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	13	0.46
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	12	0.46
(1,4095)	1:328:A:PHE:H	1:329:A:GLY:H	10	0.46
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	1	0.46
(1,4050)	1:240:A:ALA:H	1:241:A:SER:H	1	0.46
(1,4019)	1:223:B:LEU:HA	1:225:B:LEU:H	17	0.46
(1,4003)	1:221:B:GLN:HA	1:224:B:ASN:H	13	0.46
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	16	0.46
(1,3951)	1:215:B:ALA:H	1:218:B:LYS:H	12	0.46
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	12	0.46
(1,3814)	1:197:B:LEU:HD21	1:204:B:ALA:HB1	2	0.46
(1,3814)	1:197:B:LEU:HD21	1:204:B:ALA:HB2	2	0.46
(1,3814)	1:197:B:LEU:HD21	1:204:B:ALA:HB3	2	0.46
(1,3814)	1:197:B:LEU:HD22	1:204:B:ALA:HB1	2	0.46
(1,3814)	1:197:B:LEU:HD22	1:204:B:ALA:HB2	2	0.46
(1,3814)	1:197:B:LEU:HD22	1:204:B:ALA:HB3	2	0.46
(1,3814)	1:197:B:LEU:HD23	1:204:B:ALA:HB1	2	0.46
(1,3814)	1:197:B:LEU:HD23	1:204:B:ALA:HB2	2	0.46
(1,3814)	1:197:B:LEU:HD23	1:204:B:ALA:HB3	2	0.46
(1,3811)	1:197:B:LEU:HA	1:204:B:ALA:HB1	10	0.46
(1,3811)	1:197:B:LEU:HA	1:204:B:ALA:HB2	10	0.46
(1,3811)	1:197:B:LEU:HA	1:204:B:ALA:HB3	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	11	0.46
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	11	0.46
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	11	0.46
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	11	0.46
(1,3763)	1:193:B:TYR:HD1	1:211:B:ASP:HA	8	0.46
(1,3763)	1:193:B:TYR:HD2	1:211:B:ASP:HA	8	0.46
(1,3753)	1:193:B:TYR:HA	1:196:B:VAL:H	17	0.46
(1,3662)	1:181:B:TYR:HA	1:184:B:GLY:H	10	0.46
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	5	0.46
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	5	0.46
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD2	2	0.46
(1,3538)	1:170:B:PHE:HE1	1:171:B:ARG:HD3	2	0.46
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD2	2	0.46
(1,3538)	1:170:B:PHE:HE2	1:171:B:ARG:HD3	2	0.46
(1,3528)	1:170:B:PHE:HB2	1:196:B:VAL:HG11	1	0.46
(1,3528)	1:170:B:PHE:HB2	1:196:B:VAL:HG12	1	0.46
(1,3528)	1:170:B:PHE:HB2	1:196:B:VAL:HG13	1	0.46
(1,3528)	1:170:B:PHE:HB3	1:196:B:VAL:HG11	1	0.46
(1,3528)	1:170:B:PHE:HB3	1:196:B:VAL:HG12	1	0.46
(1,3528)	1:170:B:PHE:HB3	1:196:B:VAL:HG13	1	0.46
(1,3511)	1:169:B:TYR:HD2	1:171:B:ARG:H	10	0.46
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	10	0.46
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	10	0.46
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	1	0.46
(1,3357)	1:152:B:TYR:HA	1:156:B:VAL:H	12	0.46
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB2	6	0.46
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB3	6	0.46
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB2	6	0.46
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB3	6	0.46
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	6	0.46
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	6	0.46
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	12	0.46
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	12	0.46
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	12	0.46
(1,2938)	1:113:B:MET:HA	1:116:B:LYS:H	1	0.46
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	1	0.46
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	1	0.46
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	6	0.46
(1,2756)	1:96:B:ALA:H	1:98:B:THR:H	20	0.46
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	19	0.46
(1,2669)	1:218:A:LYS:H	1:221:A:GLN:H	18	0.46
(1,2615)	1:211:A:ASP:HA	1:215:A:ALA:H	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	20	0.46
(1,2573)	1:206:A:GLU:HB2	1:207:A:ALA:H	5	0.46
(1,2573)	1:206:A:GLU:HB3	1:207:A:ALA:H	5	0.46
(1,2451)	1:193:A:TYR:HA	1:212:A:TYR:HA	12	0.46
(1,2320)	1:178:A:PHE:HA	1:182:A:ALA:H	11	0.46
(1,2300)	1:177:A:GLY:H	1:189:A:ALA:HA	1	0.46
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD11	6	0.46
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD12	6	0.46
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD13	6	0.46
(1,1882)	1:137:A:ILE:HA	1:141:A:ASN:H	10	0.46
(1,1882)	1:137:A:ILE:HA	1:141:A:ASN:H	13	0.46
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE1	15	0.46
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE2	15	0.46
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE1	15	0.46
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE2	15	0.46
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	19	0.46
(1,1548)	1:106:A:LYS:H	1:128:A:ALA:HA	4	0.46
(1,1498)	1:102:A:ALA:HA	1:104:A:ASP:H	5	0.46
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	2	0.46
(1,1412)	1:67:A:ASP:HB2	1:60:B:PHE:HB2	2	0.46
(1,1412)	1:67:A:ASP:HB2	1:60:B:PHE:HB3	2	0.46
(1,1412)	1:67:A:ASP:HB3	1:60:B:PHE:HB2	2	0.46
(1,1412)	1:67:A:ASP:HB3	1:60:B:PHE:HB3	2	0.46
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	7	0.46
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB2	17	0.46
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB3	17	0.46
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB2	17	0.46
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB3	17	0.46
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB2	17	0.46
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB3	17	0.46
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	5	0.46
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	5	0.46
(1,1278)	1:16:A:PHE:HA	1:44:B:PHE:HZ	13	0.46
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	20	0.46
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	1	0.46
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	1	0.46
(1,1201)	1:68:B:ILE:HA	1:70:B:ASN:H	11	0.46
(1,1163)	1:62:B:GLY:H	1:63:B:GLN:H	4	0.46
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	5	0.46
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	5	0.46
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	3	0.46
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	3	0.46
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	3	0.46
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	1	0.46
(1,892)	1:28:B:ASP:HA	1:31:B:ASP:H	13	0.46
(1,642)	1:6:B:GLU:HA	1:10:B:ALA:H	1	0.46
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	8	0.46
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	7	0.46
(1,173)	1:16:A:PHE:HA	1:19:A:ILE:H	18	0.46
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	14	0.45
(1,4107)	1:342:A:ASN:H	1:343:A:GLU:H	17	0.45
(1,4095)	1:328:A:PHE:H	1:329:A:GLY:H	13	0.45
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	8	0.45
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	13	0.45
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	13	0.45
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	13	0.45
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	10	0.45
(1,3992)	1:220:B:GLU:H	1:222:B:SER:H	12	0.45
(1,3989)	1:219:B:VAL:HG11	1:223:B:LEU:HD11	9	0.45
(1,3989)	1:219:B:VAL:HG11	1:223:B:LEU:HD12	9	0.45
(1,3989)	1:219:B:VAL:HG11	1:223:B:LEU:HD13	9	0.45
(1,3989)	1:219:B:VAL:HG12	1:223:B:LEU:HD11	9	0.45
(1,3989)	1:219:B:VAL:HG12	1:223:B:LEU:HD12	9	0.45
(1,3989)	1:219:B:VAL:HG12	1:223:B:LEU:HD13	9	0.45
(1,3989)	1:219:B:VAL:HG13	1:223:B:LEU:HD11	9	0.45
(1,3989)	1:219:B:VAL:HG13	1:223:B:LEU:HD12	9	0.45
(1,3989)	1:219:B:VAL:HG13	1:223:B:LEU:HD13	9	0.45
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	18	0.45
(1,3858)	1:205:B:THR:H	1:208:B:MET:H	16	0.45
(1,3766)	1:193:B:TYR:HD1	1:212:B:TYR:HA	4	0.45
(1,3766)	1:193:B:TYR:HD2	1:212:B:TYR:HA	4	0.45
(1,3704)	1:188:B:GLU:HA	1:191:B:GLU:H	17	0.45
(1,3688)	1:185:B:LYS:HA	1:187:B:GLU:H	1	0.45
(1,3641)	1:180:B:LYS:H	1:189:B:ALA:HA	14	0.45
(1,3497)	1:169:B:TYR:HA	1:170:B:PHE:HA	19	0.45
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	2	0.45
(1,3442)	1:160:B:GLU:HA	1:163:B:ILE:H	3	0.45
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG2	6	0.45
(1,3237)	1:141:B:ASN:H	1:144:B:ALA:H	13	0.45
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB2	15	0.45
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB3	15	0.45
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB2	15	0.45
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB3	15	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2978)	1:116:B:LYS:HB2	1:118:B:TYR:HE1	7	0.45
(1,2978)	1:116:B:LYS:HB2	1:118:B:TYR:HE2	7	0.45
(1,2978)	1:116:B:LYS:HB3	1:118:B:TYR:HE1	7	0.45
(1,2978)	1:116:B:LYS:HB3	1:118:B:TYR:HE2	7	0.45
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	14	0.45
(1,2305)	1:177:A:GLY:HA2	1:189:A:ALA:HA	8	0.45
(1,2305)	1:177:A:GLY:HA3	1:189:A:ALA:HA	8	0.45
(1,2305)	1:177:A:GLY:HA2	1:189:A:ALA:HA	16	0.45
(1,2305)	1:177:A:GLY:HA3	1:189:A:ALA:HA	16	0.45
(1,2300)	1:177:A:GLY:H	1:189:A:ALA:HA	16	0.45
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	14	0.45
(1,2105)	1:157:A:LYS:HA	1:160:A:GLU:H	3	0.45
(1,2007)	1:147:A:SER:HA	1:152:A:TYR:HA	11	0.45
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	11	0.45
(1,1785)	1:126:A:THR:HA	1:130:A:LYS:H	3	0.45
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD2	9	0.45
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD3	9	0.45
(1,1338)	1:36:A:ALA:HA	1:36:B:ALA:HA	17	0.45
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	16	0.45
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	16	0.45
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	16	0.45
(1,1288)	1:16:A:PHE:HE1	1:12:B:ILE:HD11	7	0.45
(1,1288)	1:16:A:PHE:HE2	1:12:B:ILE:HD11	7	0.45
(1,1287)	1:16:A:PHE:HE1	1:12:B:ILE:HD11	20	0.45
(1,1287)	1:16:A:PHE:HE1	1:12:B:ILE:HD12	20	0.45
(1,1287)	1:16:A:PHE:HE1	1:12:B:ILE:HD13	20	0.45
(1,1287)	1:16:A:PHE:HE2	1:12:B:ILE:HD11	20	0.45
(1,1287)	1:16:A:PHE:HE2	1:12:B:ILE:HD12	20	0.45
(1,1287)	1:16:A:PHE:HE2	1:12:B:ILE:HD13	20	0.45
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	7	0.45
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	7	0.45
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	18	0.45
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	18	0.45
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	15	0.45
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	15	0.45
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	15	0.45
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	15	0.45
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD11	3	0.45
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD12	3	0.45
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD13	3	0.45
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD11	3	0.45
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD12	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD13	3	0.45
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	12	0.45
(1,1166)	1:63:B:GLN:H	1:64:B:HIS:H	14	0.45
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	13	0.45
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	13	0.45
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	14	0.45
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	14	0.45
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	17	0.45
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	5	0.45
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	5	0.45
(1,885)	1:27:B:GLU:HA	1:30:B:ALA:HA	12	0.45
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG11	11	0.45
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG12	11	0.45
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG13	11	0.45
(1,729)	1:13:B:VAL:HA	1:40:B:ILE:HD11	8	0.45
(1,729)	1:13:B:VAL:HA	1:40:B:ILE:HD12	8	0.45
(1,729)	1:13:B:VAL:HA	1:40:B:ILE:HD13	8	0.45
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD11	9	0.45
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD12	9	0.45
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD13	9	0.45
(1,529)	1:59:A:GLU:HA	1:64:A:HIS:HA	19	0.45
(1,344)	1:35:A:VAL:HA	1:38:A:ASP:HA	8	0.45
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	9	0.44
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	16	0.44
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	3	0.44
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	4	0.44
(1,4169)	1:300:B:GLU:H	1:301:B:GLY:H	17	0.44
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	14	0.44
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	16	0.44
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	1	0.44
(1,4064)	1:256:A:LEU:H	1:257:A:GLY:H	2	0.44
(1,4003)	1:221:B:GLN:HA	1:224:B:ASN:H	5	0.44
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD11	14	0.44
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD12	14	0.44
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD13	14	0.44
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	14	0.44
(1,3939)	1:213:B:GLU:HA	1:217:B:LYS:H	6	0.44
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	5	0.44
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	5	0.44
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	5	0.44
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	5	0.44
(1,3597)	1:176:B:LEU:HA	1:178:B:PHE:H	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3575)	1:173:B:TYR:HE2	1:199:B:ILE:HD13	19	0.44
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB2	20	0.44
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB3	20	0.44
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB2	20	0.44
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB3	20	0.44
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	3	0.44
(1,3521)	1:170:B:PHE:HA	1:174:B:SER:H	19	0.44
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	2	0.44
(1,3279)	1:144:B:ALA:HB1	1:175:B:ARG:HE	18	0.44
(1,3279)	1:144:B:ALA:HB2	1:175:B:ARG:HE	18	0.44
(1,3279)	1:144:B:ALA:HB3	1:175:B:ARG:HE	18	0.44
(1,3119)	1:129:B:ILE:HA	1:133:B:PRO:HA	2	0.44
(1,3081)	1:125:B:TYR:HE1	1:142:B:ARG:HA	15	0.44
(1,3081)	1:125:B:TYR:HE2	1:142:B:ARG:HA	15	0.44
(1,2947)	1:113:B:MET:HE1	1:141:B:ASN:HA	18	0.44
(1,2947)	1:113:B:MET:HE2	1:141:B:ASN:HA	18	0.44
(1,2947)	1:113:B:MET:HE3	1:141:B:ASN:HA	18	0.44
(1,2939)	1:113:B:MET:HA	1:116:B:LYS:HA	7	0.44
(1,2886)	1:109:B:GLY:H	1:125:B:TYR:HE1	13	0.44
(1,2828)	1:104:B:ASP:H	1:107:B:MET:H	4	0.44
(1,2828)	1:104:B:ASP:H	1:107:B:MET:H	15	0.44
(1,2796)	1:101:B:LYS:HA	1:104:B:ASP:H	17	0.44
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	11	0.44
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	13	0.44
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	13	0.44
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	10	0.44
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	10	0.44
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	10	0.44
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	6	0.44
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	20	0.44
(1,2534)	1:201:A:GLY:H	1:204:A:ALA:H	14	0.44
(1,2503)	1:197:A:LEU:HA	1:201:A:GLY:H	2	0.44
(1,2163)	1:163:A:ILE:HA	1:167:A:PRO:HA	13	0.44
(1,2113)	1:158:A:ASP:HA	1:161:A:SER:H	10	0.44
(1,2003)	1:147:A:SER:HA	1:150:A:LYS:H	1	0.44
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	16	0.44
(1,1768)	1:125:A:TYR:HB2	1:142:A:ARG:H	3	0.44
(1,1768)	1:125:A:TYR:HB3	1:142:A:ARG:H	3	0.44
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	10	0.44
(1,1535)	1:105:A:LEU:HA	1:108:A:GLN:H	1	0.44
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	15	0.44
(1,1439)	1:94:A:ASP:HA	1:96:A:ALA:H	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	18	0.44
(1,1403)	1:62:A:GLY:H	1:67:B:ASP:HA	5	0.44
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	20	0.44
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	20	0.44
(1,1289)	1:16:A:PHE:HE1	1:12:B:ILE:HD12	18	0.44
(1,1289)	1:16:A:PHE:HE2	1:12:B:ILE:HD12	18	0.44
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	12	0.44
(1,1243)	1:8:A:ILE:HG12	1:15:B:TYR:HD1	2	0.44
(1,1243)	1:8:A:ILE:HG13	1:15:B:TYR:HD1	2	0.44
(1,1229)	1:2:A:SER:HB2	1:69:B:LEU:H	18	0.44
(1,1229)	1:2:A:SER:HB3	1:69:B:LEU:H	18	0.44
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	1	0.44
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	3	0.44
(1,1127)	1:58:B:SER:H	1:59:B:GLU:HA	8	0.44
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	19	0.44
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	19	0.44
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	14	0.44
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	14	0.44
(1,877)	1:26:B:SER:HA	1:29:B:GLY:H	11	0.44
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	9	0.44
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	9	0.44
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG11	8	0.44
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG12	8	0.44
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG13	8	0.44
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD21	18	0.44
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD22	18	0.44
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD23	18	0.44
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	7	0.44
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD11	1	0.44
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD12	1	0.44
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD13	1	0.44
(1,561)	1:63:A:GLN:HA	1:67:A:ASP:H	18	0.44
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	15	0.44
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	15	0.44
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	6	0.44
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	6	0.44
(1,211)	1:18:A:SER:HA	1:22:A:LYS:H	10	0.44
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	15	0.44
(1,4206)	1:343:B:GLU:H	1:344:B:ASN:H	8	0.43
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	12	0.43
(1,4190)	1:325:B:GLY:H	1:326:B:ASN:H	4	0.43
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4162)	1:256:B:LEU:H	1:257:B:GLY:H	20	0.43
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	12	0.43
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	16	0.43
(1,4105)	1:338:A:GLU:H	1:339:A:THR:H	20	0.43
(1,4072)	1:301:A:GLY:H	1:302:A:PHE:H	14	0.43
(1,4052)	1:242:A:GLN:H	1:243:A:GLY:H	9	0.43
(1,3981)	1:218:B:LYS:HB2	1:219:B:VAL:H	11	0.43
(1,3981)	1:218:B:LYS:HB3	1:219:B:VAL:H	11	0.43
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	2	0.43
(1,3945)	1:214:B:SER:HA	1:216:B:LYS:H	4	0.43
(1,3927)	1:212:B:TYR:HA	1:215:B:ALA:HB1	5	0.43
(1,3927)	1:212:B:TYR:HA	1:215:B:ALA:HB2	5	0.43
(1,3927)	1:212:B:TYR:HA	1:215:B:ALA:HB3	5	0.43
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	7	0.43
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	11	0.43
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	11	0.43
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	15	0.43
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	15	0.43
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB2	15	0.43
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	15	0.43
(1,3511)	1:169:B:TYR:HD2	1:171:B:ARG:H	9	0.43
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	2	0.43
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	2	0.43
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	12	0.43
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	12	0.43
(1,3469)	1:163:B:ILE:HA	1:167:B:PRO:HA	4	0.43
(1,3339)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	18	0.43
(1,3279)	1:144:B:ALA:HB1	1:175:B:ARG:HE	13	0.43
(1,3279)	1:144:B:ALA:HB2	1:175:B:ARG:HE	13	0.43
(1,3279)	1:144:B:ALA:HB3	1:175:B:ARG:HE	13	0.43
(1,3225)	1:140:B:ALA:H	1:162:B:ALA:HA	7	0.43
(1,3148)	1:134:B:THR:H	1:135:B:ASN:HA	1	0.43
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB2	18	0.43
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB3	18	0.43
(1,3054)	1:124:B:LYS:H	1:127:B:GLU:H	18	0.43
(1,2977)	1:116:B:LYS:HB2	1:118:B:TYR:HD1	1	0.43
(1,2977)	1:116:B:LYS:HB2	1:118:B:TYR:HD2	1	0.43
(1,2977)	1:116:B:LYS:HB3	1:118:B:TYR:HD1	1	0.43
(1,2977)	1:116:B:LYS:HB3	1:118:B:TYR:HD2	1	0.43
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	2	0.43
(1,2842)	1:105:B:LEU:HA	1:109:B:GLY:H	15	0.43
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	20	0.43
(1,2522)	1:199:A:ILE:HA	1:201:A:GLY:H	5	0.43
(1,2457)	1:193:A:TYR:HD1	1:211:A:ASP:HA	13	0.43
(1,2457)	1:193:A:TYR:HD2	1:211:A:ASP:HA	13	0.43
(1,2390)	1:187:A:GLU:HA	1:190:A:LEU:H	16	0.43
(1,2350)	1:181:A:TYR:H	1:189:A:ALA:H	2	0.43
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	19	0.43
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	19	0.43
(1,2216)	1:170:A:PHE:HA	1:196:A:VAL:HA	4	0.43
(1,2203)	1:169:A:TYR:HE1	1:172:A:GLY:H	17	0.43
(1,2203)	1:169:A:TYR:HE2	1:172:A:GLY:H	17	0.43
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE1	6	0.43
(1,2037)	1:150:A:LYS:HZ1	1:152:A:TYR:HE2	6	0.43
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE1	6	0.43
(1,2037)	1:150:A:LYS:HZ2	1:152:A:TYR:HE2	6	0.43
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE1	6	0.43
(1,2037)	1:150:A:LYS:HZ3	1:152:A:TYR:HE2	6	0.43
(1,1985)	1:146:A:HIS:H	1:155:A:ALA:HA	11	0.43
(1,1853)	1:135:A:ASN:HB2	1:138:A:TYR:H	14	0.43
(1,1853)	1:135:A:ASN:HB3	1:138:A:TYR:H	14	0.43
(1,1802)	1:128:A:ALA:HA	1:132:A:LEU:H	3	0.43
(1,1763)	1:125:A:TYR:HA	1:138:A:TYR:HB2	14	0.43
(1,1763)	1:125:A:TYR:HA	1:138:A:TYR:HB3	14	0.43
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	14	0.43
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	14	0.43
(1,1636)	1:113:A:MET:HA	1:121:A:ALA:H	18	0.43
(1,1634)	1:113:A:MET:HA	1:117:A:ASP:H	18	0.43
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	17	0.43
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	17	0.43
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	17	0.43
(1,1401)	1:44:A:PHE:HE1	1:33:B:LEU:HD22	6	0.43
(1,1401)	1:44:A:PHE:HE2	1:33:B:LEU:HD22	6	0.43
(1,1392)	1:44:A:PHE:HE1	1:25:B:ILE:HD11	2	0.43
(1,1392)	1:44:A:PHE:HE1	1:25:B:ILE:HD12	2	0.43
(1,1392)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	2	0.43
(1,1392)	1:44:A:PHE:HE2	1:25:B:ILE:HD11	2	0.43
(1,1392)	1:44:A:PHE:HE2	1:25:B:ILE:HD12	2	0.43
(1,1392)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	2	0.43
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	10	0.43
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG21	3	0.43
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG22	3	0.43
(1,1352)	1:39:A:CYS:HB2	1:35:B:VAL:HG23	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG21	3	0.43
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG22	3	0.43
(1,1352)	1:39:A:CYS:HB3	1:35:B:VAL:HG23	3	0.43
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	16	0.43
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	16	0.43
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	2	0.43
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	2	0.43
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	2	0.43
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	2	0.43
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	5	0.43
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	5	0.43
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	5	0.43
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	5	0.43
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	5	0.43
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	1	0.43
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	15	0.43
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	12	0.43
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	5	0.43
(1,772)	1:15:B:TYR:HD1	1:18:B:SER:HB2	7	0.43
(1,772)	1:15:B:TYR:HD1	1:18:B:SER:HB3	7	0.43
(1,772)	1:15:B:TYR:HD2	1:18:B:SER:HB2	7	0.43
(1,772)	1:15:B:TYR:HD2	1:18:B:SER:HB3	7	0.43
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	6	0.43
(1,626)	1:4:B:SER:HA	1:5:B:LYS:HA	8	0.43
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	7	0.43
(1,282)	1:28:A:ASP:HA	1:30:A:ALA:H	5	0.43
(1,171)	1:16:A:PHE:HA	1:18:A:SER:H	18	0.43
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB2	10	0.43
(1,144)	1:14:A:ASN:HA	1:48:A:ARG:HB3	10	0.43
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	3	0.43
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	9	0.43
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	11	0.43
(1,4209)	1:346:B:GLN:H	1:347:B:TYR:H	5	0.42
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	7	0.42
(1,4188)	1:323:B:MET:H	1:324:B:ALA:H	2	0.42
(1,4188)	1:323:B:MET:H	1:324:B:ALA:H	10	0.42
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	13	0.42
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	20	0.42
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	20	0.42
(1,4138)	1:228:B:THR:H	1:229:B:VAL:H	8	0.42
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	15	0.42
(1,4095)	1:328:A:PHE:H	1:329:A:GLY:H	19	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	15	0.42
(1,4065)	1:257:A:GLY:H	1:258:A:GLY:H	3	0.42
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	20	0.42
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	20	0.42
(1,3951)	1:215:B:ALA:H	1:218:B:LYS:H	19	0.42
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	18	0.42
(1,3879)	1:206:B:GLU:HB2	1:207:B:ALA:H	3	0.42
(1,3879)	1:206:B:GLU:HB3	1:207:B:ALA:H	3	0.42
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE1	2	0.42
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE2	2	0.42
(1,3860)	1:205:B:THR:H	1:208:B:MET:HE3	2	0.42
(1,3808)	1:197:B:LEU:HA	1:200:B:GLU:H	14	0.42
(1,3725)	1:190:B:LEU:HD11	1:212:B:TYR:HA	12	0.42
(1,3725)	1:190:B:LEU:HD12	1:212:B:TYR:HA	12	0.42
(1,3725)	1:190:B:LEU:HD13	1:212:B:TYR:HA	12	0.42
(1,3606)	1:177:B:GLY:H	1:189:B:ALA:HA	8	0.42
(1,3355)	1:152:B:TYR:HA	1:155:B:ALA:HA	4	0.42
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB2	5	0.42
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB3	5	0.42
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB2	5	0.42
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB3	5	0.42
(1,3312)	1:147:B:SER:HA	1:152:B:TYR:H	15	0.42
(1,3225)	1:140:B:ALA:H	1:162:B:ALA:HA	6	0.42
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB2	13	0.42
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB3	13	0.42
(1,2973)	1:116:B:LYS:HA	1:118:B:TYR:HA	10	0.42
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	5	0.42
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	5	0.42
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	5	0.42
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	15	0.42
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	12	0.42
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	15	0.42
(1,2796)	1:101:B:LYS:HA	1:104:B:ASP:H	18	0.42
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	12	0.42
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	17	0.42
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	14	0.42
(1,2697)	1:221:A:GLN:HA	1:224:A:ASN:H	18	0.42
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	7	0.42
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	13	0.42
(1,2588)	1:208:A:MET:H	1:211:A:ASP:H	12	0.42
(1,2552)	1:205:A:THR:H	1:208:A:MET:H	14	0.42
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	11	0.42
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	11	0.42
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	11	0.42
(1,2416)	1:190:A:LEU:HA	1:212:A:TYR:HA	18	0.42
(1,2383)	1:185:A:LYS:HA	1:188:A:GLU:H	12	0.42
(1,2350)	1:181:A:TYR:H	1:189:A:ALA:H	1	0.42
(1,2335)	1:180:A:LYS:H	1:189:A:ALA:HA	2	0.42
(1,2304)	1:177:A:GLY:HA2	1:189:A:ALA:H	16	0.42
(1,2304)	1:177:A:GLY:HA3	1:189:A:ALA:H	16	0.42
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	3	0.42
(1,2248)	1:172:A:GLY:H	1:175:A:ARG:H	1	0.42
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	18	0.42
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	19	0.42
(1,2004)	1:147:A:SER:HA	1:150:A:LYS:HA	3	0.42
(1,1773)	1:125:A:TYR:HB2	1:142:A:ARG:HD2	12	0.42
(1,1773)	1:125:A:TYR:HB2	1:142:A:ARG:HD3	12	0.42
(1,1773)	1:125:A:TYR:HB3	1:142:A:ARG:HD2	12	0.42
(1,1773)	1:125:A:TYR:HB3	1:142:A:ARG:HD3	12	0.42
(1,1678)	1:117:A:ASP:HA	1:120:A:LEU:H	10	0.42
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE1	8	0.42
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE2	8	0.42
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE1	8	0.42
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE2	8	0.42
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	6	0.42
(1,1463)	1:98:A:THR:H	1:101:A:LYS:H	18	0.42
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	12	0.42
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	9	0.42
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	9	0.42
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	5	0.42
(1,1337)	1:36:A:ALA:HA	1:36:B:ALA:H	12	0.42
(1,1336)	1:36:A:ALA:H	1:36:B:ALA:HA	12	0.42
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	15	0.42
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	15	0.42
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	18	0.42
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	18	0.42
(1,1281)	1:16:A:PHE:HE1	1:9:B:ALA:HB1	20	0.42
(1,1281)	1:16:A:PHE:HE2	1:9:B:ALA:HB1	20	0.42
(1,1278)	1:16:A:PHE:HA	1:44:B:PHE:HZ	8	0.42
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	7	0.42
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	7	0.42
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	6	0.42
(1,1248)	1:9:A:ALA:H	1:16:B:PHE:HZ	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	15	0.42
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	15	0.42
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	14	0.42
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	16	0.42
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	16	0.42
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE1	8	0.42
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE2	8	0.42
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE3	8	0.42
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	11	0.42
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	11	0.42
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	11	0.42
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	11	0.42
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG11	8	0.42
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG12	8	0.42
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG13	8	0.42
(1,344)	1:35:A:VAL:HA	1:38:A:ASP:HA	15	0.42
(1,70)	1:10:A:ALA:H	1:54:A:ILE:HD11	14	0.42
(1,70)	1:10:A:ALA:H	1:54:A:ILE:HD12	14	0.42
(1,70)	1:10:A:ALA:H	1:54:A:ILE:HD13	14	0.42
(1,4185)	1:320:B:LEU:H	1:321:B:ARG:H	14	0.41
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	18	0.41
(1,4144)	1:236:B:ALA:H	1:237:B:ASP:H	18	0.41
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	3	0.41
(1,4065)	1:257:A:GLY:H	1:258:A:GLY:H	12	0.41
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	15	0.41
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	15	0.41
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	15	0.41
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	12	0.41
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	8	0.41
(1,3913)	1:210:B:ARG:HA	1:214:B:SER:H	20	0.41
(1,3834)	1:200:B:GLU:HB2	1:204:B:ALA:H	8	0.41
(1,3834)	1:200:B:GLU:HB3	1:204:B:ALA:H	8	0.41
(1,3802)	1:196:B:VAL:HG11	1:208:B:MET:HE1	11	0.41
(1,3802)	1:196:B:VAL:HG11	1:208:B:MET:HE2	11	0.41
(1,3802)	1:196:B:VAL:HG11	1:208:B:MET:HE3	11	0.41
(1,3802)	1:196:B:VAL:HG12	1:208:B:MET:HE1	11	0.41
(1,3802)	1:196:B:VAL:HG12	1:208:B:MET:HE2	11	0.41
(1,3802)	1:196:B:VAL:HG12	1:208:B:MET:HE3	11	0.41
(1,3802)	1:196:B:VAL:HG13	1:208:B:MET:HE1	11	0.41
(1,3802)	1:196:B:VAL:HG13	1:208:B:MET:HE2	11	0.41
(1,3802)	1:196:B:VAL:HG13	1:208:B:MET:HE3	11	0.41
(1,3657)	1:181:B:TYR:H	1:189:B:ALA:HA	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3551)	1:171:B:ARG:HA	1:175:B:ARG:H	19	0.41
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG21	20	0.41
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG22	20	0.41
(1,3529)	1:170:B:PHE:HB2	1:199:B:ILE:HG23	20	0.41
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG21	20	0.41
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG22	20	0.41
(1,3529)	1:170:B:PHE:HB3	1:199:B:ILE:HG23	20	0.41
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	8	0.41
(1,3313)	1:147:B:SER:HA	1:152:B:TYR:HA	3	0.41
(1,3313)	1:147:B:SER:HA	1:152:B:TYR:HA	7	0.41
(1,3171)	1:136:B:ALA:HA	1:166:B:ASP:H	4	0.41
(1,3168)	1:136:B:ALA:HA	1:162:B:ALA:HA	4	0.41
(1,3108)	1:128:B:ALA:HA	1:132:B:LEU:H	8	0.41
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	3	0.41
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	3	0.41
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE1	15	0.41
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE2	15	0.41
(1,2942)	1:113:B:MET:HA	1:121:B:ALA:H	20	0.41
(1,2940)	1:113:B:MET:HA	1:117:B:ASP:H	16	0.41
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD21	7	0.41
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD22	7	0.41
(1,2920)	1:112:B:ALA:HA	1:120:B:LEU:HD23	7	0.41
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	14	0.41
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	8	0.41
(1,2675)	1:218:A:LYS:HB2	1:219:A:VAL:H	7	0.41
(1,2675)	1:218:A:LYS:HB3	1:219:A:VAL:H	7	0.41
(1,2669)	1:218:A:LYS:H	1:221:A:GLN:H	11	0.41
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD21	8	0.41
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD22	8	0.41
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD23	8	0.41
(1,2287)	1:175:A:ARG:HA	1:178:A:PHE:H	16	0.41
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG21	8	0.41
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG22	8	0.41
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG23	8	0.41
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG21	8	0.41
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG22	8	0.41
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG23	8	0.41
(1,1991)	1:146:A:HIS:HA	1:151:A:GLU:H	1	0.41
(1,1962)	1:143:A:ALA:HB1	1:175:A:ARG:HB2	3	0.41
(1,1962)	1:143:A:ALA:HB1	1:175:A:ARG:HB3	3	0.41
(1,1962)	1:143:A:ALA:HB2	1:175:A:ARG:HB2	3	0.41
(1,1962)	1:143:A:ALA:HB2	1:175:A:ARG:HB3	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1962)	1:143:A:ALA:HB3	1:175:A:ARG:HB2	3	0.41
(1,1962)	1:143:A:ALA:HB3	1:175:A:ARG:HB3	3	0.41
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD1	16	0.41
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD2	16	0.41
(1,1638)	1:113:A:MET:HB2	1:125:A:TYR:HE1	8	0.41
(1,1638)	1:113:A:MET:HB2	1:125:A:TYR:HE2	8	0.41
(1,1638)	1:113:A:MET:HB3	1:125:A:TYR:HE1	8	0.41
(1,1638)	1:113:A:MET:HB3	1:125:A:TYR:HE2	8	0.41
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB1	1	0.41
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB2	1	0.41
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB3	1	0.41
(1,1522)	1:104:A:ASP:H	1:107:A:MET:H	19	0.41
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	19	0.41
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	19	0.41
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	19	0.41
(1,1439)	1:94:A:ASP:HA	1:96:A:ALA:H	13	0.41
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	2	0.41
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	2	0.41
(1,1394)	1:44:A:PHE:HE1	1:25:B:ILE:HD12	1	0.41
(1,1394)	1:44:A:PHE:HE2	1:25:B:ILE:HD12	1	0.41
(1,1358)	1:40:A:ILE:HA	1:33:B:LEU:HA	3	0.41
(1,1350)	1:39:A:CYS:HB2	1:32:B:SER:HA	8	0.41
(1,1350)	1:39:A:CYS:HB3	1:32:B:SER:HA	8	0.41
(1,1349)	1:39:A:CYS:HA	1:32:B:SER:HA	17	0.41
(1,1314)	1:29:A:GLY:HA2	1:43:B:ALA:H	15	0.41
(1,1314)	1:29:A:GLY:HA3	1:43:B:ALA:H	15	0.41
(1,1307)	1:25:A:ILE:HG12	1:44:B:PHE:HA	18	0.41
(1,1307)	1:25:A:ILE:HG13	1:44:B:PHE:HA	18	0.41
(1,1267)	1:15:A:TYR:HE1	1:5:B:LYS:HA	6	0.41
(1,1267)	1:15:A:TYR:HE2	1:5:B:LYS:HA	6	0.41
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	12	0.41
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	12	0.41
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	12	0.41
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	12	0.41
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	4	0.41
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	4	0.41
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	4	0.41
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	4	0.41
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	1	0.41
(1,1201)	1:68:B:ILE:HA	1:70:B:ASN:H	17	0.41
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	7	0.41
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1127)	1:58:B:SER:H	1:59:B:GLU:HA	18	0.41
(1,561)	1:63:A:GLN:HA	1:67:A:ASP:H	9	0.41
(1,506)	1:55:A:LEU:HD11	1:72:A:ALA:HA	1	0.41
(1,506)	1:55:A:LEU:HD12	1:72:A:ALA:HA	1	0.41
(1,506)	1:55:A:LEU:HD13	1:72:A:ALA:HA	1	0.41
(1,174)	1:16:A:PHE:HA	1:19:A:ILE:HA	18	0.41
(1,4169)	1:300:B:GLU:H	1:301:B:GLY:H	8	0.4
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	16	0.4
(1,4064)	1:256:A:LEU:H	1:257:A:GLY:H	15	0.4
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	17	0.4
(1,3951)	1:215:B:ALA:H	1:218:B:LYS:H	7	0.4
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	2	0.4
(1,3769)	1:193:B:TYR:HE2	1:211:B:ASP:HA	11	0.4
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	20	0.4
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	20	0.4
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	4	0.4
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	4	0.4
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	17	0.4
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	17	0.4
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	3	0.4
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	3	0.4
(1,3194)	1:138:B:TYR:HA	1:140:B:ALA:H	13	0.4
(1,3102)	1:128:B:ALA:H	1:131:B:VAL:H	20	0.4
(1,3091)	1:126:B:THR:HA	1:130:B:LYS:H	5	0.4
(1,2994)	1:118:B:TYR:HA	1:122:B:ILE:H	7	0.4
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE1	6	0.4
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE1	19	0.4
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE2	19	0.4
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG21	17	0.4
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG22	17	0.4
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG23	17	0.4
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG21	17	0.4
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG22	17	0.4
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG23	17	0.4
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG21	17	0.4
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG22	17	0.4
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG23	17	0.4
(1,2820)	1:103:B:GLU:H	1:106:B:LYS:H	18	0.4
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	9	0.4
(1,2746)	1:95:B:ASP:H	1:96:B:ALA:H	18	0.4
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	2	0.4
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	3	0.4
(1,2633)	1:213:A:GLU:HA	1:217:A:LYS:H	9	0.4
(1,2591)	1:208:A:MET:HA	1:210:A:ARG:H	11	0.4
(1,2529)	1:200:A:GLU:HB2	1:204:A:ALA:HA	18	0.4
(1,2529)	1:200:A:GLU:HB3	1:204:A:ALA:HA	18	0.4
(1,2463)	1:193:A:TYR:HE2	1:211:A:ASP:HA	13	0.4
(1,2261)	1:173:A:TYR:HA	1:192:A:ALA:HA	11	0.4
(1,2029)	1:150:A:LYS:HA	1:152:A:TYR:HA	3	0.4
(1,2010)	1:147:A:SER:HB2	1:178:A:PHE:HB2	16	0.4
(1,2010)	1:147:A:SER:HB2	1:178:A:PHE:HB3	16	0.4
(1,2010)	1:147:A:SER:HB3	1:178:A:PHE:HB2	16	0.4
(1,2010)	1:147:A:SER:HB3	1:178:A:PHE:HB3	16	0.4
(1,1667)	1:116:A:LYS:HA	1:118:A:TYR:HA	20	0.4
(1,1635)	1:113:A:MET:HA	1:118:A:TYR:HA	15	0.4
(1,1627)	1:113:A:MET:H	1:121:A:ALA:HA	18	0.4
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	16	0.4
(1,1483)	1:101:A:LYS:H	1:103:A:GLU:H	14	0.4
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	13	0.4
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	13	0.4
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	15	0.4
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	15	0.4
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	15	0.4
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	15	0.4
(1,1349)	1:39:A:CYS:HA	1:32:B:SER:HA	19	0.4
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	4	0.4
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	4	0.4
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	4	0.4
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	4	0.4
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	7	0.4
(1,1154)	1:60:B:PHE:HB2	1:63:B:GLN:HE21	5	0.4
(1,1154)	1:60:B:PHE:HB2	1:63:B:GLN:HE22	5	0.4
(1,1154)	1:60:B:PHE:HB3	1:63:B:GLN:HE21	5	0.4
(1,1154)	1:60:B:PHE:HB3	1:63:B:GLN:HE22	5	0.4
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	4	0.4
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	5	0.4
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	15	0.4
(1,835)	1:20:B:VAL:HA	1:24:B:GLU:H	19	0.4
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	4	0.4
(1,550)	1:61:A:LYS:H	1:63:A:GLN:H	1	0.4
(1,505)	1:55:A:LEU:HD11	1:71:A:SER:HA	3	0.4
(1,505)	1:55:A:LEU:HD12	1:71:A:SER:HA	3	0.4
(1,505)	1:55:A:LEU:HD13	1:71:A:SER:HA	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:52:A:SER:HA	1:55:A:LEU:H	5	0.4
(1,474)	1:51:A:VAL:HA	1:55:A:LEU:H	8	0.4
(1,445)	1:47:A:GLU:H	1:50:A:ALA:H	12	0.4
(1,343)	1:35:A:VAL:HA	1:38:A:ASP:H	3	0.4
(1,300)	1:30:A:ALA:HA	1:34:A:ASN:H	10	0.4
(1,4205)	1:342:B:ASN:H	1:343:B:GLU:H	14	0.39
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	17	0.39
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	15	0.39
(1,4162)	1:256:B:LEU:H	1:257:B:GLY:H	11	0.39
(1,4156)	1:248:B:GLY:H	1:249:B:LEU:H	3	0.39
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	6	0.39
(1,4110)	1:345:A:LYS:H	1:346:A:GLN:H	11	0.39
(1,4088)	1:321:A:ARG:H	1:322:A:ASN:H	5	0.39
(1,4071)	1:300:A:GLU:H	1:301:A:GLY:H	17	0.39
(1,4049)	1:239:A:ASP:H	1:240:A:ALA:H	9	0.39
(1,4025)	1:224:B:ASN:HA	1:226:B:GLU:H	20	0.39
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD11	1	0.39
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD12	1	0.39
(1,4014)	1:222:B:SER:HA	1:225:B:LEU:HD13	1	0.39
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	3	0.39
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	10	0.39
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	13	0.39
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	17	0.39
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	17	0.39
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	11	0.39
(1,3834)	1:200:B:GLU:HB2	1:204:B:ALA:H	2	0.39
(1,3834)	1:200:B:GLU:HB3	1:204:B:ALA:H	2	0.39
(1,3763)	1:193:B:TYR:HD1	1:211:B:ASP:HA	6	0.39
(1,3763)	1:193:B:TYR:HD2	1:211:B:ASP:HA	6	0.39
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	6	0.39
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	6	0.39
(1,3724)	1:190:B:LEU:HA	1:216:B:LYS:H	19	0.39
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB1	17	0.39
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB2	17	0.39
(1,3723)	1:190:B:LEU:HA	1:215:B:ALA:HB3	17	0.39
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	16	0.39
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB1	11	0.39
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB2	11	0.39
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB3	11	0.39
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	14	0.39
(1,3447)	1:161:B:SER:H	1:164:B:SER:H	3	0.39
(1,3341)	1:150:B:LYS:HG2	1:152:B:TYR:HE1	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3341)	1:150:B:LYS:HG2	1:152:B:TYR:HE2	10	0.39
(1,3341)	1:150:B:LYS:HG3	1:152:B:TYR:HE1	10	0.39
(1,3341)	1:150:B:LYS:HG3	1:152:B:TYR:HE2	10	0.39
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	6	0.39
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	12	0.39
(1,3075)	1:125:B:TYR:HB2	1:142:B:ARG:HA	1	0.39
(1,3075)	1:125:B:TYR:HB3	1:142:B:ARG:HA	1	0.39
(1,3070)	1:125:B:TYR:HA	1:138:B:TYR:HD1	13	0.39
(1,3070)	1:125:B:TYR:HA	1:138:B:TYR:HD2	13	0.39
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	1	0.39
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	1	0.39
(1,2925)	1:112:B:ALA:HB1	1:120:B:LEU:HD21	9	0.39
(1,2925)	1:112:B:ALA:HB1	1:120:B:LEU:HD22	9	0.39
(1,2925)	1:112:B:ALA:HB1	1:120:B:LEU:HD23	9	0.39
(1,2925)	1:112:B:ALA:HB2	1:120:B:LEU:HD21	9	0.39
(1,2925)	1:112:B:ALA:HB2	1:120:B:LEU:HD22	9	0.39
(1,2925)	1:112:B:ALA:HB2	1:120:B:LEU:HD23	9	0.39
(1,2925)	1:112:B:ALA:HB3	1:120:B:LEU:HD21	9	0.39
(1,2925)	1:112:B:ALA:HB3	1:120:B:LEU:HD22	9	0.39
(1,2925)	1:112:B:ALA:HB3	1:120:B:LEU:HD23	9	0.39
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	14	0.39
(1,2591)	1:208:A:MET:HA	1:210:A:ARG:H	8	0.39
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	7	0.39
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	7	0.39
(1,2517)	1:198:A:ASP:HA	1:201:A:GLY:H	5	0.39
(1,2506)	1:197:A:LEU:HD11	1:209:A:LYS:HA	15	0.39
(1,2506)	1:197:A:LEU:HD12	1:209:A:LYS:HA	15	0.39
(1,2506)	1:197:A:LEU:HD13	1:209:A:LYS:HA	15	0.39
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	7	0.39
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	7	0.39
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB2	7	0.39
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	7	0.39
(1,2432)	1:191:A:GLU:HA	1:195:A:LYS:H	3	0.39
(1,2419)	1:190:A:LEU:HD11	1:212:A:TYR:HA	6	0.39
(1,2419)	1:190:A:LEU:HD12	1:212:A:TYR:HA	6	0.39
(1,2419)	1:190:A:LEU:HD13	1:212:A:TYR:HA	6	0.39
(1,2416)	1:190:A:LEU:HA	1:212:A:TYR:HA	2	0.39
(1,2356)	1:181:A:TYR:HA	1:184:A:GLY:H	8	0.39
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	14	0.39
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	17	0.39
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	3	0.39
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1411)	1:67:A:ASP:HA	1:62:B:GLY:H	18	0.39
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	6	0.39
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	13	0.39
(1,1338)	1:36:A:ALA:HA	1:36:B:ALA:HA	12	0.39
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	18	0.39
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	18	0.39
(1,1289)	1:16:A:PHE:HE1	1:12:B:ILE:HD12	10	0.39
(1,1289)	1:16:A:PHE:HE2	1:12:B:ILE:HD12	10	0.39
(1,1262)	1:12:A:ILE:HD11	1:16:B:PHE:HE1	19	0.39
(1,1262)	1:12:A:ILE:HD11	1:16:B:PHE:HE2	19	0.39
(1,1262)	1:12:A:ILE:HD12	1:16:B:PHE:HE1	19	0.39
(1,1262)	1:12:A:ILE:HD12	1:16:B:PHE:HE2	19	0.39
(1,1262)	1:12:A:ILE:HD13	1:16:B:PHE:HE1	19	0.39
(1,1262)	1:12:A:ILE:HD13	1:16:B:PHE:HE2	19	0.39
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	4	0.39
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	15	0.39
(1,1129)	1:58:B:SER:HA	1:59:B:GLU:HA	5	0.39
(1,1114)	1:55:B:LEU:HD11	1:71:B:SER:HA	3	0.39
(1,1114)	1:55:B:LEU:HD12	1:71:B:SER:HA	3	0.39
(1,1114)	1:55:B:LEU:HD13	1:71:B:SER:HA	3	0.39
(1,1061)	1:47:B:GLU:HB2	1:49:B:GLU:H	11	0.39
(1,1061)	1:47:B:GLU:HB3	1:49:B:GLU:H	11	0.39
(1,1054)	1:47:B:GLU:H	1:50:B:ALA:H	19	0.39
(1,984)	1:39:B:CYS:H	1:42:B:GLU:H	20	0.39
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	1	0.39
(1,627)	1:4:B:SER:HA	1:6:B:GLU:H	12	0.39
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	16	0.39
(1,550)	1:61:A:LYS:H	1:63:A:GLN:H	3	0.39
(1,276)	1:27:A:GLU:HA	1:30:A:ALA:HA	6	0.39
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	6	0.39
(1,4188)	1:323:B:MET:H	1:324:B:ALA:H	5	0.38
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	7	0.38
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	9	0.38
(1,4169)	1:300:B:GLU:H	1:301:B:GLY:H	18	0.38
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	18	0.38
(1,4151)	1:243:B:GLY:H	1:244:B:ALA:H	1	0.38
(1,4151)	1:243:B:GLY:H	1:244:B:ALA:H	20	0.38
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	5	0.38
(1,4052)	1:242:A:GLN:H	1:243:A:GLY:H	5	0.38
(1,4048)	1:238:A:VAL:H	1:239:A:ASP:H	6	0.38
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	6	0.38
(1,4013)	1:222:B:SER:HA	1:225:B:LEU:H	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD11	13	0.38
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD12	13	0.38
(1,3996)	1:220:B:GLU:HA	1:223:B:LEU:HD13	13	0.38
(1,3983)	1:219:B:VAL:H	1:221:B:GLN:H	3	0.38
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	17	0.38
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	14	0.38
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	3	0.38
(1,3810)	1:197:B:LEU:HA	1:204:B:ALA:HA	17	0.38
(1,3722)	1:190:B:LEU:HA	1:212:B:TYR:HA	4	0.38
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	5	0.38
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	5	0.38
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	5	0.38
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	5	0.38
(1,3641)	1:180:B:LYS:H	1:189:B:ALA:HA	9	0.38
(1,3569)	1:173:B:TYR:HB2	1:195:B:LYS:H	15	0.38
(1,3569)	1:173:B:TYR:HB3	1:195:B:LYS:H	15	0.38
(1,3532)	1:170:B:PHE:HD1	1:171:B:ARG:HD2	13	0.38
(1,3532)	1:170:B:PHE:HD1	1:171:B:ARG:HD3	13	0.38
(1,3532)	1:170:B:PHE:HD2	1:171:B:ARG:HD2	13	0.38
(1,3532)	1:170:B:PHE:HD2	1:171:B:ARG:HD3	13	0.38
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	17	0.38
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	17	0.38
(1,3522)	1:170:B:PHE:HA	1:196:B:VAL:HA	7	0.38
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	7	0.38
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	7	0.38
(1,3452)	1:161:B:SER:HA	1:165:B:ILE:H	11	0.38
(1,3433)	1:159:B:ALA:HB1	1:176:B:LEU:HA	18	0.38
(1,3433)	1:159:B:ALA:HB2	1:176:B:LEU:HA	18	0.38
(1,3433)	1:159:B:ALA:HB3	1:176:B:LEU:HA	18	0.38
(1,3392)	1:156:B:VAL:H	1:179:B:ALA:HB1	16	0.38
(1,3392)	1:156:B:VAL:H	1:179:B:ALA:HB2	16	0.38
(1,3392)	1:156:B:VAL:H	1:179:B:ALA:HB3	16	0.38
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	2	0.38
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	15	0.38
(1,3225)	1:140:B:ALA:H	1:162:B:ALA:HA	10	0.38
(1,3158)	1:135:B:ASN:HA	1:138:B:TYR:H	6	0.38
(1,2984)	1:117:B:ASP:HA	1:120:B:LEU:H	20	0.38
(1,2973)	1:116:B:LYS:HA	1:118:B:TYR:HA	1	0.38
(1,2941)	1:113:B:MET:HA	1:118:B:TYR:HA	15	0.38
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG2	11	0.38
(1,2884)	1:109:B:GLY:H	1:124:B:LYS:HG3	11	0.38
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2837)	1:105:B:LEU:H	1:108:B:GLN:H	15	0.38
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	14	0.38
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	14	0.38
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	8	0.38
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	10	0.38
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	9	0.38
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	9	0.38
(1,2697)	1:221:A:GLN:HA	1:224:A:ASN:H	1	0.38
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	5	0.38
(1,2666)	1:217:A:LYS:HG2	1:218:A:LYS:H	7	0.38
(1,2666)	1:217:A:LYS:HG3	1:218:A:LYS:H	7	0.38
(1,2666)	1:217:A:LYS:HG2	1:218:A:LYS:H	16	0.38
(1,2666)	1:217:A:LYS:HG3	1:218:A:LYS:H	16	0.38
(1,2633)	1:213:A:GLU:HA	1:217:A:LYS:H	3	0.38
(1,2588)	1:208:A:MET:H	1:211:A:ASP:H	7	0.38
(1,2526)	1:200:A:GLU:HA	1:203:A:ASN:H	8	0.38
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG21	9	0.38
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG22	9	0.38
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG23	9	0.38
(1,2342)	1:180:A:LYS:HB2	1:185:A:LYS:H	12	0.38
(1,2342)	1:180:A:LYS:HB3	1:185:A:LYS:H	12	0.38
(1,2226)	1:170:A:PHE:HD1	1:171:A:ARG:HD2	10	0.38
(1,2226)	1:170:A:PHE:HD1	1:171:A:ARG:HD3	10	0.38
(1,2226)	1:170:A:PHE:HD2	1:171:A:ARG:HD2	10	0.38
(1,2226)	1:170:A:PHE:HD2	1:171:A:ARG:HD3	10	0.38
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	5	0.38
(1,1973)	1:144:A:ALA:HB1	1:175:A:ARG:HE	8	0.38
(1,1973)	1:144:A:ALA:HB2	1:175:A:ARG:HE	8	0.38
(1,1973)	1:144:A:ALA:HB3	1:175:A:ARG:HE	8	0.38
(1,1909)	1:139:A:TYR:HD1	1:162:A:ALA:H	20	0.38
(1,1909)	1:139:A:TYR:HD2	1:162:A:ALA:H	20	0.38
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD1	3	0.38
(1,1854)	1:135:A:ASN:HB2	1:138:A:TYR:HD2	3	0.38
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD1	3	0.38
(1,1854)	1:135:A:ASN:HB3	1:138:A:TYR:HD2	3	0.38
(1,1776)	1:125:A:TYR:HD2	1:141:A:ASN:HB3	7	0.38
(1,1646)	1:113:A:MET:HE1	1:145:A:ALA:HA	17	0.38
(1,1646)	1:113:A:MET:HE2	1:145:A:ALA:HA	17	0.38
(1,1646)	1:113:A:MET:HE3	1:145:A:ALA:HA	17	0.38
(1,1552)	1:106:A:LYS:HA	1:108:A:GLN:H	4	0.38
(1,1499)	1:102:A:ALA:HA	1:105:A:LEU:H	9	0.38
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	11	0.38
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	11	0.38
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	7	0.38
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	19	0.38
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	19	0.38
(1,1405)	1:63:A:GLN:H	1:67:B:ASP:HB2	19	0.38
(1,1405)	1:63:A:GLN:H	1:67:B:ASP:HB3	19	0.38
(1,1390)	1:44:A:PHE:HE1	1:25:B:ILE:HB	2	0.38
(1,1390)	1:44:A:PHE:HE2	1:25:B:ILE:HB	2	0.38
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	15	0.38
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	18	0.38
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	14	0.38
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	14	0.38
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	13	0.38
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	13	0.38
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	13	0.38
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	13	0.38
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	20	0.38
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	20	0.38
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	20	0.38
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	20	0.38
(1,1283)	1:16:A:PHE:HE1	1:12:B:ILE:HB	4	0.38
(1,1283)	1:16:A:PHE:HE2	1:12:B:ILE:HB	4	0.38
(1,1282)	1:16:A:PHE:HE1	1:9:B:ALA:HB2	12	0.38
(1,1282)	1:16:A:PHE:HE2	1:9:B:ALA:HB2	12	0.38
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG12	6	0.38
(1,1270)	1:15:A:TYR:HE1	1:8:B:ILE:HG13	6	0.38
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG12	6	0.38
(1,1270)	1:15:A:TYR:HE2	1:8:B:ILE:HG13	6	0.38
(1,1239)	1:8:A:ILE:HG21	1:12:B:ILE:HA	4	0.38
(1,1239)	1:8:A:ILE:HG22	1:12:B:ILE:HA	4	0.38
(1,1239)	1:8:A:ILE:HG23	1:12:B:ILE:HA	4	0.38
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	7	0.38
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	7	0.38
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	7	0.38
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	7	0.38
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	5	0.38
(1,1221)	1:2:A:SER:HA	1:67:B:ASP:HA	14	0.38
(1,1214)	1:71:B:SER:H	1:72:B:ALA:HA	14	0.38
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	13	0.38
(1,1132)	1:58:B:SER:HB2	1:59:B:GLU:HA	17	0.38
(1,1132)	1:58:B:SER:HB3	1:59:B:GLU:HA	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	20	0.38
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	11	0.38
(1,1011)	1:41:B:SER:HA	1:46:B:PHE:H	7	0.38
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	2	0.38
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE1	8	0.38
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE2	8	0.38
(1,939)	1:34:B:ASN:H	1:37:B:MET:HE3	8	0.38
(1,884)	1:27:B:GLU:HA	1:30:B:ALA:H	20	0.38
(1,834)	1:20:B:VAL:HA	1:23:B:LYS:HA	18	0.38
(1,758)	1:15:B:TYR:H	1:18:B:SER:H	3	0.38
(1,728)	1:13:B:VAL:HA	1:37:B:MET:HB2	3	0.38
(1,728)	1:13:B:VAL:HA	1:37:B:MET:HB3	3	0.38
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	3	0.38
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	16	0.38
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	5	0.38
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD11	11	0.38
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD12	11	0.38
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD13	11	0.38
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD11	11	0.38
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD12	11	0.38
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD13	11	0.38
(1,271)	1:27:A:GLU:H	1:30:A:ALA:H	6	0.38
(1,214)	1:19:A:ILE:H	1:22:A:LYS:H	10	0.38
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	5	0.38
(1,4206)	1:343:B:GLU:H	1:344:B:ASN:H	9	0.37
(1,4197)	1:332:B:GLY:H	1:333:B:ALA:H	4	0.37
(1,4197)	1:332:B:GLY:H	1:333:B:ALA:H	17	0.37
(1,4151)	1:243:B:GLY:H	1:244:B:ALA:H	7	0.37
(1,4106)	1:341:A:ASP:H	1:342:A:ASN:H	17	0.37
(1,4095)	1:328:A:PHE:H	1:329:A:GLY:H	8	0.37
(1,4073)	1:302:A:PHE:H	1:303:A:ALA:H	11	0.37
(1,4062)	1:254:A:SER:H	1:255:A:LEU:H	19	0.37
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	11	0.37
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	11	0.37
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	2	0.37
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	14	0.37
(1,3858)	1:205:B:THR:H	1:208:B:MET:H	2	0.37
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	3	0.37
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	3	0.37
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG21	12	0.37
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG22	12	0.37
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG23	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3686)	1:185:B:LYS:H	1:186:B:PRO:HA	8	0.37
(1,3619)	1:178:B:PHE:H	1:181:B:TYR:H	15	0.37
(1,3611)	1:177:B:GLY:HA2	1:189:B:ALA:HA	8	0.37
(1,3611)	1:177:B:GLY:HA3	1:189:B:ALA:HA	8	0.37
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	12	0.37
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	12	0.37
(1,3366)	1:152:B:TYR:HD1	1:182:B:ALA:HB1	1	0.37
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	8	0.37
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	8	0.37
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE1	8	0.37
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE2	8	0.37
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	3	0.37
(1,3122)	1:129:B:ILE:HA	1:138:B:TYR:HD1	11	0.37
(1,3122)	1:129:B:ILE:HA	1:138:B:TYR:HD2	11	0.37
(1,3119)	1:129:B:ILE:HA	1:133:B:PRO:HA	17	0.37
(1,3044)	1:122:B:ILE:HD11	1:146:B:HIS:HA	11	0.37
(1,3044)	1:122:B:ILE:HD12	1:146:B:HIS:HA	11	0.37
(1,3044)	1:122:B:ILE:HD13	1:146:B:HIS:HA	11	0.37
(1,3027)	1:121:B:ALA:HA	1:125:B:TYR:H	12	0.37
(1,2980)	1:117:B:ASP:H	1:118:B:TYR:HA	7	0.37
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	20	0.37
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	20	0.37
(1,2941)	1:113:B:MET:HA	1:118:B:TYR:HA	10	0.37
(1,2894)	1:110:B:ASN:H	1:113:B:MET:H	13	0.37
(1,2850)	1:105:B:LEU:HD21	1:124:B:LYS:HA	13	0.37
(1,2850)	1:105:B:LEU:HD22	1:124:B:LYS:HA	13	0.37
(1,2850)	1:105:B:LEU:HD23	1:124:B:LYS:HA	13	0.37
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG21	3	0.37
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG22	3	0.37
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG23	3	0.37
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG21	3	0.37
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG22	3	0.37
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG23	3	0.37
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG21	3	0.37
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG22	3	0.37
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG23	3	0.37
(1,2636)	1:214:A:SER:H	1:217:A:LYS:H	3	0.37
(1,2628)	1:213:A:GLU:H	1:216:A:LYS:H	7	0.37
(1,2615)	1:211:A:ASP:HA	1:215:A:ALA:H	20	0.37
(1,2529)	1:200:A:GLU:HB2	1:204:A:ALA:HA	15	0.37
(1,2529)	1:200:A:GLU:HB3	1:204:A:ALA:HA	15	0.37
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	2	0.37
(1,2527)	1:200:A:GLU:HB2	1:203:A:ASN:HA	16	0.37
(1,2527)	1:200:A:GLU:HB3	1:203:A:ASN:HA	16	0.37
(1,2464)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	10	0.37
(1,2380)	1:185:A:LYS:H	1:186:A:PRO:HA	5	0.37
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	3	0.37
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	3	0.37
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	8	0.37
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	8	0.37
(1,2055)	1:152:A:TYR:HB2	1:183:A:GLN:H	3	0.37
(1,2055)	1:152:A:TYR:HB3	1:183:A:GLN:H	3	0.37
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	12	0.37
(1,1769)	1:125:A:TYR:HB2	1:142:A:ARG:HA	3	0.37
(1,1769)	1:125:A:TYR:HB3	1:142:A:ARG:HA	3	0.37
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	5	0.37
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	5	0.37
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD1	8	0.37
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD2	8	0.37
(1,1666)	1:116:A:LYS:HA	1:118:A:TYR:H	10	0.37
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE1	11	0.37
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE2	11	0.37
(1,1643)	1:113:A:MET:HE1	1:144:A:ALA:H	3	0.37
(1,1643)	1:113:A:MET:HE2	1:144:A:ALA:H	3	0.37
(1,1643)	1:113:A:MET:HE3	1:144:A:ALA:H	3	0.37
(1,1565)	1:107:A:MET:HA	1:110:A:ASN:H	17	0.37
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG11	16	0.37
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG12	16	0.37
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG13	16	0.37
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	11	0.37
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	11	0.37
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	6	0.37
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	6	0.37
(1,1390)	1:44:A:PHE:HE1	1:25:B:ILE:HB	12	0.37
(1,1390)	1:44:A:PHE:HE2	1:25:B:ILE:HB	12	0.37
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	15	0.37
(1,1325)	1:33:A:LEU:HA	1:40:B:ILE:HA	17	0.37
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE2	11	0.37
(1,1304)	1:25:A:ILE:HA	1:5:B:LYS:HE3	11	0.37
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD11	5	0.37
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD12	5	0.37
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD13	5	0.37
(1,1256)	1:12:A:ILE:HG21	1:16:B:PHE:HZ	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	1:12:A:ILE:HG22	1:16:B:PHE:HZ	6	0.37
(1,1256)	1:12:A:ILE:HG23	1:16:B:PHE:HZ	6	0.37
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	16	0.37
(1,1149)	1:60:B:PHE:HB2	1:62:B:GLY:H	1	0.37
(1,1149)	1:60:B:PHE:HB3	1:62:B:GLY:H	1	0.37
(1,1146)	1:60:B:PHE:HA	1:63:B:GLN:H	4	0.37
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	6	0.37
(1,1074)	1:49:B:GLU:HA	1:51:B:VAL:H	2	0.37
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	3	0.37
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	3	0.37
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG11	9	0.37
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG12	9	0.37
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG13	9	0.37
(1,745)	1:14:B:ASN:H	1:17:B:SER:H	3	0.37
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	20	0.37
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	6	0.37
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	6	0.37
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE21	15	0.37
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE22	15	0.37
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE21	15	0.37
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE22	15	0.37
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	2	0.37
(1,243)	1:22:A:LYS:H	1:24:A:GLU:H	13	0.37
(1,4190)	1:325:B:GLY:H	1:326:B:ASN:H	16	0.36
(1,4176)	1:307:B:GLY:H	1:308:B:THR:H	15	0.36
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	9	0.36
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	10	0.36
(1,4105)	1:338:A:GLU:H	1:339:A:THR:H	14	0.36
(1,4088)	1:321:A:ARG:H	1:322:A:ASN:H	7	0.36
(1,4073)	1:302:A:PHE:H	1:303:A:ALA:H	5	0.36
(1,4071)	1:300:A:GLU:H	1:301:A:GLY:H	20	0.36
(1,4041)	1:231:A:GLU:H	1:232:A:GLN:H	9	0.36
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	1	0.36
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	1	0.36
(1,3921)	1:211:B:ASP:HA	1:215:B:ALA:H	12	0.36
(1,3882)	1:207:B:ALA:H	1:210:B:ARG:H	7	0.36
(1,3879)	1:206:B:GLU:HB2	1:207:B:ALA:H	4	0.36
(1,3879)	1:206:B:GLU:HB3	1:207:B:ALA:H	4	0.36
(1,3815)	1:197:B:LEU:HD21	1:209:B:LYS:H	2	0.36
(1,3815)	1:197:B:LEU:HD22	1:209:B:LYS:H	2	0.36
(1,3815)	1:197:B:LEU:HD23	1:209:B:LYS:H	2	0.36
(1,3808)	1:197:B:LEU:HA	1:200:B:GLU:H	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	19	0.36
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	19	0.36
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	14	0.36
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	17	0.36
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG21	19	0.36
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG22	19	0.36
(1,3698)	1:187:B:GLU:HA	1:219:B:VAL:HG23	19	0.36
(1,3657)	1:181:B:TYR:H	1:189:B:ALA:HA	14	0.36
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	2	0.36
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	2	0.36
(1,3507)	1:169:B:TYR:HE1	1:171:B:ARG:HB2	14	0.36
(1,3507)	1:169:B:TYR:HE1	1:171:B:ARG:HB3	14	0.36
(1,3507)	1:169:B:TYR:HE2	1:171:B:ARG:HB2	14	0.36
(1,3507)	1:169:B:TYR:HE2	1:171:B:ARG:HB3	14	0.36
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	17	0.36
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	17	0.36
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	19	0.36
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	19	0.36
(1,3444)	1:160:B:GLU:HA	1:164:B:SER:H	11	0.36
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD11	13	0.36
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD12	13	0.36
(1,3397)	1:156:B:VAL:HA	1:176:B:LEU:HD13	13	0.36
(1,3200)	1:139:B:TYR:H	1:162:B:ALA:HA	7	0.36
(1,3195)	1:138:B:TYR:HA	1:141:B:ASN:H	9	0.36
(1,3102)	1:128:B:ALA:H	1:131:B:VAL:H	8	0.36
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB2	13	0.36
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB3	13	0.36
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB2	13	0.36
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB3	13	0.36
(1,2942)	1:113:B:MET:HA	1:121:B:ALA:H	15	0.36
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	17	0.36
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	7	0.36
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	7	0.36
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	7	0.36
(1,2836)	1:105:B:LEU:H	1:107:B:MET:H	6	0.36
(1,2823)	1:103:B:GLU:HA	1:105:B:LEU:H	17	0.36
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	13	0.36
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	13	0.36
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	13	0.36
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	20	0.36
(1,2645)	1:215:A:ALA:H	1:218:A:LYS:H	6	0.36
(1,2635)	1:214:A:SER:H	1:216:A:LYS:H	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2573)	1:206:A:GLU:HB2	1:207:A:ALA:H	16	0.36
(1,2573)	1:206:A:GLU:HB3	1:207:A:ALA:H	16	0.36
(1,2526)	1:200:A:GLU:HA	1:203:A:ASN:H	17	0.36
(1,2398)	1:188:A:GLU:HA	1:191:A:GLU:H	8	0.36
(1,2367)	1:181:A:TYR:HE1	1:218:A:LYS:HE2	18	0.36
(1,2367)	1:181:A:TYR:HE1	1:218:A:LYS:HE3	18	0.36
(1,2367)	1:181:A:TYR:HE2	1:218:A:LYS:HE2	18	0.36
(1,2367)	1:181:A:TYR:HE2	1:218:A:LYS:HE3	18	0.36
(1,2359)	1:181:A:TYR:HA	1:189:A:ALA:H	7	0.36
(1,2344)	1:180:A:LYS:HB2	1:188:A:GLU:HB2	16	0.36
(1,2344)	1:180:A:LYS:HB2	1:188:A:GLU:HB3	16	0.36
(1,2344)	1:180:A:LYS:HB3	1:188:A:GLU:HB2	16	0.36
(1,2344)	1:180:A:LYS:HB3	1:188:A:GLU:HB3	16	0.36
(1,2342)	1:180:A:LYS:HB2	1:185:A:LYS:H	7	0.36
(1,2342)	1:180:A:LYS:HB3	1:185:A:LYS:H	7	0.36
(1,2261)	1:173:A:TYR:HA	1:192:A:ALA:HA	9	0.36
(1,2243)	1:171:A:ARG:HA	1:174:A:SER:H	18	0.36
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	12	0.36
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	12	0.36
(1,2181)	1:166:A:ASP:HA	1:168:A:SER:H	6	0.36
(1,2136)	1:160:A:GLU:HA	1:163:A:ILE:H	6	0.36
(1,1865)	1:136:A:ALA:HA	1:166:A:ASP:H	19	0.36
(1,1829)	1:130:A:LYS:HA	1:132:A:LEU:H	1	0.36
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	12	0.36
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	12	0.36
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	12	0.36
(1,1646)	1:113:A:MET:HE1	1:145:A:ALA:HA	11	0.36
(1,1646)	1:113:A:MET:HE2	1:145:A:ALA:HA	11	0.36
(1,1646)	1:113:A:MET:HE3	1:145:A:ALA:HA	11	0.36
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	4	0.36
(1,1490)	1:101:A:LYS:HA	1:104:A:ASP:H	8	0.36
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	16	0.36
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	16	0.36
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	16	0.36
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	15	0.36
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	15	0.36
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	20	0.36
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB2	15	0.36
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB3	15	0.36
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	10	0.36
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	10	0.36
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	3	0.36
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB2	7	0.36
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB3	7	0.36
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	2	0.36
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	10	0.36
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	10	0.36
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD11	1	0.36
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD12	1	0.36
(1,1220)	1:2:A:SER:H	1:69:B:LEU:HD13	1	0.36
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD11	8	0.36
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD12	8	0.36
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD13	8	0.36
(1,1145)	1:60:B:PHE:HA	1:62:B:GLY:H	19	0.36
(1,1121)	1:56:B:GLY:HA2	1:58:B:SER:H	16	0.36
(1,1121)	1:56:B:GLY:HA3	1:58:B:SER:H	16	0.36
(1,1117)	1:56:B:GLY:H	1:57:B:LYS:H	5	0.36
(1,1113)	1:55:B:LEU:HA	1:58:B:SER:H	1	0.36
(1,1074)	1:49:B:GLU:HA	1:51:B:VAL:H	1	0.36
(1,988)	1:39:B:CYS:HA	1:42:B:GLU:H	19	0.36
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	10	0.36
(1,595)	1:69:A:LEU:H	1:71:A:SER:H	18	0.36
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	6	0.36
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	7	0.36
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	7	0.36
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	9	0.36
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	20	0.36
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	20	0.36
(1,248)	1:23:A:LYS:H	1:25:A:ILE:H	13	0.36
(1,245)	1:22:A:LYS:HA	1:24:A:GLU:H	8	0.36
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	14	0.35
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	3	0.35
(1,4156)	1:248:B:GLY:H	1:249:B:LEU:H	17	0.35
(1,4147)	1:239:B:ASP:H	1:240:B:ALA:H	12	0.35
(1,4088)	1:321:A:ARG:H	1:322:A:ASN:H	13	0.35
(1,4060)	1:252:A:LEU:H	1:253:A:GLY:H	14	0.35
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	10	0.35
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	16	0.35
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	16	0.35
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	5	0.35
(1,3999)	1:221:B:GLN:H	1:223:B:LEU:H	10	0.35
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	19	0.35
(1,3888)	1:207:B:ALA:HA	1:210:B:ARG:HG2	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3888)	1:207:B:ALA:HA	1:210:B:ARG:HG3	12	0.35
(1,3840)	1:201:B:GLY:H	1:204:B:ALA:H	16	0.35
(1,3819)	1:198:B:ASP:H	1:201:B:GLY:H	4	0.35
(1,3716)	1:190:B:LEU:H	1:215:B:ALA:HB1	17	0.35
(1,3716)	1:190:B:LEU:H	1:215:B:ALA:HB2	17	0.35
(1,3716)	1:190:B:LEU:H	1:215:B:ALA:HB3	17	0.35
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	15	0.35
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	7	0.35
(1,3186)	1:137:B:ILE:HA	1:140:B:ALA:H	16	0.35
(1,3135)	1:130:B:LYS:HA	1:132:B:LEU:H	4	0.35
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	7	0.35
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	7	0.35
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	7	0.35
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	7	0.35
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	11	0.35
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	11	0.35
(1,2977)	1:116:B:LYS:HB2	1:118:B:TYR:HD1	7	0.35
(1,2977)	1:116:B:LYS:HB2	1:118:B:TYR:HD2	7	0.35
(1,2977)	1:116:B:LYS:HB3	1:118:B:TYR:HD1	7	0.35
(1,2977)	1:116:B:LYS:HB3	1:118:B:TYR:HD2	7	0.35
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	13	0.35
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	13	0.35
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	13	0.35
(1,2892)	1:109:B:GLY:HA2	1:113:B:MET:H	3	0.35
(1,2892)	1:109:B:GLY:HA3	1:113:B:MET:H	3	0.35
(1,2891)	1:109:B:GLY:HA2	1:112:B:ALA:HB1	13	0.35
(1,2891)	1:109:B:GLY:HA2	1:112:B:ALA:HB2	13	0.35
(1,2891)	1:109:B:GLY:HA2	1:112:B:ALA:HB3	13	0.35
(1,2891)	1:109:B:GLY:HA3	1:112:B:ALA:HB1	13	0.35
(1,2891)	1:109:B:GLY:HA3	1:112:B:ALA:HB2	13	0.35
(1,2891)	1:109:B:GLY:HA3	1:112:B:ALA:HB3	13	0.35
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	9	0.35
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	10	0.35
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE1	15	0.35
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE2	15	0.35
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE3	15	0.35
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	16	0.35
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	16	0.35
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	16	0.35
(1,2664)	1:217:A:LYS:HA	1:220:A:GLU:H	11	0.35
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	12	0.35
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	18	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2582)	1:207:A:ALA:HA	1:210:A:ARG:HG2	8	0.35
(1,2582)	1:207:A:ALA:HA	1:210:A:ARG:HG3	8	0.35
(1,2457)	1:193:A:TYR:HD1	1:211:A:ASP:HA	9	0.35
(1,2457)	1:193:A:TYR:HD2	1:211:A:ASP:HA	9	0.35
(1,2442)	1:193:A:TYR:H	1:196:A:VAL:H	15	0.35
(1,2390)	1:187:A:GLU:HA	1:190:A:LEU:H	12	0.35
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	5	0.35
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	6	0.35
(1,1998)	1:147:A:SER:H	1:155:A:ALA:HA	11	0.35
(1,1998)	1:147:A:SER:H	1:155:A:ALA:HA	14	0.35
(1,1894)	1:139:A:TYR:H	1:162:A:ALA:HA	10	0.35
(1,1872)	1:136:A:ALA:HB1	1:169:A:TYR:HB2	18	0.35
(1,1872)	1:136:A:ALA:HB1	1:169:A:TYR:HB3	18	0.35
(1,1872)	1:136:A:ALA:HB2	1:169:A:TYR:HB2	18	0.35
(1,1872)	1:136:A:ALA:HB2	1:169:A:TYR:HB3	18	0.35
(1,1872)	1:136:A:ALA:HB3	1:169:A:TYR:HB2	18	0.35
(1,1872)	1:136:A:ALA:HB3	1:169:A:TYR:HB3	18	0.35
(1,1852)	1:135:A:ASN:HA	1:138:A:TYR:H	20	0.35
(1,1776)	1:125:A:TYR:HD2	1:141:A:ASN:HB3	18	0.35
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD1	15	0.35
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD2	15	0.35
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD1	15	0.35
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD2	15	0.35
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE1	15	0.35
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE2	15	0.35
(1,1565)	1:107:A:MET:HA	1:110:A:ASN:H	4	0.35
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE1	20	0.35
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE2	20	0.35
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE3	20	0.35
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	14	0.35
(1,1385)	1:44:A:PHE:HA	1:25:B:ILE:HD13	9	0.35
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB2	2	0.35
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB3	2	0.35
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	4	0.35
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	4	0.35
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	8	0.35
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	15	0.35
(1,1321)	1:32:A:SER:HB2	1:43:B:ALA:H	17	0.35
(1,1321)	1:32:A:SER:HB3	1:43:B:ALA:H	17	0.35
(1,1321)	1:32:A:SER:HB2	1:43:B:ALA:H	19	0.35
(1,1321)	1:32:A:SER:HB3	1:43:B:ALA:H	19	0.35
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD11	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD12	4	0.35
(1,1264)	1:15:A:TYR:HB2	1:12:B:ILE:HD13	4	0.35
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD11	4	0.35
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD12	4	0.35
(1,1264)	1:15:A:TYR:HB3	1:12:B:ILE:HD13	4	0.35
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	19	0.35
(1,1150)	1:60:B:PHE:HB2	1:63:B:GLN:H	7	0.35
(1,1150)	1:60:B:PHE:HB3	1:63:B:GLN:H	7	0.35
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	9	0.35
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	14	0.35
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	18	0.35
(1,1054)	1:47:B:GLU:H	1:50:B:ALA:H	2	0.35
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG11	11	0.35
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG12	11	0.35
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG13	11	0.35
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	18	0.35
(1,626)	1:4:B:SER:HA	1:5:B:LYS:HA	1	0.35
(1,616)	1:3:B:ALA:HA	1:4:B:SER:H	6	0.35
(1,225)	1:20:A:VAL:HA	1:23:A:LYS:HA	1	0.35
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	5	0.34
(1,4092)	1:325:A:GLY:H	1:326:A:ASN:H	20	0.34
(1,4051)	1:241:A:SER:H	1:242:A:GLN:H	8	0.34
(1,4035)	1:226:B:GLU:HG2	1:227:B:LYS:H	13	0.34
(1,4035)	1:226:B:GLU:HG3	1:227:B:LYS:H	13	0.34
(1,3846)	1:202:B:ASP:HA	1:204:B:ALA:H	16	0.34
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	17	0.34
(1,3748)	1:193:B:TYR:H	1:196:B:VAL:H	17	0.34
(1,3738)	1:191:B:GLU:HA	1:195:B:LYS:H	4	0.34
(1,3724)	1:190:B:LEU:HA	1:216:B:LYS:H	13	0.34
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	19	0.34
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	18	0.34
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	18	0.34
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	18	0.34
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	18	0.34
(1,3657)	1:181:B:TYR:H	1:189:B:ALA:HA	9	0.34
(1,3546)	1:171:B:ARG:H	1:174:B:SER:H	17	0.34
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE1	11	0.34
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE2	11	0.34
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE3	11	0.34
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE1	11	0.34
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE2	11	0.34
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE3	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD11	20	0.34
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD12	20	0.34
(1,3524)	1:170:B:PHE:HA	1:199:B:ILE:HD13	20	0.34
(1,3471)	1:163:B:ILE:HD11	1:173:B:TYR:H	3	0.34
(1,3471)	1:163:B:ILE:HD12	1:173:B:TYR:H	3	0.34
(1,3471)	1:163:B:ILE:HD13	1:173:B:TYR:H	3	0.34
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	7	0.34
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	7	0.34
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE1	7	0.34
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE2	7	0.34
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	7	0.34
(1,3304)	1:147:B:SER:H	1:155:B:ALA:HA	8	0.34
(1,3262)	1:143:B:ALA:HB1	1:155:B:ALA:HA	2	0.34
(1,3262)	1:143:B:ALA:HB2	1:155:B:ALA:HA	2	0.34
(1,3262)	1:143:B:ALA:HB3	1:155:B:ALA:HA	2	0.34
(1,3135)	1:130:B:LYS:HA	1:132:B:LEU:H	18	0.34
(1,3126)	1:129:B:ILE:HD11	1:139:B:TYR:HA	5	0.34
(1,3126)	1:129:B:ILE:HD12	1:139:B:TYR:HA	5	0.34
(1,3126)	1:129:B:ILE:HD13	1:139:B:TYR:HA	5	0.34
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	20	0.34
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	20	0.34
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	20	0.34
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	20	0.34
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE2	15	0.34
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	2	0.34
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	2	0.34
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	5	0.34
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	5	0.34
(1,2973)	1:116:B:LYS:HA	1:118:B:TYR:HA	9	0.34
(1,2846)	1:105:B:LEU:HD11	1:128:B:ALA:HA	9	0.34
(1,2846)	1:105:B:LEU:HD12	1:128:B:ALA:HA	9	0.34
(1,2846)	1:105:B:LEU:HD13	1:128:B:ALA:HA	9	0.34
(1,2842)	1:105:B:LEU:HA	1:109:B:GLY:H	20	0.34
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	13	0.34
(1,2805)	1:102:B:ALA:HA	1:105:B:LEU:H	14	0.34
(1,2779)	1:99:B:LYS:HA	1:101:B:LYS:H	6	0.34
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	1	0.34
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	1	0.34
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	11	0.34
(1,2694)	1:221:A:GLN:H	1:224:A:ASN:H	12	0.34
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	16	0.34
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	5	0.34
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	16	0.34
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	16	0.34
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	8	0.34
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	8	0.34
(1,2146)	1:161:A:SER:HA	1:165:A:ILE:H	8	0.34
(1,2138)	1:160:A:GLU:HA	1:164:A:SER:H	16	0.34
(1,1880)	1:137:A:ILE:HA	1:140:A:ALA:H	20	0.34
(1,1785)	1:126:A:THR:HA	1:130:A:LYS:H	8	0.34
(1,1785)	1:126:A:THR:HA	1:130:A:LYS:H	19	0.34
(1,1748)	1:124:A:LYS:H	1:127:A:GLU:H	14	0.34
(1,1735)	1:122:A:ILE:HA	1:126:A:THR:H	14	0.34
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	2	0.34
(1,1539)	1:105:A:LEU:HD11	1:128:A:ALA:H	20	0.34
(1,1539)	1:105:A:LEU:HD12	1:128:A:ALA:H	20	0.34
(1,1539)	1:105:A:LEU:HD13	1:128:A:ALA:H	20	0.34
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	15	0.34
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	18	0.34
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	18	0.34
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG12	18	0.34
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG13	18	0.34
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	18	0.34
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	5	0.34
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	5	0.34
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	19	0.34
(1,1268)	1:15:A:TYR:HE1	1:5:B:LYS:HB2	5	0.34
(1,1268)	1:15:A:TYR:HE1	1:5:B:LYS:HB3	5	0.34
(1,1268)	1:15:A:TYR:HE2	1:5:B:LYS:HB2	5	0.34
(1,1268)	1:15:A:TYR:HE2	1:5:B:LYS:HB3	5	0.34
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD11	11	0.34
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD12	11	0.34
(1,1197)	1:68:B:ILE:H	1:69:B:LEU:HD13	11	0.34
(1,1150)	1:60:B:PHE:HB2	1:63:B:GLN:H	19	0.34
(1,1150)	1:60:B:PHE:HB3	1:63:B:GLN:H	19	0.34
(1,992)	1:40:B:ILE:H	1:42:B:GLU:H	1	0.34
(1,943)	1:34:B:ASN:HA	1:37:B:MET:H	16	0.34
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	2	0.34
(1,835)	1:20:B:VAL:HA	1:24:B:GLU:H	11	0.34
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	14	0.34
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB2	11	0.34
(1,753)	1:14:B:ASN:HA	1:48:B:ARG:HB3	11	0.34
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD11	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD12	10	0.34
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD13	10	0.34
(1,616)	1:3:B:ALA:HA	1:4:B:SER:H	15	0.34
(1,610)	1:2:B:SER:H	1:3:B:ALA:H	7	0.34
(1,595)	1:69:A:LEU:H	1:71:A:SER:H	9	0.34
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	18	0.34
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	18	0.34
(1,506)	1:55:A:LEU:HD11	1:72:A:ALA:HA	7	0.34
(1,506)	1:55:A:LEU:HD12	1:72:A:ALA:HA	7	0.34
(1,506)	1:55:A:LEU:HD13	1:72:A:ALA:HA	7	0.34
(1,474)	1:51:A:VAL:HA	1:55:A:LEU:H	7	0.34
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	11	0.34
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	2	0.34
(1,174)	1:16:A:PHE:HA	1:19:A:ILE:HA	15	0.34
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	5	0.33
(1,4188)	1:323:B:MET:H	1:324:B:ALA:H	8	0.33
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	19	0.33
(1,4176)	1:307:B:GLY:H	1:308:B:THR:H	12	0.33
(1,4162)	1:256:B:LEU:H	1:257:B:GLY:H	2	0.33
(1,4139)	1:231:B:GLU:H	1:232:B:GLN:H	18	0.33
(1,4138)	1:228:B:THR:H	1:229:B:VAL:H	1	0.33
(1,4107)	1:342:A:ASN:H	1:343:A:GLU:H	8	0.33
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	1	0.33
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	2	0.33
(1,4068)	1:260:A:LEU:H	1:261:A:GLY:H	15	0.33
(1,4050)	1:240:A:ALA:H	1:241:A:SER:H	16	0.33
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	15	0.33
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	8	0.33
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	8	0.33
(1,3992)	1:220:B:GLU:H	1:222:B:SER:H	13	0.33
(1,3978)	1:218:B:LYS:HA	1:220:B:GLU:H	5	0.33
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	15	0.33
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	15	0.33
(1,3898)	1:208:B:MET:HA	1:211:B:ASP:H	13	0.33
(1,3840)	1:201:B:GLY:H	1:204:B:ALA:H	12	0.33
(1,3828)	1:199:B:ILE:HA	1:201:B:GLY:H	1	0.33
(1,3809)	1:197:B:LEU:HA	1:201:B:GLY:H	12	0.33
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	10	0.33
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	10	0.33
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	10	0.33
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	10	0.33
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	9	0.33
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG21	8	0.33
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG22	8	0.33
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG23	8	0.33
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	4	0.33
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	4	0.33
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	4	0.33
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	4	0.33
(1,3663)	1:181:B:TYR:HA	1:185:B:LYS:H	17	0.33
(1,3651)	1:180:B:LYS:HB2	1:189:B:ALA:H	20	0.33
(1,3651)	1:180:B:LYS:HB3	1:189:B:ALA:H	20	0.33
(1,3629)	1:178:B:PHE:HB2	1:179:B:ALA:H	15	0.33
(1,3629)	1:178:B:PHE:HB3	1:179:B:ALA:H	15	0.33
(1,3605)	1:177:B:GLY:H	1:180:B:LYS:H	17	0.33
(1,3362)	1:152:B:TYR:HD1	1:179:B:ALA:HA	13	0.33
(1,3362)	1:152:B:TYR:HD2	1:179:B:ALA:HA	13	0.33
(1,3325)	1:149:B:LEU:H	1:151:B:GLU:H	5	0.33
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB2	12	0.33
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB3	12	0.33
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB2	12	0.33
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB3	12	0.33
(1,3313)	1:147:B:SER:HA	1:152:B:TYR:HA	14	0.33
(1,3106)	1:128:B:ALA:HA	1:131:B:VAL:H	17	0.33
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	1	0.33
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	1	0.33
(1,2979)	1:117:B:ASP:H	1:118:B:TYR:H	15	0.33
(1,2943)	1:113:B:MET:HA	1:121:B:ALA:HB1	2	0.33
(1,2943)	1:113:B:MET:HA	1:121:B:ALA:HB2	2	0.33
(1,2943)	1:113:B:MET:HA	1:121:B:ALA:HB3	2	0.33
(1,2796)	1:101:B:LYS:HA	1:104:B:ASP:H	20	0.33
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	13	0.33
(1,2768)	1:98:B:THR:H	1:100:B:ALA:H	8	0.33
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	1	0.33
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	1	0.33
(1,2719)	1:224:A:ASN:HA	1:226:A:GLU:H	6	0.33
(1,2669)	1:218:A:LYS:H	1:221:A:GLN:H	12	0.33
(1,2656)	1:216:A:LYS:HA	1:218:A:LYS:H	10	0.33
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	5	0.33
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	6	0.33
(1,2517)	1:198:A:ASP:HA	1:201:A:GLY:H	15	0.33
(1,2464)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	15	0.33
(1,2464)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2383)	1:185:A:LYS:HA	1:188:A:GLU:H	7	0.33
(1,2359)	1:181:A:TYR:HA	1:189:A:ALA:H	2	0.33
(1,2305)	1:177:A:GLY:HA2	1:189:A:ALA:HA	1	0.33
(1,2305)	1:177:A:GLY:HA3	1:189:A:ALA:HA	1	0.33
(1,2244)	1:171:A:ARG:HA	1:174:A:SER:HA	18	0.33
(1,2201)	1:169:A:TYR:HE1	1:171:A:ARG:HB2	8	0.33
(1,2201)	1:169:A:TYR:HE1	1:171:A:ARG:HB3	8	0.33
(1,2201)	1:169:A:TYR:HE2	1:171:A:ARG:HB2	8	0.33
(1,2201)	1:169:A:TYR:HE2	1:171:A:ARG:HB3	8	0.33
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	18	0.33
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	18	0.33
(1,2071)	1:154:A:GLN:H	1:157:A:LYS:H	11	0.33
(1,1919)	1:140:A:ALA:H	1:162:A:ALA:HA	5	0.33
(1,1645)	1:113:A:MET:HE1	1:145:A:ALA:H	14	0.33
(1,1645)	1:113:A:MET:HE2	1:145:A:ALA:H	14	0.33
(1,1645)	1:113:A:MET:HE3	1:145:A:ALA:H	14	0.33
(1,1613)	1:112:A:ALA:HA	1:117:A:ASP:H	2	0.33
(1,1544)	1:105:A:LEU:HD21	1:124:A:LYS:HA	8	0.33
(1,1544)	1:105:A:LEU:HD22	1:124:A:LYS:HA	8	0.33
(1,1544)	1:105:A:LEU:HD23	1:124:A:LYS:HA	8	0.33
(1,1518)	1:103:A:GLU:HA	1:106:A:LYS:H	13	0.33
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD11	6	0.33
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD12	6	0.33
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD13	6	0.33
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG11	2	0.33
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG12	2	0.33
(1,1495)	1:102:A:ALA:H	1:131:A:VAL:HG13	2	0.33
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	1	0.33
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	19	0.33
(1,1427)	1:69:A:LEU:HD11	1:2:B:SER:HG	2	0.33
(1,1427)	1:69:A:LEU:HD12	1:2:B:SER:HG	2	0.33
(1,1427)	1:69:A:LEU:HD13	1:2:B:SER:HG	2	0.33
(1,1374)	1:43:A:ALA:HA	1:32:B:SER:H	17	0.33
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	8	0.33
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	8	0.33
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	8	0.33
(1,1289)	1:16:A:PHE:HE1	1:12:B:ILE:HD12	4	0.33
(1,1289)	1:16:A:PHE:HE2	1:12:B:ILE:HD12	4	0.33
(1,1281)	1:16:A:PHE:HE1	1:9:B:ALA:HB1	19	0.33
(1,1281)	1:16:A:PHE:HE2	1:9:B:ALA:HB1	19	0.33
(1,1228)	1:2:A:SER:HB2	1:68:B:ILE:HA	3	0.33
(1,1228)	1:2:A:SER:HB3	1:68:B:ILE:HA	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	1	0.33
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	20	0.33
(1,1135)	1:59:B:GLU:H	1:60:B:PHE:HA	5	0.33
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD11	3	0.33
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD12	3	0.33
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD13	3	0.33
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD11	3	0.33
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD12	3	0.33
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD13	3	0.33
(1,952)	1:35:B:VAL:HA	1:38:B:ASP:H	3	0.33
(1,889)	1:28:B:ASP:H	1:31:B:ASP:H	10	0.33
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD11	11	0.33
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD12	11	0.33
(1,679)	1:10:B:ALA:H	1:54:B:ILE:HD13	11	0.33
(1,611)	1:2:B:SER:H	1:3:B:ALA:HA	5	0.33
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	12	0.33
(1,567)	1:65:A:LEU:H	1:67:A:ASP:H	3	0.33
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD11	2	0.33
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD12	2	0.33
(1,562)	1:63:A:GLN:HA	1:68:A:ILE:HD13	2	0.33
(1,277)	1:27:A:GLU:HA	1:31:A:ASP:H	4	0.33
(1,76)	1:10:A:ALA:HA	1:48:A:ARG:HA	11	0.33
(1,76)	1:10:A:ALA:HA	1:48:A:ARG:HA	13	0.33
(1,4162)	1:256:B:LEU:H	1:257:B:GLY:H	6	0.32
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	8	0.32
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	8	0.32
(1,4148)	1:240:B:ALA:H	1:241:B:SER:H	20	0.32
(1,4143)	1:235:B:ASP:H	1:236:B:ALA:H	15	0.32
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	14	0.32
(1,4077)	1:305:A:GLY:H	1:307:A:GLY:H	10	0.32
(1,4065)	1:257:A:GLY:H	1:258:A:GLY:H	15	0.32
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	9	0.32
(1,4041)	1:231:A:GLU:H	1:232:A:GLN:H	12	0.32
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	12	0.32
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	14	0.32
(1,3912)	1:210:B:ARG:HA	1:213:B:GLU:H	3	0.32
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB2	18	0.32
(1,3764)	1:193:B:TYR:HD1	1:211:B:ASP:HB3	18	0.32
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB2	18	0.32
(1,3764)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	18	0.32
(1,3724)	1:190:B:LEU:HA	1:216:B:LYS:H	12	0.32
(1,3683)	1:183:B:GLN:HA	1:185:B:LYS:H	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3671)	1:181:B:TYR:HE1	1:218:B:LYS:HB2	8	0.32
(1,3671)	1:181:B:TYR:HE1	1:218:B:LYS:HB3	8	0.32
(1,3671)	1:181:B:TYR:HE2	1:218:B:LYS:HB2	8	0.32
(1,3671)	1:181:B:TYR:HE2	1:218:B:LYS:HB3	8	0.32
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB1	3	0.32
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB2	3	0.32
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB3	3	0.32
(1,3593)	1:175:B:ARG:HA	1:178:B:PHE:H	6	0.32
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	5	0.32
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	7	0.32
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	7	0.32
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	17	0.32
(1,3420)	1:158:B:ASP:HA	1:162:B:ALA:H	9	0.32
(1,3337)	1:150:B:LYS:HB2	1:152:B:TYR:HD1	8	0.32
(1,3337)	1:150:B:LYS:HB2	1:152:B:TYR:HD2	8	0.32
(1,3337)	1:150:B:LYS:HB3	1:152:B:TYR:HD1	8	0.32
(1,3337)	1:150:B:LYS:HB3	1:152:B:TYR:HD2	8	0.32
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	6	0.32
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	1	0.32
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	11	0.32
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	11	0.32
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	11	0.32
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	11	0.32
(1,3068)	1:125:B:TYR:HA	1:138:B:TYR:HA	10	0.32
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	13	0.32
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	13	0.32
(1,2995)	1:118:B:TYR:HA	1:145:B:ALA:HA	17	0.32
(1,2979)	1:117:B:ASP:H	1:118:B:TYR:H	10	0.32
(1,2820)	1:103:B:GLU:H	1:106:B:LYS:H	11	0.32
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	17	0.32
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	17	0.32
(1,2789)	1:101:B:LYS:H	1:103:B:GLU:H	4	0.32
(1,2750)	1:95:B:ASP:HA	1:97:B:GLU:H	9	0.32
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	5	0.32
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	5	0.32
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	5	0.32
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	6	0.32
(1,2669)	1:218:A:LYS:H	1:221:A:GLN:H	4	0.32
(1,2669)	1:218:A:LYS:H	1:221:A:GLN:H	6	0.32
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	10	0.32
(1,2423)	1:190:A:LEU:HD21	1:216:A:LYS:HA	6	0.32
(1,2423)	1:190:A:LEU:HD22	1:216:A:LYS:HA	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2423)	1:190:A:LEU:HD23	1:216:A:LYS:HA	6	0.32
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	4	0.32
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	4	0.32
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	4	0.32
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	4	0.32
(1,2279)	1:174:A:SER:HA	1:193:A:TYR:HA	8	0.32
(1,2277)	1:174:A:SER:HA	1:177:A:GLY:H	18	0.32
(1,2273)	1:174:A:SER:H	1:196:A:VAL:HG21	12	0.32
(1,2273)	1:174:A:SER:H	1:196:A:VAL:HG22	12	0.32
(1,2273)	1:174:A:SER:H	1:196:A:VAL:HG23	12	0.32
(1,2206)	1:169:A:TYR:HE2	1:171:A:ARG:HB2	8	0.32
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	5	0.32
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	13	0.32
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	13	0.32
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	17	0.32
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	17	0.32
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	10	0.32
(1,1998)	1:147:A:SER:H	1:155:A:ALA:HA	5	0.32
(1,1985)	1:146:A:HIS:H	1:155:A:ALA:HA	8	0.32
(1,1882)	1:137:A:ILE:HA	1:141:A:ASN:H	3	0.32
(1,1862)	1:136:A:ALA:HA	1:162:A:ALA:HA	7	0.32
(1,1767)	1:125:A:TYR:HB2	1:139:A:TYR:H	4	0.32
(1,1767)	1:125:A:TYR:HB3	1:139:A:TYR:H	4	0.32
(1,1594)	1:110:A:ASN:HA	1:113:A:MET:HE1	10	0.32
(1,1594)	1:110:A:ASN:HA	1:113:A:MET:HE2	10	0.32
(1,1594)	1:110:A:ASN:HA	1:113:A:MET:HE3	10	0.32
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	7	0.32
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	11	0.32
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	20	0.32
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	20	0.32
(1,1374)	1:43:A:ALA:HA	1:32:B:SER:H	6	0.32
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	10	0.32
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	2	0.32
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	2	0.32
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB2	12	0.32
(1,1302)	1:19:A:ILE:HD11	1:5:B:LYS:HB3	12	0.32
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB2	12	0.32
(1,1302)	1:19:A:ILE:HD12	1:5:B:LYS:HB3	12	0.32
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB2	12	0.32
(1,1302)	1:19:A:ILE:HD13	1:5:B:LYS:HB3	12	0.32
(1,1290)	1:16:A:PHE:HE1	1:12:B:ILE:HD13	10	0.32
(1,1290)	1:16:A:PHE:HE2	1:12:B:ILE:HD13	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:16:A:PHE:HA	1:44:B:PHE:HZ	9	0.32
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	18	0.32
(1,992)	1:40:B:ILE:H	1:42:B:GLU:H	20	0.32
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	16	0.32
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	10	0.32
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	12	0.32
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	15	0.32
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	15	0.32
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	15	0.32
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB1	12	0.32
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB2	12	0.32
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB3	12	0.32
(1,379)	1:39:A:CYS:HA	1:42:A:GLU:H	8	0.32
(1,336)	1:34:A:ASN:HA	1:38:A:ASP:H	5	0.32
(1,218)	1:19:A:ILE:HA	1:22:A:LYS:H	10	0.32
(1,174)	1:16:A:PHE:HA	1:19:A:ILE:HA	9	0.32
(1,4208)	1:345:B:LYS:H	1:346:B:GLN:H	6	0.31
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	6	0.31
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	6	0.31
(1,4167)	1:294:B:SER:H	1:295:B:ILE:H	16	0.31
(1,4042)	1:232:A:GLN:H	1:233:A:SER:H	10	0.31
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	5	0.31
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	9	0.31
(1,3912)	1:210:B:ARG:HA	1:213:B:GLU:H	9	0.31
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	15	0.31
(1,3879)	1:206:B:GLU:HB2	1:207:B:ALA:H	15	0.31
(1,3879)	1:206:B:GLU:HB3	1:207:B:ALA:H	15	0.31
(1,3816)	1:197:B:LEU:HD21	1:209:B:LYS:HA	3	0.31
(1,3816)	1:197:B:LEU:HD22	1:209:B:LYS:HA	3	0.31
(1,3816)	1:197:B:LEU:HD23	1:209:B:LYS:HA	3	0.31
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	9	0.31
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	4	0.31
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	4	0.31
(1,3724)	1:190:B:LEU:HA	1:216:B:LYS:H	9	0.31
(1,3646)	1:180:B:LYS:HA	1:185:B:LYS:H	9	0.31
(1,3646)	1:180:B:LYS:HA	1:185:B:LYS:H	14	0.31
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB1	2	0.31
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB2	2	0.31
(1,3607)	1:177:B:GLY:H	1:192:B:ALA:HB3	2	0.31
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB1	10	0.31
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB2	10	0.31
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB3	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3355)	1:152:B:TYR:HA	1:155:B:ALA:HA	14	0.31
(1,3354)	1:152:B:TYR:HA	1:155:B:ALA:H	8	0.31
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	7	0.31
(1,3335)	1:150:B:LYS:HA	1:152:B:TYR:HA	20	0.31
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	11	0.31
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	13	0.31
(1,3252)	1:143:B:ALA:H	1:155:B:ALA:HA	12	0.31
(1,3167)	1:136:B:ALA:HA	1:138:B:TYR:H	6	0.31
(1,3135)	1:130:B:LYS:HA	1:132:B:LEU:H	3	0.31
(1,3094)	1:127:B:GLU:H	1:130:B:LYS:H	8	0.31
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB2	5	0.31
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB3	5	0.31
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB2	5	0.31
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB3	5	0.31
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB2	1	0.31
(1,3069)	1:125:B:TYR:HA	1:138:B:TYR:HB3	1	0.31
(1,3068)	1:125:B:TYR:HA	1:138:B:TYR:HA	11	0.31
(1,2940)	1:113:B:MET:HA	1:117:B:ASP:H	9	0.31
(1,2907)	1:111:B:LYS:H	1:114:B:ALA:H	12	0.31
(1,2890)	1:109:B:GLY:HA2	1:112:B:ALA:H	13	0.31
(1,2890)	1:109:B:GLY:HA3	1:112:B:ALA:H	13	0.31
(1,2850)	1:105:B:LEU:HD21	1:124:B:LYS:HA	8	0.31
(1,2850)	1:105:B:LEU:HD22	1:124:B:LYS:HA	8	0.31
(1,2850)	1:105:B:LEU:HD23	1:124:B:LYS:HA	8	0.31
(1,2837)	1:105:B:LEU:H	1:108:B:GLN:H	7	0.31
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG11	17	0.31
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG12	17	0.31
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG13	17	0.31
(1,2798)	1:102:B:ALA:H	1:103:B:GLU:H	4	0.31
(1,2768)	1:98:B:THR:H	1:100:B:ALA:H	19	0.31
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB2	15	0.31
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB3	15	0.31
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	7	0.31
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD11	18	0.31
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD12	18	0.31
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD13	18	0.31
(1,2645)	1:215:A:ALA:H	1:218:A:LYS:H	18	0.31
(1,2632)	1:213:A:GLU:HA	1:216:A:LYS:H	8	0.31
(1,2632)	1:213:A:GLU:HA	1:216:A:LYS:H	15	0.31
(1,2579)	1:207:A:ALA:HA	1:209:A:LYS:H	8	0.31
(1,2502)	1:197:A:LEU:HA	1:200:A:GLU:H	12	0.31
(1,2485)	1:195:A:LYS:HA	1:199:A:ILE:H	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2463)	1:193:A:TYR:HE2	1:211:A:ASP:HA	7	0.31
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	4	0.31
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	4	0.31
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	4	0.31
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	4	0.31
(1,2264)	1:173:A:TYR:HB2	1:195:A:LYS:HB2	6	0.31
(1,2264)	1:173:A:TYR:HB2	1:195:A:LYS:HB3	6	0.31
(1,2264)	1:173:A:TYR:HB3	1:195:A:LYS:HB2	6	0.31
(1,2264)	1:173:A:TYR:HB3	1:195:A:LYS:HB3	6	0.31
(1,2245)	1:171:A:ARG:HA	1:175:A:ARG:H	18	0.31
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	1	0.31
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	4	0.31
(1,2029)	1:150:A:LYS:HA	1:152:A:TYR:HA	2	0.31
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	11	0.31
(1,1490)	1:101:A:LYS:HA	1:104:A:ASP:H	5	0.31
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	15	0.31
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	15	0.31
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE21	8	0.31
(1,1420)	1:68:A:ILE:HA	1:63:B:GLN:HE22	8	0.31
(1,1418)	1:68:A:ILE:HG21	1:2:B:SER:HA	8	0.31
(1,1418)	1:68:A:ILE:HG22	1:2:B:SER:HA	8	0.31
(1,1418)	1:68:A:ILE:HG23	1:2:B:SER:HA	8	0.31
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	20	0.31
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	20	0.31
(1,1405)	1:63:A:GLN:H	1:67:B:ASP:HB2	3	0.31
(1,1405)	1:63:A:GLN:H	1:67:B:ASP:HB3	3	0.31
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	10	0.31
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	10	0.31
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	10	0.31
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	10	0.31
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	16	0.31
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	16	0.31
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	16	0.31
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	16	0.31
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD11	6	0.31
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD12	6	0.31
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD13	6	0.31
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG21	17	0.31
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG22	17	0.31
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG23	17	0.31
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	1	0.31
(1,1178)	1:65:B:LEU:HA	1:66:B:ALA:HA	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	1	0.31
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	5	0.31
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	15	0.31
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	15	0.31
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD11	19	0.31
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD12	19	0.31
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD13	19	0.31
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	14	0.31
(1,669)	1:9:B:ALA:HA	1:13:B:VAL:H	10	0.31
(1,659)	1:8:B:ILE:HD11	1:60:B:PHE:HE1	19	0.31
(1,659)	1:8:B:ILE:HD11	1:60:B:PHE:HE2	19	0.31
(1,659)	1:8:B:ILE:HD12	1:60:B:PHE:HE1	19	0.31
(1,659)	1:8:B:ILE:HD12	1:60:B:PHE:HE2	19	0.31
(1,659)	1:8:B:ILE:HD13	1:60:B:PHE:HE1	19	0.31
(1,659)	1:8:B:ILE:HD13	1:60:B:PHE:HE2	19	0.31
(1,642)	1:6:B:GLU:HA	1:10:B:ALA:H	10	0.31
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	9	0.31
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	11	0.31
(1,379)	1:39:A:CYS:HA	1:42:A:GLU:H	2	0.31
(1,375)	1:39:A:CYS:H	1:42:A:GLU:H	2	0.31
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	19	0.31
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	19	0.31
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB2	3	0.31
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB3	3	0.31
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	1	0.31
(1,92)	1:11:A:LEU:HA	1:55:A:LEU:HD11	3	0.31
(1,92)	1:11:A:LEU:HA	1:55:A:LEU:HD12	3	0.31
(1,92)	1:11:A:LEU:HA	1:55:A:LEU:HD13	3	0.31
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB1	14	0.3
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB2	14	0.3
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB3	14	0.3
(1,4202)	1:337:B:ASP:H	1:338:B:GLU:H	11	0.3
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	12	0.3
(1,4143)	1:235:B:ASP:H	1:236:B:ALA:H	17	0.3
(1,4138)	1:228:B:THR:H	1:229:B:VAL:H	14	0.3
(1,4110)	1:345:A:LYS:H	1:346:A:GLN:H	4	0.3
(1,4092)	1:325:A:GLY:H	1:326:A:ASN:H	14	0.3
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	1	0.3
(1,4000)	1:221:B:GLN:H	1:224:B:ASN:H	17	0.3
(1,3822)	1:198:B:ASP:HA	1:200:B:GLU:H	11	0.3
(1,3807)	1:197:B:LEU:HA	1:199:B:ILE:H	8	0.3
(1,3757)	1:193:B:TYR:HA	1:212:B:TYR:HA	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3686)	1:185:B:LYS:H	1:186:B:PRO:HA	10	0.3
(1,3677)	1:182:B:ALA:HA	1:184:B:GLY:H	11	0.3
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB1	9	0.3
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB2	9	0.3
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB3	9	0.3
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	12	0.3
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	17	0.3
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	17	0.3
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	19	0.3
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	19	0.3
(1,3367)	1:152:B:TYR:HD1	1:183:B:GLN:HG3	19	0.3
(1,3303)	1:147:B:SER:H	1:151:B:GLU:H	8	0.3
(1,3291)	1:146:B:HIS:H	1:155:B:ALA:HA	2	0.3
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	9	0.3
(1,2984)	1:117:B:ASP:HA	1:120:B:LEU:H	10	0.3
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	1	0.3
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	1	0.3
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	19	0.3
(1,2940)	1:113:B:MET:HA	1:117:B:ASP:H	2	0.3
(1,2934)	1:113:B:MET:H	1:121:B:ALA:HB1	2	0.3
(1,2934)	1:113:B:MET:H	1:121:B:ALA:HB2	2	0.3
(1,2934)	1:113:B:MET:H	1:121:B:ALA:HB3	2	0.3
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB2	8	0.3
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB3	8	0.3
(1,2773)	1:98:B:THR:HA	1:101:B:LYS:H	12	0.3
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	16	0.3
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	18	0.3
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB1	16	0.3
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB2	16	0.3
(1,2740)	1:93:B:GLU:HA	1:96:B:ALA:HB3	16	0.3
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	13	0.3
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	13	0.3
(1,2721)	1:225:A:LEU:H	1:226:A:GLU:H	5	0.3
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	4	0.3
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	9	0.3
(1,2583)	1:207:A:ALA:HA	1:211:A:ASP:H	20	0.3
(1,2343)	1:180:A:LYS:HB2	1:188:A:GLU:H	14	0.3
(1,2343)	1:180:A:LYS:HB3	1:188:A:GLU:H	14	0.3
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE1	7	0.3
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE2	7	0.3
(1,2252)	1:173:A:TYR:H	1:175:A:ARG:H	1	0.3
(1,2230)	1:170:A:PHE:HE1	1:171:A:ARG:H	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2230)	1:170:A:PHE:HE2	1:171:A:ARG:H	6	0.3
(1,2216)	1:170:A:PHE:HA	1:196:A:VAL:HA	12	0.3
(1,2175)	1:164:A:SER:HA	1:166:A:ASP:H	13	0.3
(1,2029)	1:150:A:LYS:HA	1:152:A:TYR:HA	17	0.3
(1,2010)	1:147:A:SER:HB2	1:178:A:PHE:HB2	3	0.3
(1,2010)	1:147:A:SER:HB2	1:178:A:PHE:HB3	3	0.3
(1,2010)	1:147:A:SER:HB3	1:178:A:PHE:HB2	3	0.3
(1,2010)	1:147:A:SER:HB3	1:178:A:PHE:HB3	3	0.3
(1,2007)	1:147:A:SER:HA	1:152:A:TYR:HA	4	0.3
(1,1890)	1:138:A:TYR:HA	1:142:A:ARG:H	14	0.3
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD11	7	0.3
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD12	7	0.3
(1,1845)	1:134:A:THR:HA	1:165:A:ILE:HD13	7	0.3
(1,1752)	1:124:A:LYS:HA	1:127:A:GLU:H	1	0.3
(1,1491)	1:101:A:LYS:HA	1:105:A:LEU:H	13	0.3
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	14	0.3
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	5	0.3
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	16	0.3
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	4	0.3
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	13	0.3
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	16	0.3
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	8	0.3
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	8	0.3
(1,1350)	1:39:A:CYS:HB2	1:32:B:SER:HA	12	0.3
(1,1350)	1:39:A:CYS:HB3	1:32:B:SER:HA	12	0.3
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	17	0.3
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	10	0.3
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	10	0.3
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	1	0.3
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	4	0.3
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE1	4	0.3
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE2	4	0.3
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	15	0.3
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	7	0.3
(1,1180)	1:65:B:LEU:HA	1:71:B:SER:H	11	0.3
(1,896)	1:29:B:GLY:H	1:32:B:SER:H	2	0.3
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	20	0.3
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	20	0.3
(1,599)	1:70:A:ASN:H	1:71:A:SER:H	18	0.3
(1,578)	1:66:A:ALA:HA	1:68:A:ILE:H	18	0.3
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	10	0.3
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	11	0.3
(1,458)	1:48:A:ARG:HA	1:50:A:ALA:H	2	0.3
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	3	0.3
(1,310)	1:31:A:ASP:HA	1:35:A:VAL:H	9	0.3
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	11	0.3
(1,173)	1:16:A:PHE:HA	1:19:A:ILE:H	15	0.3
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	16	0.3
(1,14)	1:4:A:SER:H	1:7:A:GLU:H	2	0.3
(1,4196)	1:331:B:ALA:H	1:332:B:GLY:H	6	0.29
(1,4163)	1:257:B:GLY:H	1:258:B:GLY:H	8	0.29
(1,4160)	1:254:B:SER:H	1:255:B:LEU:H	5	0.29
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	19	0.29
(1,4108)	1:343:A:GLU:H	1:344:A:ASN:H	8	0.29
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	11	0.29
(1,4052)	1:242:A:GLN:H	1:243:A:GLY:H	14	0.29
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	9	0.29
(1,4006)	1:221:B:GLN:HB2	1:222:B:SER:HA	9	0.29
(1,4006)	1:221:B:GLN:HB3	1:222:B:SER:HA	9	0.29
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	12	0.29
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	12	0.29
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	16	0.29
(1,3921)	1:211:B:ASP:HA	1:215:B:ALA:H	8	0.29
(1,3894)	1:208:B:MET:H	1:211:B:ASP:H	13	0.29
(1,3810)	1:197:B:LEU:HA	1:204:B:ALA:HA	7	0.29
(1,3721)	1:190:B:LEU:HA	1:194:B:LYS:H	3	0.29
(1,3704)	1:188:B:GLU:HA	1:191:B:GLU:H	1	0.29
(1,3686)	1:185:B:LYS:H	1:186:B:PRO:HA	11	0.29
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	11	0.29
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	11	0.29
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	11	0.29
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	11	0.29
(1,3574)	1:173:B:TYR:HD1	1:199:B:ILE:HD11	19	0.29
(1,3574)	1:173:B:TYR:HD1	1:199:B:ILE:HD12	19	0.29
(1,3574)	1:173:B:TYR:HD1	1:199:B:ILE:HD13	19	0.29
(1,3574)	1:173:B:TYR:HD2	1:199:B:ILE:HD11	19	0.29
(1,3574)	1:173:B:TYR:HD2	1:199:B:ILE:HD12	19	0.29
(1,3574)	1:173:B:TYR:HD2	1:199:B:ILE:HD13	19	0.29
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE1	3	0.29
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE2	3	0.29
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE3	3	0.29
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE1	3	0.29
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE2	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE3	3	0.29
(1,3533)	1:170:B:PHE:HD1	1:196:B:VAL:HA	9	0.29
(1,3533)	1:170:B:PHE:HD2	1:196:B:VAL:HA	9	0.29
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG2	11	0.29
(1,3525)	1:170:B:PHE:HA	1:200:B:GLU:HG3	11	0.29
(1,3511)	1:169:B:TYR:HD2	1:171:B:ARG:H	11	0.29
(1,3256)	1:143:B:ALA:HA	1:155:B:ALA:H	9	0.29
(1,3203)	1:139:B:TYR:HA	1:141:B:ASN:H	8	0.29
(1,3130)	1:129:B:ILE:HD11	1:142:B:ARG:HB2	13	0.29
(1,3130)	1:129:B:ILE:HD11	1:142:B:ARG:HB3	13	0.29
(1,3130)	1:129:B:ILE:HD12	1:142:B:ARG:HB2	13	0.29
(1,3130)	1:129:B:ILE:HD12	1:142:B:ARG:HB3	13	0.29
(1,3130)	1:129:B:ILE:HD13	1:142:B:ARG:HB2	13	0.29
(1,3130)	1:129:B:ILE:HD13	1:142:B:ARG:HB3	13	0.29
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	13	0.29
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	15	0.29
(1,3080)	1:125:B:TYR:HE1	1:141:B:ASN:HB3	15	0.29
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB2	15	0.29
(1,3080)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	15	0.29
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB2	2	0.29
(1,3076)	1:125:B:TYR:HB2	1:142:B:ARG:HB3	2	0.29
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB2	2	0.29
(1,3076)	1:125:B:TYR:HB3	1:142:B:ARG:HB3	2	0.29
(1,3074)	1:125:B:TYR:HB2	1:142:B:ARG:H	1	0.29
(1,3074)	1:125:B:TYR:HB3	1:142:B:ARG:H	1	0.29
(1,3074)	1:125:B:TYR:HB2	1:142:B:ARG:H	15	0.29
(1,3074)	1:125:B:TYR:HB3	1:142:B:ARG:H	15	0.29
(1,3048)	1:123:B:ASN:H	1:126:B:THR:H	18	0.29
(1,2894)	1:110:B:ASN:H	1:113:B:MET:H	12	0.29
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	10	0.29
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB2	15	0.29
(1,2791)	1:101:B:LYS:HA	1:105:B:LEU:HB3	15	0.29
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	3	0.29
(1,2739)	1:93:B:GLU:HA	1:96:B:ALA:HA	16	0.29
(1,2738)	1:93:B:GLU:HA	1:96:B:ALA:H	3	0.29
(1,2675)	1:218:A:LYS:HB2	1:219:A:VAL:H	8	0.29
(1,2675)	1:218:A:LYS:HB3	1:219:A:VAL:H	8	0.29
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	8	0.29
(1,2660)	1:217:A:LYS:H	1:220:A:GLU:H	3	0.29
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	17	0.29
(1,2573)	1:206:A:GLU:HB2	1:207:A:ALA:H	12	0.29
(1,2573)	1:206:A:GLU:HB3	1:207:A:ALA:H	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2475)	1:194:A:LYS:HA	1:198:A:ASP:H	13	0.29
(1,2464)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	14	0.29
(1,2447)	1:193:A:TYR:HA	1:196:A:VAL:H	15	0.29
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD21	3	0.29
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD22	3	0.29
(1,2391)	1:187:A:GLU:HA	1:190:A:LEU:HD23	3	0.29
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	16	0.29
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	16	0.29
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	16	0.29
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	16	0.29
(1,2138)	1:160:A:GLU:HA	1:164:A:SER:H	4	0.29
(1,2136)	1:160:A:GLU:HA	1:163:A:ILE:H	12	0.29
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	17	0.29
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE1	10	0.29
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE2	10	0.29
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE1	10	0.29
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE2	10	0.29
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE2	20	0.29
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	6	0.29
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	6	0.29
(1,1576)	1:109:A:GLY:H	1:121:A:ALA:HA	3	0.29
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE1	13	0.29
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE2	13	0.29
(1,1528)	1:104:A:ASP:HA	1:107:A:MET:HE3	13	0.29
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	6	0.29
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	18	0.29
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	18	0.29
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	1	0.29
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	1	0.29
(1,1349)	1:39:A:CYS:HA	1:32:B:SER:HA	11	0.29
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	4	0.29
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	4	0.29
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	4	0.29
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	4	0.29
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	7	0.29
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	7	0.29
(1,1266)	1:15:A:TYR:HE1	1:5:B:LYS:H	2	0.29
(1,1266)	1:15:A:TYR:HE2	1:5:B:LYS:H	2	0.29
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE1	17	0.29
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE2	17	0.29
(1,1191)	1:67:B:ASP:H	1:68:B:ILE:H	6	0.29
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	13	0.29
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	13	0.29
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	13	0.29
(1,1178)	1:65:B:LEU:HA	1:66:B:ALA:HA	19	0.29
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	8	0.29
(1,1060)	1:47:B:GLU:HB2	1:48:B:ARG:H	2	0.29
(1,1060)	1:47:B:GLU:HB3	1:48:B:ARG:H	2	0.29
(1,934)	1:33:B:LEU:HA	1:37:B:MET:H	18	0.29
(1,885)	1:27:B:GLU:HA	1:30:B:ALA:HA	11	0.29
(1,876)	1:26:B:SER:HA	1:28:B:ASP:H	11	0.29
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD11	10	0.29
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD12	10	0.29
(1,688)	1:10:B:ALA:HA	1:54:B:ILE:HD13	10	0.29
(1,658)	1:8:B:ILE:HA	1:12:B:ILE:H	17	0.29
(1,645)	1:7:B:GLU:H	1:10:B:ALA:H	17	0.29
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	8	0.29
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	19	0.29
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	10	0.29
(1,339)	1:35:A:VAL:H	1:38:A:ASP:H	3	0.29
(1,339)	1:35:A:VAL:H	1:38:A:ASP:H	19	0.29
(1,248)	1:23:A:LYS:H	1:25:A:ILE:H	10	0.29
(1,224)	1:20:A:VAL:HA	1:23:A:LYS:H	14	0.29
(1,149)	1:15:A:TYR:H	1:18:A:SER:H	10	0.29
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	7	0.29
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	9	0.28
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	11	0.28
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	17	0.28
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	1	0.28
(1,4146)	1:238:B:VAL:H	1:239:B:ASP:H	6	0.28
(1,4092)	1:325:A:GLY:H	1:326:A:ASN:H	11	0.28
(1,4071)	1:300:A:GLU:H	1:301:A:GLY:H	10	0.28
(1,4068)	1:260:A:LEU:H	1:261:A:GLY:H	16	0.28
(1,4050)	1:240:A:ALA:H	1:241:A:SER:H	2	0.28
(1,4048)	1:238:A:VAL:H	1:239:A:ASP:H	10	0.28
(1,4039)	1:227:B:LYS:HB2	1:228:B:THR:HA	9	0.28
(1,4039)	1:227:B:LYS:HB3	1:228:B:THR:HA	9	0.28
(1,4037)	1:227:B:LYS:HA	1:228:B:THR:HA	9	0.28
(1,3898)	1:208:B:MET:HA	1:211:B:ASP:H	18	0.28
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	5	0.28
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	5	0.28
(1,3825)	1:199:B:ILE:H	1:201:B:GLY:H	10	0.28
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3800)	1:196:B:VAL:HG11	1:208:B:MET:HA	11	0.28
(1,3800)	1:196:B:VAL:HG12	1:208:B:MET:HA	11	0.28
(1,3800)	1:196:B:VAL:HG13	1:208:B:MET:HA	11	0.28
(1,3749)	1:193:B:TYR:H	1:212:B:TYR:HA	8	0.28
(1,3729)	1:190:B:LEU:HD21	1:216:B:LYS:HA	3	0.28
(1,3729)	1:190:B:LEU:HD22	1:216:B:LYS:HA	3	0.28
(1,3729)	1:190:B:LEU:HD23	1:216:B:LYS:HA	3	0.28
(1,3646)	1:180:B:LYS:HA	1:185:B:LYS:H	16	0.28
(1,3626)	1:178:B:PHE:HA	1:182:B:ALA:H	3	0.28
(1,3593)	1:175:B:ARG:HA	1:178:B:PHE:H	5	0.28
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG21	1	0.28
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG22	1	0.28
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG23	1	0.28
(1,3509)	1:169:B:TYR:HE1	1:172:B:GLY:H	15	0.28
(1,3509)	1:169:B:TYR:HE2	1:172:B:GLY:H	15	0.28
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD11	16	0.28
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD12	16	0.28
(1,3438)	1:160:B:GLU:H	1:176:B:LEU:HD13	16	0.28
(1,3420)	1:158:B:ASP:HA	1:162:B:ALA:H	13	0.28
(1,3411)	1:157:B:LYS:HA	1:160:B:GLU:H	1	0.28
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG3	1	0.28
(1,3343)	1:150:B:LYS:HZ1	1:152:B:TYR:HE1	6	0.28
(1,3343)	1:150:B:LYS:HZ1	1:152:B:TYR:HE2	6	0.28
(1,3343)	1:150:B:LYS:HZ2	1:152:B:TYR:HE1	6	0.28
(1,3343)	1:150:B:LYS:HZ2	1:152:B:TYR:HE2	6	0.28
(1,3343)	1:150:B:LYS:HZ3	1:152:B:TYR:HE1	6	0.28
(1,3343)	1:150:B:LYS:HZ3	1:152:B:TYR:HE2	6	0.28
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	9	0.28
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	9	0.28
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE1	9	0.28
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE2	9	0.28
(1,3335)	1:150:B:LYS:HA	1:152:B:TYR:HA	4	0.28
(1,3248)	1:142:B:ARG:HA	1:145:B:ALA:H	6	0.28
(1,3041)	1:122:B:ILE:HA	1:126:B:THR:H	13	0.28
(1,2991)	1:118:B:TYR:HA	1:120:B:LEU:H	7	0.28
(1,2980)	1:117:B:ASP:H	1:118:B:TYR:HA	15	0.28
(1,2979)	1:117:B:ASP:H	1:118:B:TYR:H	7	0.28
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB2	9	0.28
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB3	9	0.28
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	8	0.28
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	8	0.28
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	14	0.28
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	14	0.28
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	14	0.28
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	11	0.28
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	20	0.28
(1,2645)	1:215:A:ALA:H	1:218:A:LYS:H	4	0.28
(1,2628)	1:213:A:GLU:H	1:216:A:LYS:H	3	0.28
(1,2502)	1:197:A:LEU:HA	1:200:A:GLU:H	4	0.28
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	14	0.28
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	14	0.28
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	14	0.28
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	14	0.28
(1,2358)	1:181:A:TYR:HA	1:186:A:PRO:HA	11	0.28
(1,2245)	1:171:A:ARG:HA	1:175:A:ARG:H	19	0.28
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	14	0.28
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	14	0.28
(1,1951)	1:143:A:ALA:HA	1:155:A:ALA:HA	17	0.28
(1,1852)	1:135:A:ASN:HA	1:138:A:TYR:H	14	0.28
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB2	8	0.28
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB3	8	0.28
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB2	8	0.28
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB3	8	0.28
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB2	8	0.28
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB3	8	0.28
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	10	0.28
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	10	0.28
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD1	10	0.28
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD2	10	0.28
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD1	10	0.28
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD2	10	0.28
(1,1645)	1:113:A:MET:HE1	1:145:A:ALA:H	5	0.28
(1,1645)	1:113:A:MET:HE2	1:145:A:ALA:H	5	0.28
(1,1645)	1:113:A:MET:HE3	1:145:A:ALA:H	5	0.28
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB2	5	0.28
(1,1485)	1:101:A:LYS:HA	1:105:A:LEU:HB3	5	0.28
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB2	18	0.28
(1,1423)	1:69:A:LEU:H	1:2:B:SER:HB3	18	0.28
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	15	0.28
(1,1393)	1:44:A:PHE:HE1	1:25:B:ILE:HD11	11	0.28
(1,1393)	1:44:A:PHE:HE2	1:25:B:ILE:HD11	11	0.28
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	16	0.28
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	13	0.28
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	13	0.28
(1,1283)	1:16:A:PHE:HE1	1:12:B:ILE:HB	9	0.28
(1,1283)	1:16:A:PHE:HE2	1:12:B:ILE:HB	9	0.28
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	17	0.28
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	17	0.28
(1,1248)	1:9:A:ALA:H	1:16:B:PHE:HZ	20	0.28
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE1	6	0.28
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE2	6	0.28
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	2	0.28
(1,1164)	1:62:B:GLY:H	1:63:B:GLN:HA	4	0.28
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	2	0.28
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	2	0.28
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	7	0.28
(1,1145)	1:60:B:PHE:HA	1:62:B:GLY:H	16	0.28
(1,1009)	1:41:B:SER:HA	1:44:B:PHE:H	2	0.28
(1,1009)	1:41:B:SER:HA	1:44:B:PHE:H	9	0.28
(1,854)	1:22:B:LYS:HA	1:24:B:GLU:H	17	0.28
(1,827)	1:19:B:ILE:HA	1:22:B:LYS:H	10	0.28
(1,624)	1:4:B:SER:H	1:8:B:ILE:H	15	0.28
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	6	0.28
(1,578)	1:66:A:ALA:HA	1:68:A:ILE:H	15	0.28
(1,491)	1:54:A:ILE:H	1:57:A:LYS:H	11	0.28
(1,291)	1:29:A:GLY:HA2	1:32:A:SER:H	5	0.28
(1,291)	1:29:A:GLY:HA3	1:32:A:SER:H	5	0.28
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	4	0.28
(1,4207)	1:344:B:ASN:H	1:345:B:LYS:H	2	0.27
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	13	0.27
(1,4162)	1:256:B:LEU:H	1:257:B:GLY:H	10	0.27
(1,4147)	1:239:B:ASP:H	1:240:B:ALA:H	8	0.27
(1,4091)	1:324:A:ALA:H	1:325:A:GLY:H	16	0.27
(1,4089)	1:322:A:ASN:H	1:323:A:MET:H	13	0.27
(1,4088)	1:321:A:ARG:H	1:322:A:ASN:H	15	0.27
(1,4072)	1:301:A:GLY:H	1:302:A:PHE:H	3	0.27
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	4	0.27
(1,3948)	1:214:B:SER:HB2	1:215:B:ALA:H	16	0.27
(1,3948)	1:214:B:SER:HB3	1:215:B:ALA:H	16	0.27
(1,3913)	1:210:B:ARG:HA	1:214:B:SER:H	5	0.27
(1,3858)	1:205:B:THR:H	1:208:B:MET:H	17	0.27
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	14	0.27
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	14	0.27
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	4	0.27
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB2	4	0.27
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	4	0.27
(1,3748)	1:193:B:TYR:H	1:196:B:VAL:H	4	0.27
(1,3729)	1:190:B:LEU:HD21	1:216:B:LYS:HA	14	0.27
(1,3729)	1:190:B:LEU:HD22	1:216:B:LYS:HA	14	0.27
(1,3729)	1:190:B:LEU:HD23	1:216:B:LYS:HA	14	0.27
(1,3727)	1:190:B:LEU:HD11	1:216:B:LYS:H	6	0.27
(1,3727)	1:190:B:LEU:HD12	1:216:B:LYS:H	6	0.27
(1,3727)	1:190:B:LEU:HD13	1:216:B:LYS:H	6	0.27
(1,3689)	1:185:B:LYS:HA	1:188:B:GLU:H	14	0.27
(1,3627)	1:178:B:PHE:HA	1:193:B:TYR:HE1	11	0.27
(1,3627)	1:178:B:PHE:HA	1:193:B:TYR:HE2	11	0.27
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	15	0.27
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	15	0.27
(1,3551)	1:171:B:ARG:HA	1:175:B:ARG:H	2	0.27
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG21	10	0.27
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG22	10	0.27
(1,3523)	1:170:B:PHE:HA	1:196:B:VAL:HG23	10	0.27
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	5	0.27
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	5	0.27
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	9	0.27
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	9	0.27
(1,3159)	1:135:B:ASN:HB2	1:138:B:TYR:H	20	0.27
(1,3159)	1:135:B:ASN:HB3	1:138:B:TYR:H	20	0.27
(1,3082)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	7	0.27
(1,3074)	1:125:B:TYR:HB2	1:142:B:ARG:H	9	0.27
(1,3074)	1:125:B:TYR:HB3	1:142:B:ARG:H	9	0.27
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	14	0.27
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	14	0.27
(1,3058)	1:124:B:LYS:HA	1:127:B:GLU:H	14	0.27
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE1	7	0.27
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE2	7	0.27
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	7	0.27
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	7	0.27
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	7	0.27
(1,2949)	1:113:B:MET:HE1	1:144:B:ALA:H	18	0.27
(1,2949)	1:113:B:MET:HE2	1:144:B:ALA:H	18	0.27
(1,2949)	1:113:B:MET:HE3	1:144:B:ALA:H	18	0.27
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	1	0.27
(1,2836)	1:105:B:LEU:H	1:107:B:MET:H	19	0.27
(1,2824)	1:103:B:GLU:HA	1:106:B:LYS:H	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	11	0.27
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	2	0.27
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	2	0.27
(1,2686)	1:220:A:GLU:H	1:222:A:SER:H	19	0.27
(1,2666)	1:217:A:LYS:HG2	1:218:A:LYS:H	19	0.27
(1,2666)	1:217:A:LYS:HG3	1:218:A:LYS:H	19	0.27
(1,2645)	1:215:A:ALA:H	1:218:A:LYS:H	1	0.27
(1,2640)	1:214:A:SER:HA	1:217:A:LYS:H	1	0.27
(1,2640)	1:214:A:SER:HA	1:217:A:LYS:H	3	0.27
(1,2570)	1:206:A:GLU:HA	1:209:A:LYS:H	18	0.27
(1,2558)	1:205:A:THR:HA	1:207:A:ALA:H	18	0.27
(1,2502)	1:197:A:LEU:HA	1:200:A:GLU:H	18	0.27
(1,2485)	1:195:A:LYS:HA	1:199:A:ILE:H	3	0.27
(1,2289)	1:176:A:LEU:H	1:178:A:PHE:H	16	0.27
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	4	0.27
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	4	0.27
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	7	0.27
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	7	0.27
(1,2114)	1:158:A:ASP:HA	1:162:A:ALA:H	2	0.27
(1,2075)	1:154:A:GLN:HA	1:157:A:LYS:H	11	0.27
(1,2051)	1:152:A:TYR:HA	1:156:A:VAL:H	5	0.27
(1,2031)	1:150:A:LYS:HB2	1:152:A:TYR:HD1	2	0.27
(1,2031)	1:150:A:LYS:HB2	1:152:A:TYR:HD2	2	0.27
(1,2031)	1:150:A:LYS:HB3	1:152:A:TYR:HD1	2	0.27
(1,2031)	1:150:A:LYS:HB3	1:152:A:TYR:HD2	2	0.27
(1,2009)	1:147:A:SER:HA	1:179:A:ALA:HA	4	0.27
(1,1853)	1:135:A:ASN:HB2	1:138:A:TYR:H	20	0.27
(1,1853)	1:135:A:ASN:HB3	1:138:A:TYR:H	20	0.27
(1,1813)	1:129:A:ILE:HA	1:133:A:PRO:HA	12	0.27
(1,1792)	1:127:A:GLU:HA	1:130:A:LYS:H	3	0.27
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE1	16	0.27
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE2	16	0.27
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE1	16	0.27
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE2	16	0.27
(1,1553)	1:106:A:LYS:HA	1:109:A:GLY:H	7	0.27
(1,1474)	1:99:A:LYS:HA	1:102:A:ALA:H	4	0.27
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	16	0.27
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	7	0.27
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	7	0.27
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	6	0.27
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	6	0.27
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB2	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:32:A:SER:HB2	1:42:B:GLU:HB3	15	0.27
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB2	15	0.27
(1,1320)	1:32:A:SER:HB3	1:42:B:GLU:HB3	15	0.27
(1,1301)	1:19:A:ILE:HD11	1:5:B:LYS:HA	9	0.27
(1,1301)	1:19:A:ILE:HD12	1:5:B:LYS:HA	9	0.27
(1,1301)	1:19:A:ILE:HD13	1:5:B:LYS:HA	9	0.27
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	15	0.27
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	15	0.27
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	15	0.27
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	15	0.27
(1,1225)	1:2:A:SER:HA	1:69:B:LEU:H	12	0.27
(1,1214)	1:71:B:SER:H	1:72:B:ALA:HA	16	0.27
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	3	0.27
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	6	0.27
(1,1110)	1:55:B:LEU:H	1:57:B:LYS:H	16	0.27
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	11	0.27
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	7	0.27
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	6	0.27
(1,834)	1:20:B:VAL:HA	1:23:B:LYS:HA	8	0.27
(1,634)	1:5:B:LYS:HA	1:8:B:ILE:H	4	0.27
(1,624)	1:4:B:SER:H	1:8:B:ILE:H	14	0.27
(1,616)	1:3:B:ALA:HA	1:4:B:SER:H	12	0.27
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	18	0.27
(1,567)	1:65:A:LEU:H	1:67:A:ASP:H	7	0.27
(1,251)	1:23:A:LYS:HA	1:25:A:ILE:H	14	0.27
(1,245)	1:22:A:LYS:HA	1:24:A:GLU:H	10	0.27
(1,178)	1:16:A:PHE:HA	1:20:A:VAL:H	15	0.27
(1,171)	1:16:A:PHE:HA	1:18:A:SER:H	15	0.27
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD21	18	0.27
(1,157)	1:15:A:TYR:HA	1:70:A:ASN:HD22	18	0.27
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	10	0.27
(1,4205)	1:342:B:ASN:H	1:343:B:GLU:H	3	0.26
(1,4189)	1:324:B:ALA:H	1:325:B:GLY:H	9	0.26
(1,4159)	1:253:B:GLY:H	1:254:B:SER:H	14	0.26
(1,4143)	1:235:B:ASP:H	1:236:B:ALA:H	14	0.26
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	18	0.26
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	6	0.26
(1,3938)	1:213:B:GLU:HA	1:216:B:LYS:H	6	0.26
(1,3916)	1:211:B:ASP:H	1:214:B:SER:H	16	0.26
(1,3913)	1:210:B:ARG:HA	1:214:B:SER:H	18	0.26
(1,3833)	1:200:B:GLU:HB2	1:203:B:ASN:HA	12	0.26
(1,3833)	1:200:B:GLU:HB3	1:203:B:ASN:HA	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3825)	1:199:B:ILE:H	1:201:B:GLY:H	6	0.26
(1,3779)	1:194:B:LYS:HA	1:197:B:LEU:H	19	0.26
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	7	0.26
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB2	12	0.26
(1,3768)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	12	0.26
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB2	12	0.26
(1,3768)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	12	0.26
(1,3655)	1:181:B:TYR:H	1:186:B:PRO:HA	16	0.26
(1,3641)	1:180:B:LYS:H	1:189:B:ALA:HA	1	0.26
(1,3599)	1:176:B:LEU:HA	1:180:B:LYS:H	16	0.26
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	4	0.26
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	17	0.26
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE1	19	0.26
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE2	19	0.26
(1,3539)	1:170:B:PHE:HE1	1:208:B:MET:HE3	19	0.26
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE1	19	0.26
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE2	19	0.26
(1,3539)	1:170:B:PHE:HE2	1:208:B:MET:HE3	19	0.26
(1,3532)	1:170:B:PHE:HD1	1:171:B:ARG:HD2	19	0.26
(1,3532)	1:170:B:PHE:HD1	1:171:B:ARG:HD3	19	0.26
(1,3532)	1:170:B:PHE:HD2	1:171:B:ARG:HD2	19	0.26
(1,3532)	1:170:B:PHE:HD2	1:171:B:ARG:HD3	19	0.26
(1,3481)	1:164:B:SER:HA	1:166:B:ASP:H	10	0.26
(1,3382)	1:154:B:GLN:HA	1:158:B:ASP:H	10	0.26
(1,3377)	1:154:B:GLN:H	1:157:B:LYS:H	4	0.26
(1,3358)	1:152:B:TYR:HA	1:179:B:ALA:HA	16	0.26
(1,3355)	1:152:B:TYR:HA	1:155:B:ALA:HA	9	0.26
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	10	0.26
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	10	0.26
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE1	10	0.26
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE2	10	0.26
(1,3309)	1:147:B:SER:HA	1:150:B:LYS:H	4	0.26
(1,3291)	1:146:B:HIS:H	1:155:B:ALA:HA	12	0.26
(1,3256)	1:143:B:ALA:HA	1:155:B:ALA:H	11	0.26
(1,3204)	1:139:B:TYR:HA	1:142:B:ARG:H	8	0.26
(1,3196)	1:138:B:TYR:HA	1:142:B:ARG:H	10	0.26
(1,3171)	1:136:B:ALA:HA	1:166:B:ASP:H	16	0.26
(1,3159)	1:135:B:ASN:HB2	1:138:B:TYR:H	19	0.26
(1,3159)	1:135:B:ASN:HB3	1:138:B:TYR:H	19	0.26
(1,3124)	1:129:B:ILE:HD11	1:138:B:TYR:HD2	11	0.26
(1,3124)	1:129:B:ILE:HD12	1:138:B:TYR:HD2	11	0.26
(1,3124)	1:129:B:ILE:HD13	1:138:B:TYR:HD2	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3082)	1:125:B:TYR:HE2	1:141:B:ASN:HB3	15	0.26
(1,3061)	1:125:B:TYR:H	1:128:B:ALA:H	11	0.26
(1,2984)	1:117:B:ASP:HA	1:120:B:LEU:H	7	0.26
(1,2980)	1:117:B:ASP:H	1:118:B:TYR:HA	3	0.26
(1,2978)	1:116:B:LYS:HB2	1:118:B:TYR:HE1	11	0.26
(1,2978)	1:116:B:LYS:HB2	1:118:B:TYR:HE2	11	0.26
(1,2978)	1:116:B:LYS:HB3	1:118:B:TYR:HE1	11	0.26
(1,2978)	1:116:B:LYS:HB3	1:118:B:TYR:HE2	11	0.26
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE2	5	0.26
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE1	6	0.26
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE2	6	0.26
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	2	0.26
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	2	0.26
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	2	0.26
(1,2911)	1:111:B:LYS:HA	1:114:B:ALA:H	1	0.26
(1,2885)	1:109:B:GLY:H	1:125:B:TYR:HD1	12	0.26
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB2	13	0.26
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB3	13	0.26
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	7	0.26
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	7	0.26
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	7	0.26
(1,2824)	1:103:B:GLU:HA	1:106:B:LYS:H	4	0.26
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	13	0.26
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	20	0.26
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	10	0.26
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	13	0.26
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	5	0.26
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	5	0.26
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	14	0.26
(1,2696)	1:221:A:GLN:HA	1:223:A:LEU:H	13	0.26
(1,2694)	1:221:A:GLN:H	1:224:A:ASN:H	1	0.26
(1,2694)	1:221:A:GLN:H	1:224:A:ASN:H	9	0.26
(1,2660)	1:217:A:LYS:H	1:220:A:GLU:H	10	0.26
(1,2640)	1:214:A:SER:HA	1:217:A:LYS:H	15	0.26
(1,2529)	1:200:A:GLU:HB2	1:204:A:ALA:HA	12	0.26
(1,2529)	1:200:A:GLU:HB3	1:204:A:ALA:HA	12	0.26
(1,2504)	1:197:A:LEU:HA	1:204:A:ALA:HA	14	0.26
(1,2345)	1:180:A:LYS:HB2	1:189:A:ALA:H	14	0.26
(1,2345)	1:180:A:LYS:HB3	1:189:A:ALA:H	14	0.26
(1,2335)	1:180:A:LYS:H	1:189:A:ALA:HA	10	0.26
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE1	10	0.26
(1,2321)	1:178:A:PHE:HA	1:193:A:TYR:HE2	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:173:A:TYR:H	1:176:A:LEU:H	8	0.26
(1,2240)	1:171:A:ARG:H	1:174:A:SER:H	9	0.26
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG2	5	0.26
(1,2219)	1:170:A:PHE:HA	1:200:A:GLU:HG3	5	0.26
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	6	0.26
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	6	0.26
(1,2164)	1:163:A:ILE:HA	1:169:A:TYR:H	8	0.26
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	2	0.26
(1,1923)	1:140:A:ALA:HA	1:143:A:ALA:H	2	0.26
(1,1898)	1:139:A:TYR:HA	1:142:A:ARG:H	12	0.26
(1,1755)	1:125:A:TYR:H	1:128:A:ALA:H	3	0.26
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD1	11	0.26
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD2	11	0.26
(1,1636)	1:113:A:MET:HA	1:121:A:ALA:H	15	0.26
(1,1577)	1:109:A:GLY:H	1:124:A:LYS:HB2	14	0.26
(1,1577)	1:109:A:GLY:H	1:124:A:LYS:HB3	14	0.26
(1,1518)	1:103:A:GLU:HA	1:106:A:LYS:H	6	0.26
(1,1467)	1:98:A:THR:HA	1:101:A:LYS:H	16	0.26
(1,1463)	1:98:A:THR:H	1:101:A:LYS:H	2	0.26
(1,1424)	1:69:A:LEU:HD11	1:2:B:SER:H	8	0.26
(1,1424)	1:69:A:LEU:HD12	1:2:B:SER:H	8	0.26
(1,1424)	1:69:A:LEU:HD13	1:2:B:SER:H	8	0.26
(1,1422)	1:69:A:LEU:H	1:2:B:SER:HA	5	0.26
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	15	0.26
(1,1391)	1:44:A:PHE:HE1	1:19:B:ILE:HG12	4	0.26
(1,1391)	1:44:A:PHE:HE1	1:19:B:ILE:HG13	4	0.26
(1,1391)	1:44:A:PHE:HE2	1:19:B:ILE:HG12	4	0.26
(1,1391)	1:44:A:PHE:HE2	1:19:B:ILE:HG13	4	0.26
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	2	0.26
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	19	0.26
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	19	0.26
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD11	10	0.26
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD12	10	0.26
(1,1226)	1:2:A:SER:HA	1:69:B:LEU:HD13	10	0.26
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	15	0.26
(1,1221)	1:2:A:SER:HA	1:67:B:ASP:HA	16	0.26
(1,1216)	1:71:B:SER:HA	1:72:B:ALA:HA	10	0.26
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	17	0.26
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	9	0.26
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	15	0.26
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	8	0.26
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB1	19	0.26
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB2	19	0.26
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB3	19	0.26
(1,1013)	1:41:B:SER:HA	1:46:B:PHE:HD1	3	0.26
(1,1013)	1:41:B:SER:HA	1:46:B:PHE:HD2	3	0.26
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	4	0.26
(1,988)	1:39:B:CYS:HA	1:42:B:GLU:H	20	0.26
(1,953)	1:35:B:VAL:HA	1:38:B:ASP:HA	9	0.26
(1,945)	1:34:B:ASN:HA	1:38:B:ASP:H	11	0.26
(1,876)	1:26:B:SER:HA	1:28:B:ASP:H	20	0.26
(1,833)	1:20:B:VAL:HA	1:23:B:LYS:H	7	0.26
(1,814)	1:18:B:SER:H	1:21:B:GLU:H	8	0.26
(1,764)	1:15:B:TYR:HA	1:19:B:ILE:H	8	0.26
(1,726)	1:13:B:VAL:HA	1:17:B:SER:H	7	0.26
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	19	0.26
(1,616)	1:3:B:ALA:HA	1:4:B:SER:H	13	0.26
(1,616)	1:3:B:ALA:HA	1:4:B:SER:H	16	0.26
(1,595)	1:69:A:LEU:H	1:71:A:SER:H	13	0.26
(1,495)	1:54:A:ILE:HA	1:57:A:LYS:H	8	0.26
(1,487)	1:53:A:GLY:H	1:56:A:GLY:H	3	0.26
(1,474)	1:51:A:VAL:HA	1:55:A:LEU:H	15	0.26
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	14	0.26
(1,381)	1:39:A:CYS:HA	1:43:A:ALA:H	12	0.26
(1,379)	1:39:A:CYS:HA	1:42:A:GLU:H	18	0.26
(1,299)	1:30:A:ALA:HA	1:33:A:LEU:HD11	6	0.26
(1,299)	1:30:A:ALA:HA	1:33:A:LEU:HD12	6	0.26
(1,299)	1:30:A:ALA:HA	1:33:A:LEU:HD13	6	0.26
(1,286)	1:29:A:GLY:H	1:31:A:ASP:H	4	0.26
(1,245)	1:22:A:LYS:HA	1:24:A:GLU:H	13	0.26
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	9	0.26
(1,25)	1:5:A:LYS:HA	1:8:A:ILE:H	7	0.26
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	2	0.26
(1,4197)	1:332:B:GLY:H	1:333:B:ALA:H	15	0.25
(1,4190)	1:325:B:GLY:H	1:326:B:ASN:H	5	0.25
(1,4186)	1:321:B:ARG:H	1:322:B:ASN:H	10	0.25
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	1	0.25
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	20	0.25
(1,4171)	1:302:B:PHE:H	1:303:B:ALA:H	17	0.25
(1,4107)	1:342:A:ASN:H	1:343:A:GLU:H	11	0.25
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	14	0.25
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	17	0.25
(1,4051)	1:241:A:SER:H	1:242:A:GLN:H	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	18	0.25
(1,4032)	1:226:B:GLU:HA	1:227:B:LYS:H	5	0.25
(1,4016)	1:223:B:LEU:H	1:225:B:LEU:H	20	0.25
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	9	0.25
(1,3800)	1:196:B:VAL:HG11	1:208:B:MET:HA	17	0.25
(1,3800)	1:196:B:VAL:HG12	1:208:B:MET:HA	17	0.25
(1,3800)	1:196:B:VAL:HG13	1:208:B:MET:HA	17	0.25
(1,3781)	1:194:B:LYS:HA	1:198:B:ASP:H	17	0.25
(1,3770)	1:193:B:TYR:HE1	1:211:B:ASP:HB3	10	0.25
(1,3756)	1:193:B:TYR:HA	1:197:B:LEU:H	12	0.25
(1,3605)	1:177:B:GLY:H	1:180:B:LYS:H	12	0.25
(1,3595)	1:176:B:LEU:H	1:178:B:PHE:H	7	0.25
(1,3512)	1:169:B:TYR:HE2	1:171:B:ARG:HB2	4	0.25
(1,3507)	1:169:B:TYR:HE1	1:171:B:ARG:HB2	17	0.25
(1,3507)	1:169:B:TYR:HE1	1:171:B:ARG:HB3	17	0.25
(1,3507)	1:169:B:TYR:HE2	1:171:B:ARG:HB2	17	0.25
(1,3507)	1:169:B:TYR:HE2	1:171:B:ARG:HB3	17	0.25
(1,3442)	1:160:B:GLU:HA	1:163:B:ILE:H	14	0.25
(1,3361)	1:152:B:TYR:HB2	1:183:B:GLN:H	15	0.25
(1,3361)	1:152:B:TYR:HB3	1:183:B:GLN:H	15	0.25
(1,3148)	1:134:B:THR:H	1:135:B:ASN:HA	3	0.25
(1,3099)	1:127:B:GLU:HA	1:131:B:VAL:H	10	0.25
(1,2991)	1:118:B:TYR:HA	1:120:B:LEU:H	15	0.25
(1,2938)	1:113:B:MET:HA	1:116:B:LYS:H	7	0.25
(1,2818)	1:103:B:GLU:H	1:104:B:ASP:H	11	0.25
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG11	4	0.25
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG12	4	0.25
(1,2809)	1:102:B:ALA:HA	1:131:B:VAL:HG13	4	0.25
(1,2750)	1:95:B:ASP:HA	1:97:B:GLU:H	17	0.25
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	17	0.25
(1,2735)	1:93:B:GLU:H	1:95:B:ASP:H	1	0.25
(1,2719)	1:224:A:ASN:HA	1:226:A:GLU:H	13	0.25
(1,2694)	1:221:A:GLN:H	1:224:A:ASN:H	15	0.25
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	14	0.25
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	10	0.25
(1,2555)	1:205:A:THR:H	1:209:A:LYS:H	9	0.25
(1,2495)	1:196:A:VAL:HG11	1:208:A:MET:HB2	14	0.25
(1,2495)	1:196:A:VAL:HG11	1:208:A:MET:HB3	14	0.25
(1,2495)	1:196:A:VAL:HG12	1:208:A:MET:HB2	14	0.25
(1,2495)	1:196:A:VAL:HG12	1:208:A:MET:HB3	14	0.25
(1,2495)	1:196:A:VAL:HG13	1:208:A:MET:HB2	14	0.25
(1,2495)	1:196:A:VAL:HG13	1:208:A:MET:HB3	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2485)	1:195:A:LYS:HA	1:199:A:ILE:H	8	0.25
(1,2357)	1:181:A:TYR:HA	1:185:A:LYS:H	7	0.25
(1,2340)	1:180:A:LYS:HA	1:185:A:LYS:H	1	0.25
(1,2291)	1:176:A:LEU:HA	1:178:A:PHE:H	16	0.25
(1,2261)	1:173:A:TYR:HA	1:192:A:ALA:HA	7	0.25
(1,2245)	1:171:A:ARG:HA	1:175:A:ARG:H	15	0.25
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	3	0.25
(1,2051)	1:152:A:TYR:HA	1:156:A:VAL:H	3	0.25
(1,2004)	1:147:A:SER:HA	1:150:A:LYS:HA	2	0.25
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE1	16	0.25
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE2	16	0.25
(1,1646)	1:113:A:MET:HE1	1:145:A:ALA:HA	14	0.25
(1,1646)	1:113:A:MET:HE2	1:145:A:ALA:HA	14	0.25
(1,1646)	1:113:A:MET:HE3	1:145:A:ALA:HA	14	0.25
(1,1638)	1:113:A:MET:HB2	1:125:A:TYR:HE1	5	0.25
(1,1638)	1:113:A:MET:HB2	1:125:A:TYR:HE2	5	0.25
(1,1638)	1:113:A:MET:HB3	1:125:A:TYR:HE1	5	0.25
(1,1638)	1:113:A:MET:HB3	1:125:A:TYR:HE2	5	0.25
(1,1593)	1:110:A:ASN:HA	1:113:A:MET:H	11	0.25
(1,1553)	1:106:A:LYS:HA	1:109:A:GLY:H	19	0.25
(1,1534)	1:105:A:LEU:HA	1:107:A:MET:H	1	0.25
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD11	9	0.25
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD12	9	0.25
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD13	9	0.25
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	19	0.25
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	1	0.25
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	3	0.25
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	5	0.25
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	5	0.25
(1,1373)	1:43:A:ALA:HA	1:29:B:GLY:H	13	0.25
(1,1313)	1:29:A:GLY:H	1:43:B:ALA:HA	7	0.25
(1,1231)	1:5:A:LYS:H	1:15:B:TYR:HE1	18	0.25
(1,1231)	1:5:A:LYS:H	1:15:B:TYR:HE2	18	0.25
(1,1223)	1:2:A:SER:HA	1:68:B:ILE:HA	9	0.25
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	17	0.25
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	5	0.25
(1,1214)	1:71:B:SER:H	1:72:B:ALA:HA	17	0.25
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	1	0.25
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	2	0.25
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	8	0.25
(1,1179)	1:65:B:LEU:HA	1:67:B:ASP:H	5	0.25
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:41:B:SER:H	1:46:B:PHE:HE1	3	0.25
(1,1004)	1:41:B:SER:H	1:46:B:PHE:HE2	3	0.25
(1,990)	1:39:B:CYS:HA	1:43:B:ALA:H	18	0.25
(1,945)	1:34:B:ASN:HA	1:38:B:ASP:H	19	0.25
(1,892)	1:28:B:ASP:HA	1:31:B:ASP:H	5	0.25
(1,892)	1:28:B:ASP:HA	1:31:B:ASP:H	12	0.25
(1,884)	1:27:B:GLU:HA	1:30:B:ALA:H	12	0.25
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	18	0.25
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	17	0.25
(1,634)	1:5:B:LYS:HA	1:8:B:ILE:H	5	0.25
(1,634)	1:5:B:LYS:HA	1:8:B:ILE:H	16	0.25
(1,623)	1:4:B:SER:H	1:7:B:GLU:H	8	0.25
(1,595)	1:69:A:LEU:H	1:71:A:SER:H	17	0.25
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	7	0.25
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	11	0.25
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	14	0.25
(1,4208)	1:345:B:LYS:H	1:346:B:GLN:H	7	0.24
(1,4193)	1:328:B:PHE:H	1:329:B:GLY:H	10	0.24
(1,4190)	1:325:B:GLY:H	1:326:B:ASN:H	3	0.24
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	3	0.24
(1,4140)	1:232:B:GLN:H	1:233:B:SER:H	18	0.24
(1,4139)	1:231:B:GLU:H	1:232:B:GLN:H	8	0.24
(1,4138)	1:228:B:THR:H	1:229:B:VAL:H	5	0.24
(1,4064)	1:256:A:LEU:H	1:257:A:GLY:H	9	0.24
(1,4052)	1:242:A:GLN:H	1:243:A:GLY:H	6	0.24
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	15	0.24
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	15	0.24
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	19	0.24
(1,4000)	1:221:B:GLN:H	1:224:B:ASN:H	11	0.24
(1,4000)	1:221:B:GLN:H	1:224:B:ASN:H	16	0.24
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	1	0.24
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	1	0.24
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	2	0.24
(1,3783)	1:194:B:LYS:HB2	1:212:B:TYR:HE1	10	0.24
(1,3783)	1:194:B:LYS:HB2	1:212:B:TYR:HE2	10	0.24
(1,3783)	1:194:B:LYS:HB3	1:212:B:TYR:HE1	10	0.24
(1,3783)	1:194:B:LYS:HB3	1:212:B:TYR:HE2	10	0.24
(1,3727)	1:190:B:LEU:HD11	1:216:B:LYS:H	17	0.24
(1,3727)	1:190:B:LEU:HD12	1:216:B:LYS:H	17	0.24
(1,3727)	1:190:B:LEU:HD13	1:216:B:LYS:H	17	0.24
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	8	0.24
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	8	0.24
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	8	0.24
(1,3651)	1:180:B:LYS:HB2	1:189:B:ALA:H	10	0.24
(1,3651)	1:180:B:LYS:HB3	1:189:B:ALA:H	10	0.24
(1,3572)	1:173:B:TYR:HB2	1:196:B:VAL:H	11	0.24
(1,3572)	1:173:B:TYR:HB3	1:196:B:VAL:H	11	0.24
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG2	15	0.24
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG3	15	0.24
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG2	15	0.24
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG3	15	0.24
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE1	1	0.24
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE2	1	0.24
(1,3535)	1:170:B:PHE:HD1	1:208:B:MET:HE3	1	0.24
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE1	1	0.24
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE2	1	0.24
(1,3535)	1:170:B:PHE:HD2	1:208:B:MET:HE3	1	0.24
(1,3512)	1:169:B:TYR:HE1	1:171:B:ARG:HB3	17	0.24
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	8	0.24
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	8	0.24
(1,3474)	1:163:B:ILE:HD11	1:176:B:LEU:H	8	0.24
(1,3474)	1:163:B:ILE:HD12	1:176:B:LEU:H	8	0.24
(1,3474)	1:163:B:ILE:HD13	1:176:B:LEU:H	8	0.24
(1,3381)	1:154:B:GLN:HA	1:157:B:LYS:H	11	0.24
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	20	0.24
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	1	0.24
(1,3291)	1:146:B:HIS:H	1:155:B:ALA:HA	7	0.24
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	17	0.24
(1,3256)	1:143:B:ALA:HA	1:155:B:ALA:H	12	0.24
(1,3212)	1:139:B:TYR:HB2	1:162:B:ALA:HA	7	0.24
(1,3212)	1:139:B:TYR:HB3	1:162:B:ALA:HA	7	0.24
(1,3191)	1:138:B:TYR:H	1:141:B:ASN:H	13	0.24
(1,3188)	1:137:B:ILE:HA	1:141:B:ASN:H	16	0.24
(1,3159)	1:135:B:ASN:HB2	1:138:B:TYR:H	15	0.24
(1,3159)	1:135:B:ASN:HB3	1:138:B:TYR:H	15	0.24
(1,3118)	1:129:B:ILE:HA	1:132:B:LEU:H	11	0.24
(1,3068)	1:125:B:TYR:HA	1:138:B:TYR:HA	13	0.24
(1,3058)	1:124:B:LYS:HA	1:127:B:GLU:H	2	0.24
(1,2979)	1:117:B:ASP:H	1:118:B:TYR:H	3	0.24
(1,2938)	1:113:B:MET:HA	1:116:B:LYS:H	9	0.24
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	10	0.24
(1,2824)	1:103:B:GLU:HA	1:106:B:LYS:H	18	0.24
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG11	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG12	19	0.24
(1,2792)	1:101:B:LYS:H	1:131:B:VAL:HG13	19	0.24
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB2	19	0.24
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB3	19	0.24
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	14	0.24
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	14	0.24
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	16	0.24
(1,2694)	1:221:A:GLN:H	1:224:A:ASN:H	7	0.24
(1,2673)	1:218:A:LYS:HA	1:221:A:GLN:H	2	0.24
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	13	0.24
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	13	0.24
(1,2517)	1:198:A:ASP:HA	1:201:A:GLY:H	13	0.24
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG21	5	0.24
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG22	5	0.24
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG23	5	0.24
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG21	10	0.24
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG22	10	0.24
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG23	10	0.24
(1,2279)	1:174:A:SER:HA	1:193:A:TYR:HA	16	0.24
(1,2243)	1:171:A:ARG:HA	1:174:A:SER:H	9	0.24
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	11	0.24
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	11	0.24
(1,1916)	1:139:A:TYR:HD2	1:161:A:SER:HB2	10	0.24
(1,1814)	1:129:A:ILE:HA	1:135:A:ASN:H	3	0.24
(1,1770)	1:125:A:TYR:HB2	1:142:A:ARG:HB2	3	0.24
(1,1770)	1:125:A:TYR:HB2	1:142:A:ARG:HB3	3	0.24
(1,1770)	1:125:A:TYR:HB3	1:142:A:ARG:HB2	3	0.24
(1,1770)	1:125:A:TYR:HB3	1:142:A:ARG:HB3	3	0.24
(1,1678)	1:117:A:ASP:HA	1:120:A:LEU:H	12	0.24
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	13	0.24
(1,1635)	1:113:A:MET:HA	1:118:A:TYR:HA	2	0.24
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG2	5	0.24
(1,1578)	1:109:A:GLY:H	1:124:A:LYS:HG3	5	0.24
(1,1536)	1:105:A:LEU:HA	1:109:A:GLY:H	9	0.24
(1,1474)	1:99:A:LYS:HA	1:102:A:ALA:H	11	0.24
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	15	0.24
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	15	0.24
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	15	0.24
(1,1418)	1:68:A:ILE:HG21	1:2:B:SER:HA	3	0.24
(1,1418)	1:68:A:ILE:HG22	1:2:B:SER:HA	3	0.24
(1,1418)	1:68:A:ILE:HG23	1:2:B:SER:HA	3	0.24
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	12	0.24
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	15	0.24
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	15	0.24
(1,1350)	1:39:A:CYS:HB2	1:32:B:SER:HA	19	0.24
(1,1350)	1:39:A:CYS:HB3	1:32:B:SER:HA	19	0.24
(1,1325)	1:33:A:LEU:HA	1:40:B:ILE:HA	13	0.24
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	13	0.24
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	13	0.24
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	5	0.24
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	7	0.24
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	2	0.24
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	2	0.24
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	2	0.24
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	2	0.24
(1,1236)	1:5:A:LYS:HB2	1:15:B:TYR:HE1	12	0.24
(1,1236)	1:5:A:LYS:HB2	1:15:B:TYR:HE2	12	0.24
(1,1236)	1:5:A:LYS:HB3	1:15:B:TYR:HE1	12	0.24
(1,1236)	1:5:A:LYS:HB3	1:15:B:TYR:HE2	12	0.24
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	19	0.24
(1,1127)	1:58:B:SER:H	1:59:B:GLU:HA	9	0.24
(1,1100)	1:54:B:ILE:H	1:57:B:LYS:H	20	0.24
(1,857)	1:23:B:LYS:H	1:25:B:ILE:H	6	0.24
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD21	9	0.24
(1,771)	1:15:B:TYR:HB2	1:70:B:ASN:HD22	9	0.24
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD21	9	0.24
(1,771)	1:15:B:TYR:HB3	1:70:B:ASN:HD22	9	0.24
(1,762)	1:15:B:TYR:HA	1:18:B:SER:H	4	0.24
(1,752)	1:14:B:ASN:HA	1:18:B:SER:H	7	0.24
(1,725)	1:13:B:VAL:HA	1:16:B:PHE:H	4	0.24
(1,669)	1:9:B:ALA:HA	1:13:B:VAL:H	8	0.24
(1,616)	1:3:B:ALA:HA	1:4:B:SER:H	18	0.24
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	14	0.24
(1,570)	1:65:A:LEU:HA	1:67:A:ASP:H	10	0.24
(1,531)	1:59:A:GLU:HB2	1:64:A:HIS:HA	2	0.24
(1,531)	1:59:A:GLU:HB3	1:64:A:HIS:HA	2	0.24
(1,474)	1:51:A:VAL:HA	1:55:A:LEU:H	13	0.24
(1,466)	1:50:A:ALA:H	1:51:A:VAL:H	20	0.24
(1,452)	1:47:A:GLU:HB2	1:49:A:GLU:H	9	0.24
(1,452)	1:47:A:GLU:HB3	1:49:A:GLU:H	9	0.24
(1,325)	1:33:A:LEU:HA	1:37:A:MET:H	13	0.24
(1,287)	1:29:A:GLY:H	1:32:A:SER:H	4	0.24
(1,284)	1:28:A:ASP:HA	1:32:A:SER:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4205)	1:342:B:ASN:H	1:343:B:GLU:H	11	0.23
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	7	0.23
(1,4181)	1:314:B:LEU:H	1:315:B:MET:H	16	0.23
(1,4176)	1:307:B:GLY:H	1:308:B:THR:H	20	0.23
(1,4175)	1:305:B:GLY:H	1:307:B:GLY:H	13	0.23
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	7	0.23
(1,4158)	1:252:B:LEU:H	1:253:B:GLY:H	7	0.23
(1,4108)	1:343:A:GLU:H	1:344:A:ASN:H	20	0.23
(1,4060)	1:252:A:LEU:H	1:253:A:GLY:H	2	0.23
(1,4016)	1:223:B:LEU:H	1:225:B:LEU:H	9	0.23
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	16	0.23
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	13	0.23
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	20	0.23
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	20	0.23
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	20	0.23
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	20	0.23
(1,3583)	1:174:B:SER:HA	1:177:B:GLY:H	6	0.23
(1,3583)	1:174:B:SER:HA	1:177:B:GLY:H	11	0.23
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG21	9	0.23
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG22	9	0.23
(1,3579)	1:174:B:SER:H	1:196:B:VAL:HG23	9	0.23
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	6	0.23
(1,3382)	1:154:B:GLN:HA	1:158:B:ASP:H	18	0.23
(1,3367)	1:152:B:TYR:HD2	1:183:B:GLN:HG3	20	0.23
(1,3354)	1:152:B:TYR:HA	1:155:B:ALA:H	4	0.23
(1,3354)	1:152:B:TYR:HA	1:155:B:ALA:H	9	0.23
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB2	16	0.23
(1,3316)	1:147:B:SER:HB2	1:178:B:PHE:HB3	16	0.23
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB2	16	0.23
(1,3316)	1:147:B:SER:HB3	1:178:B:PHE:HB3	16	0.23
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	8	0.23
(1,3252)	1:143:B:ALA:H	1:155:B:ALA:HA	9	0.23
(1,3204)	1:139:B:TYR:HA	1:142:B:ARG:H	3	0.23
(1,3148)	1:134:B:THR:H	1:135:B:ASN:HA	18	0.23
(1,3124)	1:129:B:ILE:HD11	1:138:B:TYR:HD2	10	0.23
(1,3124)	1:129:B:ILE:HD12	1:138:B:TYR:HD2	10	0.23
(1,3124)	1:129:B:ILE:HD13	1:138:B:TYR:HD2	10	0.23
(1,3102)	1:128:B:ALA:H	1:131:B:VAL:H	2	0.23
(1,3075)	1:125:B:TYR:HB2	1:142:B:ARG:HA	7	0.23
(1,3075)	1:125:B:TYR:HB3	1:142:B:ARG:HA	7	0.23
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	7	0.23
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB1	6	0.23
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB2	6	0.23
(1,2953)	1:113:B:MET:HE1	1:145:B:ALA:HB3	6	0.23
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB1	6	0.23
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB2	6	0.23
(1,2953)	1:113:B:MET:HE2	1:145:B:ALA:HB3	6	0.23
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB1	6	0.23
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB2	6	0.23
(1,2953)	1:113:B:MET:HE3	1:145:B:ALA:HB3	6	0.23
(1,2882)	1:109:B:GLY:H	1:121:B:ALA:HA	6	0.23
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB1	11	0.23
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB2	11	0.23
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB3	11	0.23
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	12	0.23
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	7	0.23
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	7	0.23
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	7	0.23
(1,2660)	1:217:A:LYS:H	1:220:A:GLU:H	9	0.23
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	19	0.23
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	1	0.23
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	1	0.23
(1,2504)	1:197:A:LEU:HA	1:204:A:ALA:HA	3	0.23
(1,2504)	1:197:A:LEU:HA	1:204:A:ALA:HA	5	0.23
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	9	0.23
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	9	0.23
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB2	9	0.23
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	9	0.23
(1,2418)	1:190:A:LEU:HA	1:216:A:LYS:H	10	0.23
(1,2415)	1:190:A:LEU:HA	1:194:A:LYS:H	11	0.23
(1,2294)	1:176:A:LEU:HD11	1:180:A:LYS:H	20	0.23
(1,2294)	1:176:A:LEU:HD12	1:180:A:LYS:H	20	0.23
(1,2294)	1:176:A:LEU:HD13	1:180:A:LYS:H	20	0.23
(1,2244)	1:171:A:ARG:HA	1:174:A:SER:HA	9	0.23
(1,2216)	1:170:A:PHE:HA	1:196:A:VAL:HA	6	0.23
(1,2215)	1:170:A:PHE:HA	1:174:A:SER:H	7	0.23
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	9	0.23
(1,2175)	1:164:A:SER:HA	1:166:A:ASP:H	10	0.23
(1,2155)	1:162:A:ALA:HB1	1:172:A:GLY:H	7	0.23
(1,2155)	1:162:A:ALA:HB2	1:172:A:GLY:H	7	0.23
(1,2155)	1:162:A:ALA:HB3	1:172:A:GLY:H	7	0.23
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	2	0.23
(1,1946)	1:143:A:ALA:H	1:155:A:ALA:HA	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1894)	1:139:A:TYR:H	1:162:A:ALA:HA	5	0.23
(1,1889)	1:138:A:TYR:HA	1:141:A:ASN:H	2	0.23
(1,1853)	1:135:A:ASN:HB2	1:138:A:TYR:H	9	0.23
(1,1853)	1:135:A:ASN:HB3	1:138:A:TYR:H	9	0.23
(1,1841)	1:134:A:THR:H	1:135:A:ASN:H	15	0.23
(1,1667)	1:116:A:LYS:HA	1:118:A:TYR:HA	8	0.23
(1,1663)	1:116:A:LYS:H	1:118:A:TYR:HE1	4	0.23
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE1	12	0.23
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE2	12	0.23
(1,1645)	1:113:A:MET:HE1	1:145:A:ALA:H	17	0.23
(1,1645)	1:113:A:MET:HE2	1:145:A:ALA:H	17	0.23
(1,1645)	1:113:A:MET:HE3	1:145:A:ALA:H	17	0.23
(1,1588)	1:110:A:ASN:H	1:113:A:MET:H	18	0.23
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	7	0.23
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	15	0.23
(1,1572)	1:108:A:GLN:HA	1:111:A:LYS:H	20	0.23
(1,1565)	1:107:A:MET:HA	1:110:A:ASN:H	7	0.23
(1,1555)	1:106:A:LYS:HA	1:125:A:TYR:HA	2	0.23
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	16	0.23
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	12	0.23
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	12	0.23
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	12	0.23
(1,1406)	1:63:A:GLN:HA	1:63:B:GLN:H	19	0.23
(1,1374)	1:43:A:ALA:HA	1:32:B:SER:H	15	0.23
(1,1311)	1:25:A:ILE:HD11	1:44:B:PHE:HA	15	0.23
(1,1311)	1:25:A:ILE:HD12	1:44:B:PHE:HA	15	0.23
(1,1311)	1:25:A:ILE:HD13	1:44:B:PHE:HA	15	0.23
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE2	14	0.23
(1,1303)	1:25:A:ILE:H	1:5:B:LYS:HE3	14	0.23
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	2	0.23
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	2	0.23
(1,1211)	1:70:B:ASN:HA	1:71:B:SER:HA	17	0.23
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	10	0.23
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD11	19	0.23
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD12	19	0.23
(1,1171)	1:63:B:GLN:HA	1:68:B:ILE:HD13	19	0.23
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	20	0.23
(1,1096)	1:53:B:GLY:H	1:56:B:GLY:H	11	0.23
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD11	9	0.23
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD12	9	0.23
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD13	9	0.23
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD11	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD12	9	0.23
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD13	9	0.23
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	17	0.23
(1,988)	1:39:B:CYS:HA	1:42:B:GLU:H	5	0.23
(1,884)	1:27:B:GLU:HA	1:30:B:ALA:H	11	0.23
(1,834)	1:20:B:VAL:HA	1:23:B:LYS:HA	19	0.23
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB2	1	0.23
(1,765)	1:15:B:TYR:HA	1:70:B:ASN:HB3	1	0.23
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG11	2	0.23
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG12	2	0.23
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG13	2	0.23
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG11	10	0.23
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG12	10	0.23
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG13	10	0.23
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	4	0.23
(1,578)	1:66:A:ALA:HA	1:68:A:ILE:H	6	0.23
(1,578)	1:66:A:ALA:HA	1:68:A:ILE:H	11	0.23
(1,553)	1:61:A:LYS:HG2	1:62:A:GLY:H	17	0.23
(1,553)	1:61:A:LYS:HG3	1:62:A:GLY:H	17	0.23
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	13	0.23
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	13	0.23
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	14	0.23
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	14	0.23
(1,431)	1:45:A:GLY:H	1:46:A:PHE:HD1	14	0.23
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	13	0.23
(1,175)	1:16:A:PHE:HA	1:19:A:ILE:HG12	18	0.23
(1,175)	1:16:A:PHE:HA	1:19:A:ILE:HG13	18	0.23
(1,26)	1:5:A:LYS:HA	1:9:A:ALA:H	15	0.23
(1,4207)	1:344:B:ASN:H	1:345:B:LYS:H	13	0.22
(1,4207)	1:344:B:ASN:H	1:345:B:LYS:H	16	0.22
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	16	0.22
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	9	0.22
(1,4138)	1:228:B:THR:H	1:229:B:VAL:H	9	0.22
(1,4110)	1:345:A:LYS:H	1:346:A:GLN:H	2	0.22
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	17	0.22
(1,4089)	1:322:A:ASN:H	1:323:A:MET:H	18	0.22
(1,4074)	1:303:A:ALA:H	1:304:A:SER:H	10	0.22
(1,4071)	1:300:A:GLU:H	1:301:A:GLY:H	15	0.22
(1,4061)	1:253:A:GLY:H	1:254:A:SER:H	19	0.22
(1,4044)	1:234:A:ARG:H	1:235:A:ASP:H	3	0.22
(1,4020)	1:223:B:LEU:HA	1:226:B:GLU:H	16	0.22
(1,4003)	1:221:B:GLN:HA	1:224:B:ASN:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	10	0.22
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	7	0.22
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	9	0.22
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	9	0.22
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	20	0.22
(1,3939)	1:213:B:GLU:HA	1:217:B:LYS:H	1	0.22
(1,3938)	1:213:B:GLU:HA	1:216:B:LYS:H	4	0.22
(1,3898)	1:208:B:MET:HA	1:211:B:ASP:H	11	0.22
(1,3898)	1:208:B:MET:HA	1:211:B:ASP:H	15	0.22
(1,3894)	1:208:B:MET:H	1:211:B:ASP:H	12	0.22
(1,3801)	1:196:B:VAL:HG11	1:208:B:MET:HB2	19	0.22
(1,3801)	1:196:B:VAL:HG11	1:208:B:MET:HB3	19	0.22
(1,3801)	1:196:B:VAL:HG12	1:208:B:MET:HB2	19	0.22
(1,3801)	1:196:B:VAL:HG12	1:208:B:MET:HB3	19	0.22
(1,3801)	1:196:B:VAL:HG13	1:208:B:MET:HB2	19	0.22
(1,3801)	1:196:B:VAL:HG13	1:208:B:MET:HB3	19	0.22
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	15	0.22
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD2	6	0.22
(1,3669)	1:181:B:TYR:HD1	1:218:B:LYS:HD3	6	0.22
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD2	6	0.22
(1,3669)	1:181:B:TYR:HD2	1:218:B:LYS:HD3	6	0.22
(1,3645)	1:180:B:LYS:HA	1:183:B:GLN:H	13	0.22
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG21	17	0.22
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG22	17	0.22
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG23	17	0.22
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB1	15	0.22
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB2	15	0.22
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB3	15	0.22
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	16	0.22
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	16	0.22
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	2	0.22
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	2	0.22
(1,3468)	1:163:B:ILE:HA	1:166:B:ASP:H	7	0.22
(1,3337)	1:150:B:LYS:HB2	1:152:B:TYR:HD1	7	0.22
(1,3337)	1:150:B:LYS:HB2	1:152:B:TYR:HD2	7	0.22
(1,3337)	1:150:B:LYS:HB3	1:152:B:TYR:HD1	7	0.22
(1,3337)	1:150:B:LYS:HB3	1:152:B:TYR:HD2	7	0.22
(1,3335)	1:150:B:LYS:HA	1:152:B:TYR:HA	6	0.22
(1,3313)	1:147:B:SER:HA	1:152:B:TYR:HA	11	0.22
(1,3079)	1:125:B:TYR:HB2	1:142:B:ARG:HD2	4	0.22
(1,3079)	1:125:B:TYR:HB2	1:142:B:ARG:HD3	4	0.22
(1,3079)	1:125:B:TYR:HB3	1:142:B:ARG:HD2	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3079)	1:125:B:TYR:HB3	1:142:B:ARG:HD3	4	0.22
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	16	0.22
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	16	0.22
(1,3044)	1:122:B:ILE:HD11	1:146:B:HIS:HA	5	0.22
(1,3044)	1:122:B:ILE:HD12	1:146:B:HIS:HA	5	0.22
(1,3044)	1:122:B:ILE:HD13	1:146:B:HIS:HA	5	0.22
(1,2892)	1:109:B:GLY:HA2	1:113:B:MET:H	15	0.22
(1,2892)	1:109:B:GLY:HA3	1:113:B:MET:H	15	0.22
(1,2837)	1:105:B:LEU:H	1:108:B:GLN:H	19	0.22
(1,2828)	1:104:B:ASP:H	1:107:B:MET:H	17	0.22
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	20	0.22
(1,2614)	1:211:A:ASP:HA	1:214:A:SER:H	3	0.22
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB2	14	0.22
(1,2458)	1:193:A:TYR:HD1	1:211:A:ASP:HB3	14	0.22
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB2	14	0.22
(1,2458)	1:193:A:TYR:HD2	1:211:A:ASP:HB3	14	0.22
(1,2457)	1:193:A:TYR:HD1	1:211:A:ASP:HA	6	0.22
(1,2457)	1:193:A:TYR:HD2	1:211:A:ASP:HA	6	0.22
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG21	10	0.22
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG22	10	0.22
(1,2411)	1:190:A:LEU:H	1:219:A:VAL:HG23	10	0.22
(1,2383)	1:185:A:LYS:HA	1:188:A:GLU:H	16	0.22
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	11	0.22
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	11	0.22
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	11	0.22
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	11	0.22
(1,2345)	1:180:A:LYS:HB2	1:189:A:ALA:H	2	0.22
(1,2345)	1:180:A:LYS:HB3	1:189:A:ALA:H	2	0.22
(1,2278)	1:174:A:SER:HA	1:178:A:PHE:H	1	0.22
(1,2236)	1:170:A:PHE:HE1	1:171:A:ARG:HD3	16	0.22
(1,2236)	1:170:A:PHE:HE2	1:171:A:ARG:HD3	20	0.22
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG21	6	0.22
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG22	6	0.22
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG23	6	0.22
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG21	6	0.22
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG22	6	0.22
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG23	6	0.22
(1,2205)	1:169:A:TYR:HD1	1:171:A:ARG:H	1	0.22
(1,2205)	1:169:A:TYR:HD1	1:171:A:ARG:H	16	0.22
(1,2146)	1:161:A:SER:HA	1:165:A:ILE:H	13	0.22
(1,2138)	1:160:A:GLU:HA	1:164:A:SER:H	10	0.22
(1,2076)	1:154:A:GLN:HA	1:158:A:ASP:H	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1951)	1:143:A:ALA:HA	1:155:A:ALA:HA	5	0.22
(1,1909)	1:139:A:TYR:HD1	1:162:A:ALA:H	3	0.22
(1,1909)	1:139:A:TYR:HD2	1:162:A:ALA:H	3	0.22
(1,1900)	1:139:A:TYR:HA	1:158:A:ASP:HA	20	0.22
(1,1862)	1:136:A:ALA:HA	1:162:A:ALA:HA	9	0.22
(1,1773)	1:125:A:TYR:HB2	1:142:A:ARG:HD2	2	0.22
(1,1773)	1:125:A:TYR:HB2	1:142:A:ARG:HD3	2	0.22
(1,1773)	1:125:A:TYR:HB3	1:142:A:ARG:HD2	2	0.22
(1,1773)	1:125:A:TYR:HB3	1:142:A:ARG:HD3	2	0.22
(1,1680)	1:118:A:TYR:H	1:120:A:LEU:H	12	0.22
(1,1593)	1:110:A:ASN:HA	1:113:A:MET:H	6	0.22
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	2	0.22
(1,1575)	1:109:A:GLY:H	1:112:A:ALA:H	18	0.22
(1,1553)	1:106:A:LYS:HA	1:109:A:GLY:H	1	0.22
(1,1518)	1:103:A:GLU:HA	1:106:A:LYS:H	7	0.22
(1,1510)	1:102:A:ALA:HB1	1:132:A:LEU:H	6	0.22
(1,1510)	1:102:A:ALA:HB2	1:132:A:LEU:H	6	0.22
(1,1510)	1:102:A:ALA:HB3	1:132:A:LEU:H	6	0.22
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	14	0.22
(1,1448)	1:95:A:ASP:HB2	1:99:A:LYS:H	13	0.22
(1,1448)	1:95:A:ASP:HB3	1:99:A:LYS:H	13	0.22
(1,1436)	1:94:A:ASP:H	1:96:A:ALA:H	10	0.22
(1,1429)	1:93:A:GLU:H	1:95:A:ASP:H	7	0.22
(1,1424)	1:69:A:LEU:HD11	1:2:B:SER:H	5	0.22
(1,1424)	1:69:A:LEU:HD12	1:2:B:SER:H	5	0.22
(1,1424)	1:69:A:LEU:HD13	1:2:B:SER:H	5	0.22
(1,1389)	1:44:A:PHE:HE1	1:19:B:ILE:HG22	18	0.22
(1,1389)	1:44:A:PHE:HE2	1:19:B:ILE:HG22	18	0.22
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB2	16	0.22
(1,1371)	1:43:A:ALA:H	1:32:B:SER:HB3	16	0.22
(1,1364)	1:40:A:ILE:HG12	1:36:B:ALA:HA	3	0.22
(1,1364)	1:40:A:ILE:HG13	1:36:B:ALA:HA	3	0.22
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	8	0.22
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	19	0.22
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	19	0.22
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	19	0.22
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	12	0.22
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	12	0.22
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	12	0.22
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	12	0.22
(1,1301)	1:19:A:ILE:HD11	1:5:B:LYS:HA	15	0.22
(1,1301)	1:19:A:ILE:HD12	1:5:B:LYS:HA	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1301)	1:19:A:ILE:HD13	1:5:B:LYS:HA	15	0.22
(1,1285)	1:16:A:PHE:HE1	1:12:B:ILE:HG21	20	0.22
(1,1285)	1:16:A:PHE:HE2	1:12:B:ILE:HG21	20	0.22
(1,1276)	1:15:A:TYR:HH	1:8:B:ILE:H	11	0.22
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	10	0.22
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	10	0.22
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD11	18	0.22
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD12	18	0.22
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD13	18	0.22
(1,1209)	1:70:B:ASN:H	1:71:B:SER:HA	9	0.22
(1,1181)	1:65:B:LEU:HD21	1:66:B:ALA:H	2	0.22
(1,1181)	1:65:B:LEU:HD22	1:66:B:ALA:H	2	0.22
(1,1181)	1:65:B:LEU:HD23	1:66:B:ALA:H	2	0.22
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	7	0.22
(1,1164)	1:62:B:GLY:H	1:63:B:GLN:HA	10	0.22
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	20	0.22
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	20	0.22
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	6	0.22
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	6	0.22
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	6	0.22
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	6	0.22
(1,1096)	1:53:B:GLY:H	1:56:B:GLY:H	5	0.22
(1,1063)	1:48:B:ARG:H	1:49:B:GLU:HA	1	0.22
(1,1054)	1:47:B:GLU:H	1:50:B:ALA:H	15	0.22
(1,1011)	1:41:B:SER:HA	1:46:B:PHE:H	1	0.22
(1,1011)	1:41:B:SER:HA	1:46:B:PHE:H	17	0.22
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	17	0.22
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	17	0.22
(1,892)	1:28:B:ASP:HA	1:31:B:ASP:H	9	0.22
(1,885)	1:27:B:GLU:HA	1:30:B:ALA:HA	1	0.22
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG11	12	0.22
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG12	12	0.22
(1,754)	1:14:B:ASN:HA	1:51:B:VAL:HG13	12	0.22
(1,623)	1:4:B:SER:H	1:7:B:GLU:H	6	0.22
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	20	0.22
(1,587)	1:68:A:ILE:H	1:69:A:LEU:HA	12	0.22
(1,549)	1:61:A:LYS:H	1:62:A:GLY:H	18	0.22
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	6	0.22
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	1	0.22
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	1	0.22
(1,251)	1:23:A:LYS:HA	1:25:A:ILE:H	19	0.22
(1,178)	1:16:A:PHE:HA	1:20:A:VAL:H	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:16:A:PHE:HA	1:19:A:ILE:H	9	0.22
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB2	10	0.22
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB3	10	0.22
(1,60)	1:9:A:ALA:HA	1:13:A:VAL:H	17	0.22
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	1	0.22
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB1	1	0.21
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB2	1	0.21
(1,4222)	1:321:B:ARG:H	1:319:B:ALA:HB3	1	0.21
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	8	0.21
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	8	0.21
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	8	0.21
(1,4163)	1:257:B:GLY:H	1:258:B:GLY:H	14	0.21
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	2	0.21
(1,4054)	1:244:A:ALA:H	1:245:A:SER:H	9	0.21
(1,4051)	1:241:A:SER:H	1:242:A:GLN:H	4	0.21
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	6	0.21
(1,3966)	1:217:B:LYS:H	1:220:B:GLU:H	6	0.21
(1,3939)	1:213:B:GLU:HA	1:217:B:LYS:H	7	0.21
(1,3894)	1:208:B:MET:H	1:211:B:ASP:H	5	0.21
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	14	0.21
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	5	0.21
(1,3770)	1:193:B:TYR:HD2	1:211:B:ASP:HB3	9	0.21
(1,3760)	1:193:B:TYR:HB2	1:212:B:TYR:HB2	4	0.21
(1,3760)	1:193:B:TYR:HB2	1:212:B:TYR:HB3	4	0.21
(1,3760)	1:193:B:TYR:HB3	1:212:B:TYR:HB2	4	0.21
(1,3760)	1:193:B:TYR:HB3	1:212:B:TYR:HB3	4	0.21
(1,3753)	1:193:B:TYR:HA	1:196:B:VAL:H	4	0.21
(1,3725)	1:190:B:LEU:HD11	1:212:B:TYR:HA	7	0.21
(1,3725)	1:190:B:LEU:HD12	1:212:B:TYR:HA	7	0.21
(1,3725)	1:190:B:LEU:HD13	1:212:B:TYR:HA	7	0.21
(1,3722)	1:190:B:LEU:HA	1:212:B:TYR:HA	10	0.21
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	2	0.21
(1,3681)	1:183:B:GLN:H	1:185:B:LYS:H	13	0.21
(1,3671)	1:181:B:TYR:HE1	1:218:B:LYS:HB2	1	0.21
(1,3671)	1:181:B:TYR:HE1	1:218:B:LYS:HB3	1	0.21
(1,3671)	1:181:B:TYR:HE2	1:218:B:LYS:HB2	1	0.21
(1,3671)	1:181:B:TYR:HE2	1:218:B:LYS:HB3	1	0.21
(1,3646)	1:180:B:LYS:HA	1:185:B:LYS:H	8	0.21
(1,3626)	1:178:B:PHE:HA	1:182:B:ALA:H	14	0.21
(1,3572)	1:173:B:TYR:HB2	1:196:B:VAL:H	9	0.21
(1,3572)	1:173:B:TYR:HB3	1:196:B:VAL:H	9	0.21
(1,3572)	1:173:B:TYR:HB2	1:196:B:VAL:H	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3572)	1:173:B:TYR:HB3	1:196:B:VAL:H	15	0.21
(1,3551)	1:171:B:ARG:HA	1:175:B:ARG:H	20	0.21
(1,3461)	1:162:B:ALA:HB1	1:172:B:GLY:H	11	0.21
(1,3461)	1:162:B:ALA:HB2	1:172:B:GLY:H	11	0.21
(1,3461)	1:162:B:ALA:HB3	1:172:B:GLY:H	11	0.21
(1,3419)	1:158:B:ASP:HA	1:161:B:SER:H	3	0.21
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	14	0.21
(1,3259)	1:143:B:ALA:HA	1:158:B:ASP:H	12	0.21
(1,3159)	1:135:B:ASN:HB2	1:138:B:TYR:H	17	0.21
(1,3159)	1:135:B:ASN:HB3	1:138:B:TYR:H	17	0.21
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD11	17	0.21
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD12	17	0.21
(1,3090)	1:126:B:THR:HA	1:129:B:ILE:HD13	17	0.21
(1,3079)	1:125:B:TYR:HB2	1:142:B:ARG:HD2	20	0.21
(1,3079)	1:125:B:TYR:HB2	1:142:B:ARG:HD3	20	0.21
(1,3079)	1:125:B:TYR:HB3	1:142:B:ARG:HD2	20	0.21
(1,3079)	1:125:B:TYR:HB3	1:142:B:ARG:HD3	20	0.21
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	2	0.21
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	2	0.21
(1,3067)	1:125:B:TYR:HA	1:129:B:ILE:H	9	0.21
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB1	5	0.21
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB2	5	0.21
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB3	5	0.21
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB1	5	0.21
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB2	5	0.21
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB3	5	0.21
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB1	5	0.21
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB2	5	0.21
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB3	5	0.21
(1,2941)	1:113:B:MET:HA	1:118:B:TYR:HA	7	0.21
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	20	0.21
(1,2926)	1:112:B:ALA:HB1	1:121:B:ALA:H	9	0.21
(1,2926)	1:112:B:ALA:HB2	1:121:B:ALA:H	9	0.21
(1,2926)	1:112:B:ALA:HB3	1:121:B:ALA:H	9	0.21
(1,2919)	1:112:B:ALA:HA	1:117:B:ASP:H	15	0.21
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB1	4	0.21
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB2	4	0.21
(1,2862)	1:106:B:LYS:HA	1:128:B:ALA:HB3	4	0.21
(1,2816)	1:102:B:ALA:HB1	1:132:B:LEU:H	2	0.21
(1,2816)	1:102:B:ALA:HB2	1:132:B:LEU:H	2	0.21
(1,2816)	1:102:B:ALA:HB3	1:132:B:LEU:H	2	0.21
(1,2816)	1:102:B:ALA:HB1	1:132:B:LEU:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2816)	1:102:B:ALA:HB2	1:132:B:LEU:H	9	0.21
(1,2816)	1:102:B:ALA:HB3	1:132:B:LEU:H	9	0.21
(1,2789)	1:101:B:LYS:H	1:103:B:GLU:H	11	0.21
(1,2775)	1:99:B:LYS:H	1:100:B:ALA:H	9	0.21
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	11	0.21
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB2	17	0.21
(1,2751)	1:95:B:ASP:HA	1:97:B:GLU:HB3	17	0.21
(1,2707)	1:222:A:SER:HA	1:225:A:LEU:H	9	0.21
(1,2598)	1:209:A:LYS:HA	1:211:A:ASP:H	11	0.21
(1,2573)	1:206:A:GLU:HB2	1:207:A:ALA:H	19	0.21
(1,2573)	1:206:A:GLU:HB3	1:207:A:ALA:H	19	0.21
(1,2572)	1:206:A:GLU:HA	1:210:A:ARG:H	10	0.21
(1,2522)	1:199:A:ILE:HA	1:201:A:GLY:H	16	0.21
(1,2512)	1:198:A:ASP:H	1:200:A:GLU:H	8	0.21
(1,2502)	1:197:A:LEU:HA	1:200:A:GLU:H	15	0.21
(1,2451)	1:193:A:TYR:HA	1:212:A:TYR:HA	4	0.21
(1,2422)	1:190:A:LEU:HD11	1:216:A:LYS:HA	8	0.21
(1,2422)	1:190:A:LEU:HD12	1:216:A:LYS:HA	8	0.21
(1,2422)	1:190:A:LEU:HD13	1:216:A:LYS:HA	8	0.21
(1,2380)	1:185:A:LYS:H	1:186:A:PRO:HA	10	0.21
(1,2359)	1:181:A:TYR:HA	1:189:A:ALA:H	11	0.21
(1,2236)	1:170:A:PHE:HE2	1:171:A:ARG:HD2	2	0.21
(1,2232)	1:170:A:PHE:HE1	1:171:A:ARG:HD2	14	0.21
(1,2232)	1:170:A:PHE:HE1	1:171:A:ARG:HD3	14	0.21
(1,2232)	1:170:A:PHE:HE2	1:171:A:ARG:HD2	14	0.21
(1,2232)	1:170:A:PHE:HE2	1:171:A:ARG:HD3	14	0.21
(1,2227)	1:170:A:PHE:HD1	1:196:A:VAL:HA	3	0.21
(1,2227)	1:170:A:PHE:HD2	1:196:A:VAL:HA	3	0.21
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG21	3	0.21
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG22	3	0.21
(1,2223)	1:170:A:PHE:HB2	1:199:A:ILE:HG23	3	0.21
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG21	3	0.21
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG22	3	0.21
(1,2223)	1:170:A:PHE:HB3	1:199:A:ILE:HG23	3	0.21
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	1	0.21
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	7	0.21
(1,1946)	1:143:A:ALA:H	1:155:A:ALA:HA	15	0.21
(1,1919)	1:140:A:ALA:H	1:162:A:ALA:HA	2	0.21
(1,1862)	1:136:A:ALA:HA	1:162:A:ALA:HA	3	0.21
(1,1853)	1:135:A:ASN:HB2	1:138:A:TYR:H	8	0.21
(1,1853)	1:135:A:ASN:HB3	1:138:A:TYR:H	8	0.21
(1,1820)	1:129:A:ILE:HD11	1:139:A:TYR:HA	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:129:A:ILE:HD12	1:139:A:TYR:HA	3	0.21
(1,1820)	1:129:A:ILE:HD13	1:139:A:TYR:HA	3	0.21
(1,1788)	1:127:A:GLU:H	1:130:A:LYS:H	3	0.21
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB2	12	0.21
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	12	0.21
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB2	12	0.21
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB3	12	0.21
(1,1773)	1:125:A:TYR:HB2	1:142:A:ARG:HD2	4	0.21
(1,1773)	1:125:A:TYR:HB2	1:142:A:ARG:HD3	4	0.21
(1,1773)	1:125:A:TYR:HB3	1:142:A:ARG:HD2	4	0.21
(1,1773)	1:125:A:TYR:HB3	1:142:A:ARG:HD3	4	0.21
(1,1721)	1:121:A:ALA:HA	1:125:A:TYR:H	4	0.21
(1,1689)	1:118:A:TYR:HA	1:145:A:ALA:HA	3	0.21
(1,1645)	1:113:A:MET:HE1	1:145:A:ALA:H	19	0.21
(1,1645)	1:113:A:MET:HE2	1:145:A:ALA:H	19	0.21
(1,1645)	1:113:A:MET:HE3	1:145:A:ALA:H	19	0.21
(1,1642)	1:113:A:MET:HE1	1:142:A:ARG:HA	3	0.21
(1,1642)	1:113:A:MET:HE2	1:142:A:ARG:HA	3	0.21
(1,1642)	1:113:A:MET:HE3	1:142:A:ARG:HA	3	0.21
(1,1593)	1:110:A:ASN:HA	1:113:A:MET:H	17	0.21
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	11	0.21
(1,1565)	1:107:A:MET:HA	1:110:A:ASN:H	11	0.21
(1,1490)	1:101:A:LYS:HA	1:104:A:ASP:H	9	0.21
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	4	0.21
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	4	0.21
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	4	0.21
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	20	0.21
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	20	0.21
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	20	0.21
(1,1440)	1:95:A:ASP:H	1:96:A:ALA:H	10	0.21
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	1	0.21
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	1	0.21
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	1	0.21
(1,1370)	1:42:A:GLU:HB2	1:32:B:SER:HG	20	0.21
(1,1370)	1:42:A:GLU:HB3	1:32:B:SER:HG	20	0.21
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	19	0.21
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	19	0.21
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	19	0.21
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	19	0.21
(1,1290)	1:16:A:PHE:HE1	1:12:B:ILE:HD13	20	0.21
(1,1290)	1:16:A:PHE:HE2	1:12:B:ILE:HD13	20	0.21
(1,1252)	1:12:A:ILE:HA	1:12:B:ILE:HD11	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1252)	1:12:A:ILE:HA	1:12:B:ILE:HD12	8	0.21
(1,1252)	1:12:A:ILE:HA	1:12:B:ILE:HD13	8	0.21
(1,1247)	1:9:A:ALA:H	1:16:B:PHE:HE1	19	0.21
(1,1222)	1:2:A:SER:HA	1:68:B:ILE:H	9	0.21
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD11	16	0.21
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD12	16	0.21
(1,1189)	1:66:B:ALA:HA	1:69:B:LEU:HD13	16	0.21
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	7	0.21
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	7	0.21
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	7	0.21
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	17	0.21
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	11	0.21
(1,1146)	1:60:B:PHE:HA	1:63:B:GLN:H	13	0.21
(1,1127)	1:58:B:SER:H	1:59:B:GLU:HA	12	0.21
(1,1127)	1:58:B:SER:H	1:59:B:GLU:HA	13	0.21
(1,1121)	1:56:B:GLY:HA2	1:58:B:SER:H	13	0.21
(1,1121)	1:56:B:GLY:HA3	1:58:B:SER:H	13	0.21
(1,1116)	1:55:B:LEU:HD21	1:71:B:SER:HA	1	0.21
(1,1116)	1:55:B:LEU:HD22	1:71:B:SER:HA	1	0.21
(1,1116)	1:55:B:LEU:HD23	1:71:B:SER:HA	1	0.21
(1,1064)	1:48:B:ARG:H	1:50:B:ALA:H	2	0.21
(1,1025)	1:43:B:ALA:HA	1:45:B:GLY:H	14	0.21
(1,852)	1:22:B:LYS:H	1:24:B:GLU:H	18	0.21
(1,725)	1:13:B:VAL:HA	1:16:B:PHE:H	8	0.21
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD21	20	0.21
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD22	20	0.21
(1,702)	1:11:B:LEU:HA	1:55:B:LEU:HD23	20	0.21
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD21	11	0.21
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD22	11	0.21
(1,699)	1:11:B:LEU:H	1:55:B:LEU:HD23	11	0.21
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	1	0.21
(1,561)	1:63:A:GLN:HA	1:67:A:ASP:H	5	0.21
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE21	7	0.21
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE22	7	0.21
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE21	7	0.21
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE22	7	0.21
(1,348)	1:36:A:ALA:H	1:38:A:ASP:H	3	0.21
(1,94)	1:11:A:LEU:HA	1:71:A:SER:HA	3	0.21
(1,77)	1:10:A:ALA:HA	1:51:A:VAL:HA	14	0.21
(1,4188)	1:323:B:MET:H	1:324:B:ALA:H	12	0.2
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	2	0.2
(1,4169)	1:300:B:GLU:H	1:301:B:GLY:H	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4147)	1:239:B:ASP:H	1:240:B:ALA:H	16	0.2
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	11	0.2
(1,4092)	1:325:A:GLY:H	1:326:A:ASN:H	10	0.2
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	3	0.2
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	11	0.2
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	14	0.2
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	16	0.2
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	16	0.2
(1,3966)	1:217:B:LYS:H	1:220:B:GLU:H	17	0.2
(1,3946)	1:214:B:SER:HA	1:217:B:LYS:H	20	0.2
(1,3908)	1:210:B:ARG:H	1:213:B:GLU:H	11	0.2
(1,3894)	1:208:B:MET:H	1:211:B:ASP:H	18	0.2
(1,3765)	1:193:B:TYR:HD1	1:212:B:TYR:H	10	0.2
(1,3765)	1:193:B:TYR:HD2	1:212:B:TYR:H	10	0.2
(1,3721)	1:190:B:LEU:HA	1:194:B:LYS:H	2	0.2
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG21	19	0.2
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG22	19	0.2
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG23	19	0.2
(1,3704)	1:188:B:GLU:HA	1:191:B:GLU:H	12	0.2
(1,3597)	1:176:B:LEU:HA	1:178:B:PHE:H	5	0.2
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB1	20	0.2
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB2	20	0.2
(1,3568)	1:173:B:TYR:HA	1:192:B:ALA:HB3	20	0.2
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	10	0.2
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	10	0.2
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	7	0.2
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	14	0.2
(1,3420)	1:158:B:ASP:HA	1:162:B:ALA:H	3	0.2
(1,3419)	1:158:B:ASP:HA	1:161:B:SER:H	6	0.2
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	10	0.2
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB2	16	0.2
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB3	16	0.2
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB2	16	0.2
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB3	16	0.2
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB2	16	0.2
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB3	16	0.2
(1,3248)	1:142:B:ARG:HA	1:145:B:ALA:H	8	0.2
(1,3148)	1:134:B:THR:H	1:135:B:ASN:HA	6	0.2
(1,3118)	1:129:B:ILE:HA	1:132:B:LEU:H	3	0.2
(1,3114)	1:129:B:ILE:H	1:138:B:TYR:HB2	18	0.2
(1,3114)	1:129:B:ILE:H	1:138:B:TYR:HB3	18	0.2
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	18	0.2
(1,3067)	1:125:B:TYR:HA	1:129:B:ILE:H	20	0.2
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	15	0.2
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	15	0.2
(1,2933)	1:113:B:MET:H	1:121:B:ALA:HA	4	0.2
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	2	0.2
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG21	11	0.2
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG22	11	0.2
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG23	11	0.2
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG21	11	0.2
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG22	11	0.2
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG23	11	0.2
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG21	11	0.2
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG22	11	0.2
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG23	11	0.2
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE1	11	0.2
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE2	11	0.2
(1,2834)	1:104:B:ASP:HA	1:107:B:MET:HE3	11	0.2
(1,2833)	1:104:B:ASP:HA	1:107:B:MET:H	15	0.2
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD11	3	0.2
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD12	3	0.2
(1,2690)	1:220:A:GLU:HA	1:223:A:LEU:HD13	3	0.2
(1,2666)	1:217:A:LYS:HG2	1:218:A:LYS:H	18	0.2
(1,2666)	1:217:A:LYS:HG3	1:218:A:LYS:H	18	0.2
(1,2645)	1:215:A:ALA:H	1:218:A:LYS:H	17	0.2
(1,2517)	1:198:A:ASP:HA	1:201:A:GLY:H	16	0.2
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD11	13	0.2
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD12	13	0.2
(1,2474)	1:194:A:LYS:HA	1:197:A:LEU:HD13	13	0.2
(1,2390)	1:187:A:GLU:HA	1:190:A:LEU:H	14	0.2
(1,2335)	1:180:A:LYS:H	1:189:A:ALA:HA	16	0.2
(1,2304)	1:177:A:GLY:HA2	1:189:A:ALA:H	1	0.2
(1,2304)	1:177:A:GLY:HA3	1:189:A:ALA:H	1	0.2
(1,2261)	1:173:A:TYR:HA	1:192:A:ALA:HA	15	0.2
(1,2175)	1:164:A:SER:HA	1:166:A:ASP:H	17	0.2
(1,1997)	1:147:A:SER:H	1:151:A:GLU:H	7	0.2
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB2	15	0.2
(1,1774)	1:125:A:TYR:HE1	1:141:A:ASN:HB3	15	0.2
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB2	15	0.2
(1,1774)	1:125:A:TYR:HE2	1:141:A:ASN:HB3	15	0.2
(1,1713)	1:120:A:LEU:HA	1:123:A:ASN:H	11	0.2
(1,1696)	1:118:A:TYR:HB2	1:148:A:SER:HB2	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1696)	1:118:A:TYR:HB2	1:148:A:SER:HB3	16	0.2
(1,1696)	1:118:A:TYR:HB3	1:148:A:SER:HB2	16	0.2
(1,1696)	1:118:A:TYR:HB3	1:148:A:SER:HB3	16	0.2
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	13	0.2
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	13	0.2
(1,1680)	1:118:A:TYR:H	1:120:A:LEU:H	10	0.2
(1,1518)	1:103:A:GLU:HA	1:106:A:LYS:H	2	0.2
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	16	0.2
(1,1409)	1:63:A:GLN:HE21	1:68:B:ILE:HA	9	0.2
(1,1409)	1:63:A:GLN:HE22	1:68:B:ILE:HA	9	0.2
(1,1374)	1:43:A:ALA:HA	1:32:B:SER:H	2	0.2
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	1	0.2
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	1	0.2
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	1	0.2
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	1	0.2
(1,1353)	1:39:A:CYS:HB2	1:36:B:ALA:H	19	0.2
(1,1353)	1:39:A:CYS:HB3	1:36:B:ALA:H	19	0.2
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	14	0.2
(1,1336)	1:36:A:ALA:H	1:36:B:ALA:HA	9	0.2
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB2	11	0.2
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB3	11	0.2
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB2	11	0.2
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB3	11	0.2
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB2	11	0.2
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB3	11	0.2
(1,1319)	1:32:A:SER:HB2	1:42:B:GLU:H	3	0.2
(1,1319)	1:32:A:SER:HB3	1:42:B:GLU:H	3	0.2
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB2	12	0.2
(1,1317)	1:32:A:SER:HA	1:39:B:CYS:HB3	12	0.2
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	15	0.2
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	15	0.2
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	5	0.2
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	5	0.2
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	13	0.2
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	13	0.2
(1,1291)	1:16:A:PHE:HE1	1:40:B:ILE:HA	17	0.2
(1,1291)	1:16:A:PHE:HE2	1:40:B:ILE:HA	17	0.2
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD11	6	0.2
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD12	6	0.2
(1,1277)	1:15:A:TYR:HH	1:8:B:ILE:HD13	6	0.2
(1,1274)	1:15:A:TYR:HH	1:5:B:LYS:HA	3	0.2
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD11	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD12	2	0.2
(1,1232)	1:5:A:LYS:H	1:19:B:ILE:HD13	2	0.2
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	1	0.2
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	2	0.2
(1,1170)	1:63:B:GLN:HA	1:67:B:ASP:H	5	0.2
(1,1127)	1:58:B:SER:H	1:59:B:GLU:HA	7	0.2
(1,1112)	1:55:B:LEU:HA	1:57:B:LYS:H	1	0.2
(1,1104)	1:54:B:ILE:HA	1:57:B:LYS:H	8	0.2
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	12	0.2
(1,1054)	1:47:B:GLU:H	1:50:B:ALA:H	8	0.2
(1,953)	1:35:B:VAL:HA	1:38:B:ASP:HA	17	0.2
(1,860)	1:23:B:LYS:HA	1:25:B:ILE:H	16	0.2
(1,781)	1:16:B:PHE:HA	1:18:B:SER:HB2	4	0.2
(1,781)	1:16:B:PHE:HA	1:18:B:SER:HB3	4	0.2
(1,780)	1:16:B:PHE:HA	1:18:B:SER:H	7	0.2
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	2	0.2
(1,550)	1:61:A:LYS:H	1:63:A:GLN:H	13	0.2
(1,524)	1:58:A:SER:HB2	1:60:A:PHE:H	3	0.2
(1,524)	1:58:A:SER:HB3	1:60:A:PHE:H	3	0.2
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB2	6	0.2
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB3	6	0.2
(1,401)	1:41:A:SER:HA	1:45:A:GLY:H	3	0.2
(1,211)	1:18:A:SER:HA	1:22:A:LYS:H	15	0.2
(1,201)	1:17:A:SER:HA	1:21:A:GLU:H	17	0.2
(1,4205)	1:342:B:ASN:H	1:343:B:GLU:H	4	0.19
(1,4204)	1:341:B:ASP:H	1:342:B:ASN:H	11	0.19
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	15	0.19
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	18	0.19
(1,4167)	1:294:B:SER:H	1:295:B:ILE:H	3	0.19
(1,4162)	1:256:B:LEU:H	1:257:B:GLY:H	9	0.19
(1,4109)	1:344:A:ASN:H	1:345:A:LYS:H	8	0.19
(1,4074)	1:303:A:ALA:H	1:304:A:SER:H	6	0.19
(1,4072)	1:301:A:GLY:H	1:302:A:PHE:H	2	0.19
(1,4068)	1:260:A:LEU:H	1:261:A:GLY:H	10	0.19
(1,4052)	1:242:A:GLN:H	1:243:A:GLY:H	17	0.19
(1,4045)	1:235:A:ASP:H	1:236:A:ALA:H	2	0.19
(1,3980)	1:218:B:LYS:HA	1:222:B:SER:H	8	0.19
(1,3938)	1:213:B:GLU:HA	1:216:B:LYS:H	16	0.19
(1,3876)	1:206:B:GLU:HA	1:209:B:LYS:H	14	0.19
(1,3832)	1:200:B:GLU:HA	1:203:B:ASN:H	12	0.19
(1,3823)	1:198:B:ASP:HA	1:201:B:GLY:H	14	0.19
(1,3809)	1:197:B:LEU:HA	1:201:B:GLY:H	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3801)	1:196:B:VAL:HG11	1:208:B:MET:HB2	9	0.19
(1,3801)	1:196:B:VAL:HG11	1:208:B:MET:HB3	9	0.19
(1,3801)	1:196:B:VAL:HG12	1:208:B:MET:HB2	9	0.19
(1,3801)	1:196:B:VAL:HG12	1:208:B:MET:HB3	9	0.19
(1,3801)	1:196:B:VAL:HG13	1:208:B:MET:HB2	9	0.19
(1,3801)	1:196:B:VAL:HG13	1:208:B:MET:HB3	9	0.19
(1,3791)	1:195:B:LYS:HA	1:199:B:ILE:H	5	0.19
(1,3775)	1:194:B:LYS:H	1:212:B:TYR:HA	1	0.19
(1,3765)	1:193:B:TYR:HD1	1:212:B:TYR:H	5	0.19
(1,3765)	1:193:B:TYR:HD2	1:212:B:TYR:H	5	0.19
(1,3763)	1:193:B:TYR:HD1	1:211:B:ASP:HA	11	0.19
(1,3763)	1:193:B:TYR:HD2	1:211:B:ASP:HA	11	0.19
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	11	0.19
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	4	0.19
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	4	0.19
(1,3452)	1:161:B:SER:HA	1:165:B:ILE:H	9	0.19
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	6	0.19
(1,3343)	1:150:B:LYS:HZ1	1:152:B:TYR:HE1	5	0.19
(1,3343)	1:150:B:LYS:HZ1	1:152:B:TYR:HE2	5	0.19
(1,3343)	1:150:B:LYS:HZ2	1:152:B:TYR:HE1	5	0.19
(1,3343)	1:150:B:LYS:HZ2	1:152:B:TYR:HE2	5	0.19
(1,3343)	1:150:B:LYS:HZ3	1:152:B:TYR:HE1	5	0.19
(1,3343)	1:150:B:LYS:HZ3	1:152:B:TYR:HE2	5	0.19
(1,3275)	1:144:B:ALA:HA	1:147:B:SER:H	1	0.19
(1,3195)	1:138:B:TYR:HA	1:141:B:ASN:H	1	0.19
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	5	0.19
(1,3145)	1:132:B:LEU:HD11	1:134:B:THR:H	12	0.19
(1,3145)	1:132:B:LEU:HD12	1:134:B:THR:H	12	0.19
(1,3145)	1:132:B:LEU:HD13	1:134:B:THR:H	12	0.19
(1,3082)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	11	0.19
(1,3081)	1:125:B:TYR:HE1	1:142:B:ARG:HA	3	0.19
(1,3081)	1:125:B:TYR:HE2	1:142:B:ARG:HA	3	0.19
(1,3002)	1:118:B:TYR:HB2	1:148:B:SER:HB2	5	0.19
(1,3002)	1:118:B:TYR:HB2	1:148:B:SER:HB3	5	0.19
(1,3002)	1:118:B:TYR:HB3	1:148:B:SER:HB2	5	0.19
(1,3002)	1:118:B:TYR:HB3	1:148:B:SER:HB3	5	0.19
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE1	20	0.19
(1,2975)	1:116:B:LYS:HA	1:118:B:TYR:HE2	20	0.19
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	10	0.19
(1,2919)	1:112:B:ALA:HA	1:117:B:ASP:H	3	0.19
(1,2871)	1:107:B:MET:HA	1:110:B:ASN:H	3	0.19
(1,2843)	1:105:B:LEU:HA	1:124:B:LYS:HA	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2828)	1:104:B:ASP:H	1:107:B:MET:H	18	0.19
(1,2790)	1:101:B:LYS:H	1:104:B:ASP:H	3	0.19
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	4	0.19
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD11	19	0.19
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD12	19	0.19
(1,2708)	1:222:A:SER:HA	1:225:A:LEU:HD13	19	0.19
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	11	0.19
(1,2664)	1:217:A:LYS:HA	1:220:A:GLU:H	12	0.19
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	1	0.19
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	8	0.19
(1,2606)	1:210:A:ARG:HA	1:213:A:GLU:H	11	0.19
(1,2558)	1:205:A:THR:HA	1:207:A:ALA:H	20	0.19
(1,2502)	1:197:A:LEU:HA	1:200:A:GLU:H	8	0.19
(1,2469)	1:194:A:LYS:H	1:212:A:TYR:HA	10	0.19
(1,2443)	1:193:A:TYR:H	1:212:A:TYR:HA	13	0.19
(1,2432)	1:191:A:GLU:HA	1:195:A:LYS:H	19	0.19
(1,2423)	1:190:A:LEU:HD21	1:216:A:LYS:HA	18	0.19
(1,2423)	1:190:A:LEU:HD22	1:216:A:LYS:HA	18	0.19
(1,2423)	1:190:A:LEU:HD23	1:216:A:LYS:HA	18	0.19
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD2	20	0.19
(1,2366)	1:181:A:TYR:HE1	1:218:A:LYS:HD3	20	0.19
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD2	20	0.19
(1,2366)	1:181:A:TYR:HE2	1:218:A:LYS:HD3	20	0.19
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD2	1	0.19
(1,2363)	1:181:A:TYR:HD1	1:218:A:LYS:HD3	1	0.19
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD2	1	0.19
(1,2363)	1:181:A:TYR:HD2	1:218:A:LYS:HD3	1	0.19
(1,2349)	1:181:A:TYR:H	1:186:A:PRO:HA	1	0.19
(1,2205)	1:169:A:TYR:HD1	1:171:A:ARG:H	10	0.19
(1,2205)	1:169:A:TYR:HD2	1:171:A:ARG:H	19	0.19
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	13	0.19
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	13	0.19
(1,2138)	1:160:A:GLU:HA	1:164:A:SER:H	3	0.19
(1,2136)	1:160:A:GLU:HA	1:163:A:ILE:H	15	0.19
(1,2131)	1:160:A:GLU:H	1:163:A:ILE:H	12	0.19
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	5	0.19
(1,2029)	1:150:A:LYS:HA	1:152:A:TYR:HA	1	0.19
(1,2010)	1:147:A:SER:HB2	1:178:A:PHE:HB2	14	0.19
(1,2010)	1:147:A:SER:HB2	1:178:A:PHE:HB3	14	0.19
(1,2010)	1:147:A:SER:HB3	1:178:A:PHE:HB2	14	0.19
(1,2010)	1:147:A:SER:HB3	1:178:A:PHE:HB3	14	0.19
(1,1900)	1:139:A:TYR:HA	1:158:A:ASP:HA	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1892)	1:139:A:TYR:H	1:141:A:ASN:H	2	0.19
(1,1889)	1:138:A:TYR:HA	1:141:A:ASN:H	12	0.19
(1,1876)	1:137:A:ILE:H	1:169:A:TYR:HE2	3	0.19
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB2	14	0.19
(1,1824)	1:129:A:ILE:HD11	1:142:A:ARG:HB3	14	0.19
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB2	14	0.19
(1,1824)	1:129:A:ILE:HD12	1:142:A:ARG:HB3	14	0.19
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB2	14	0.19
(1,1824)	1:129:A:ILE:HD13	1:142:A:ARG:HB3	14	0.19
(1,1808)	1:129:A:ILE:H	1:138:A:TYR:HB2	14	0.19
(1,1808)	1:129:A:ILE:H	1:138:A:TYR:HB3	14	0.19
(1,1762)	1:125:A:TYR:HA	1:138:A:TYR:HA	3	0.19
(1,1738)	1:122:A:ILE:HD11	1:146:A:HIS:HA	3	0.19
(1,1738)	1:122:A:ILE:HD12	1:146:A:HIS:HA	3	0.19
(1,1738)	1:122:A:ILE:HD13	1:146:A:HIS:HA	3	0.19
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD1	2	0.19
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD2	2	0.19
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD1	20	0.19
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD2	20	0.19
(1,1646)	1:113:A:MET:HE1	1:145:A:ALA:HA	6	0.19
(1,1646)	1:113:A:MET:HE2	1:145:A:ALA:HA	6	0.19
(1,1646)	1:113:A:MET:HE3	1:145:A:ALA:HA	6	0.19
(1,1537)	1:105:A:LEU:HA	1:124:A:LYS:HA	8	0.19
(1,1519)	1:103:A:GLU:HA	1:107:A:MET:H	7	0.19
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD11	3	0.19
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD12	3	0.19
(1,1500)	1:102:A:ALA:HA	1:105:A:LEU:HD13	3	0.19
(1,1444)	1:95:A:ASP:HA	1:97:A:GLU:H	17	0.19
(1,1432)	1:93:A:GLU:HA	1:96:A:ALA:H	11	0.19
(1,1399)	1:44:A:PHE:HE1	1:33:B:LEU:HD13	13	0.19
(1,1399)	1:44:A:PHE:HE2	1:33:B:LEU:HD13	13	0.19
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	4	0.19
(1,1338)	1:36:A:ALA:HA	1:36:B:ALA:HA	13	0.19
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	6	0.19
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	6	0.19
(1,1248)	1:9:A:ALA:H	1:16:B:PHE:HZ	15	0.19
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG12	14	0.19
(1,1237)	1:5:A:LYS:HB2	1:19:B:ILE:HG13	14	0.19
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG12	14	0.19
(1,1237)	1:5:A:LYS:HB3	1:19:B:ILE:HG13	14	0.19
(1,1214)	1:71:B:SER:H	1:72:B:ALA:HA	15	0.19
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:67:B:ASP:H	1:68:B:ILE:H	1	0.19
(1,1170)	1:63:B:GLN:HA	1:67:B:ASP:H	18	0.19
(1,1165)	1:62:B:GLY:H	1:64:B:HIS:H	11	0.19
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	18	0.19
(1,1133)	1:58:B:SER:HB2	1:60:B:PHE:H	9	0.19
(1,1133)	1:58:B:SER:HB3	1:60:B:PHE:H	9	0.19
(1,1133)	1:58:B:SER:HB2	1:60:B:PHE:H	11	0.19
(1,1133)	1:58:B:SER:HB3	1:60:B:PHE:H	11	0.19
(1,1121)	1:56:B:GLY:HA2	1:58:B:SER:H	7	0.19
(1,1121)	1:56:B:GLY:HA3	1:58:B:SER:H	7	0.19
(1,1110)	1:55:B:LEU:H	1:57:B:LYS:H	18	0.19
(1,1110)	1:55:B:LEU:H	1:57:B:LYS:H	20	0.19
(1,1059)	1:47:B:GLU:HA	1:50:B:ALA:H	1	0.19
(1,1054)	1:47:B:GLU:H	1:50:B:ALA:H	4	0.19
(1,1015)	1:41:B:SER:HA	1:46:B:PHE:HE1	3	0.19
(1,857)	1:23:B:LYS:H	1:25:B:ILE:H	1	0.19
(1,777)	1:16:B:PHE:H	1:19:B:ILE:H	7	0.19
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	6	0.19
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	6	0.19
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD21	12	0.19
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD22	12	0.19
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD23	12	0.19
(1,623)	1:4:B:SER:H	1:7:B:GLU:H	3	0.19
(1,579)	1:66:A:ALA:HA	1:69:A:LEU:HA	10	0.19
(1,561)	1:63:A:GLN:HA	1:67:A:ASP:H	20	0.19
(1,554)	1:62:A:GLY:H	1:63:A:GLN:H	1	0.19
(1,537)	1:60:A:PHE:HA	1:63:A:GLN:H	5	0.19
(1,529)	1:59:A:GLU:HA	1:64:A:HIS:HA	15	0.19
(1,503)	1:55:A:LEU:HA	1:57:A:LYS:H	12	0.19
(1,458)	1:48:A:ARG:HA	1:50:A:ALA:H	8	0.19
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	12	0.19
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	8	0.19
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	8	0.19
(1,362)	1:37:A:MET:HA	1:40:A:ILE:H	8	0.19
(1,336)	1:34:A:ASN:HA	1:38:A:ASP:H	8	0.19
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	10	0.19
(1,211)	1:18:A:SER:HA	1:22:A:LYS:H	8	0.19
(1,163)	1:15:A:TYR:HD1	1:18:A:SER:HB2	18	0.19
(1,163)	1:15:A:TYR:HD1	1:18:A:SER:HB3	18	0.19
(1,163)	1:15:A:TYR:HD2	1:18:A:SER:HB2	18	0.19
(1,163)	1:15:A:TYR:HD2	1:18:A:SER:HB3	18	0.19
(1,4207)	1:344:B:ASN:H	1:345:B:LYS:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4199)	1:334:B:GLN:H	1:335:B:SER:H	20	0.18
(1,4168)	1:299:B:ALA:H	1:300:B:GLU:H	20	0.18
(1,4161)	1:255:B:LEU:H	1:256:B:LEU:H	17	0.18
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	3	0.18
(1,4111)	1:346:A:GLN:H	1:347:A:TYR:H	10	0.18
(1,4107)	1:342:A:ASN:H	1:343:A:GLU:H	20	0.18
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	3	0.18
(1,4092)	1:325:A:GLY:H	1:326:A:ASN:H	8	0.18
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	19	0.18
(1,4002)	1:221:B:GLN:HA	1:223:B:LEU:H	10	0.18
(1,3948)	1:214:B:SER:HB2	1:215:B:ALA:H	5	0.18
(1,3948)	1:214:B:SER:HB3	1:215:B:ALA:H	5	0.18
(1,3946)	1:214:B:SER:HA	1:217:B:LYS:H	12	0.18
(1,3721)	1:190:B:LEU:HA	1:194:B:LYS:H	11	0.18
(1,3686)	1:185:B:LYS:H	1:186:B:PRO:HA	19	0.18
(1,3665)	1:181:B:TYR:HA	1:189:B:ALA:H	5	0.18
(1,3627)	1:178:B:PHE:HA	1:193:B:TYR:HE1	3	0.18
(1,3627)	1:178:B:PHE:HA	1:193:B:TYR:HE2	3	0.18
(1,3600)	1:176:B:LEU:HD11	1:180:B:LYS:H	5	0.18
(1,3600)	1:176:B:LEU:HD12	1:180:B:LYS:H	5	0.18
(1,3600)	1:176:B:LEU:HD13	1:180:B:LYS:H	5	0.18
(1,3567)	1:173:B:TYR:HA	1:192:B:ALA:HA	16	0.18
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	6	0.18
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	6	0.18
(1,3502)	1:169:B:TYR:HD1	1:170:B:PHE:H	14	0.18
(1,3502)	1:169:B:TYR:HD2	1:170:B:PHE:H	14	0.18
(1,3410)	1:157:B:LYS:HA	1:159:B:ALA:H	3	0.18
(1,3337)	1:150:B:LYS:HB2	1:152:B:TYR:HD1	9	0.18
(1,3337)	1:150:B:LYS:HB2	1:152:B:TYR:HD2	9	0.18
(1,3337)	1:150:B:LYS:HB3	1:152:B:TYR:HD1	9	0.18
(1,3337)	1:150:B:LYS:HB3	1:152:B:TYR:HD2	9	0.18
(1,3241)	1:141:B:ASN:HA	1:145:B:ALA:H	4	0.18
(1,3194)	1:138:B:TYR:HA	1:140:B:ALA:H	7	0.18
(1,3119)	1:129:B:ILE:HA	1:133:B:PRO:HA	8	0.18
(1,3000)	1:118:B:TYR:HB2	1:145:B:ALA:HB2	5	0.18
(1,3000)	1:118:B:TYR:HB3	1:145:B:ALA:HB2	5	0.18
(1,2992)	1:118:B:TYR:HA	1:121:B:ALA:H	9	0.18
(1,2977)	1:116:B:LYS:HB2	1:118:B:TYR:HD1	11	0.18
(1,2977)	1:116:B:LYS:HB2	1:118:B:TYR:HD2	11	0.18
(1,2977)	1:116:B:LYS:HB3	1:118:B:TYR:HD1	11	0.18
(1,2977)	1:116:B:LYS:HB3	1:118:B:TYR:HD2	11	0.18
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE1	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2968)	1:116:B:LYS:H	1:118:B:TYR:HE2	5	0.18
(1,2951)	1:113:B:MET:HE1	1:145:B:ALA:H	4	0.18
(1,2951)	1:113:B:MET:HE2	1:145:B:ALA:H	4	0.18
(1,2951)	1:113:B:MET:HE3	1:145:B:ALA:H	4	0.18
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	8	0.18
(1,2861)	1:106:B:LYS:HA	1:125:B:TYR:HA	18	0.18
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG21	3	0.18
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG22	3	0.18
(1,2810)	1:102:B:ALA:HA	1:131:B:VAL:HG23	3	0.18
(1,2800)	1:102:B:ALA:H	1:105:B:LEU:H	20	0.18
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB1	1	0.18
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB2	1	0.18
(1,2781)	1:99:B:LYS:HA	1:102:B:ALA:HB3	1	0.18
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG11	4	0.18
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG12	4	0.18
(1,2774)	1:98:B:THR:HA	1:131:B:VAL:HG13	4	0.18
(1,2756)	1:96:B:ALA:H	1:98:B:THR:H	9	0.18
(1,2732)	1:227:A:LYS:HB2	1:228:A:THR:H	11	0.18
(1,2732)	1:227:A:LYS:HB3	1:228:A:THR:H	11	0.18
(1,2716)	1:224:A:ASN:H	1:226:A:GLU:H	5	0.18
(1,2713)	1:223:A:LEU:HA	1:225:A:LEU:H	7	0.18
(1,2710)	1:223:A:LEU:H	1:225:A:LEU:H	14	0.18
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	14	0.18
(1,2653)	1:216:A:LYS:H	1:218:A:LYS:H	6	0.18
(1,2649)	1:215:A:ALA:HA	1:218:A:LYS:H	13	0.18
(1,2642)	1:214:A:SER:HB2	1:215:A:ALA:H	6	0.18
(1,2642)	1:214:A:SER:HB3	1:215:A:ALA:H	6	0.18
(1,2555)	1:205:A:THR:H	1:209:A:LYS:H	6	0.18
(1,2552)	1:205:A:THR:H	1:208:A:MET:H	2	0.18
(1,2418)	1:190:A:LEU:HA	1:216:A:LYS:H	4	0.18
(1,2416)	1:190:A:LEU:HA	1:212:A:TYR:HA	20	0.18
(1,2383)	1:185:A:LYS:HA	1:188:A:GLU:H	14	0.18
(1,2350)	1:181:A:TYR:H	1:189:A:ALA:H	11	0.18
(1,2300)	1:177:A:GLY:H	1:189:A:ALA:HA	3	0.18
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	19	0.18
(1,2243)	1:171:A:ARG:HA	1:174:A:SER:H	6	0.18
(1,2067)	1:153:A:ASP:HA	1:156:A:VAL:H	2	0.18
(1,2051)	1:152:A:TYR:HA	1:156:A:VAL:H	8	0.18
(1,2051)	1:152:A:TYR:HA	1:156:A:VAL:H	9	0.18
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	15	0.18
(1,1919)	1:140:A:ALA:H	1:162:A:ALA:HA	4	0.18
(1,1898)	1:139:A:TYR:HA	1:142:A:ARG:H	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1796)	1:128:A:ALA:H	1:131:A:VAL:H	8	0.18
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE1	2	0.18
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE2	2	0.18
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE1	2	0.18
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE2	2	0.18
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD1	10	0.18
(1,1668)	1:116:A:LYS:HA	1:118:A:TYR:HD2	10	0.18
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE1	8	0.18
(1,1662)	1:116:A:LYS:H	1:118:A:TYR:HE2	8	0.18
(1,1537)	1:105:A:LEU:HA	1:124:A:LYS:HA	5	0.18
(1,1537)	1:105:A:LEU:HA	1:124:A:LYS:HA	9	0.18
(1,1484)	1:101:A:LYS:H	1:104:A:ASP:H	17	0.18
(1,1474)	1:99:A:LYS:HA	1:102:A:ALA:H	19	0.18
(1,1444)	1:95:A:ASP:HA	1:97:A:GLU:H	9	0.18
(1,1440)	1:95:A:ASP:H	1:96:A:ALA:H	6	0.18
(1,1421)	1:69:A:LEU:H	1:2:B:SER:H	18	0.18
(1,1415)	1:68:A:ILE:H	1:2:B:SER:HA	1	0.18
(1,1410)	1:67:A:ASP:HA	1:61:B:LYS:H	2	0.18
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	10	0.18
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	18	0.18
(1,1311)	1:25:A:ILE:HD11	1:44:B:PHE:HA	9	0.18
(1,1311)	1:25:A:ILE:HD12	1:44:B:PHE:HA	9	0.18
(1,1311)	1:25:A:ILE:HD13	1:44:B:PHE:HA	9	0.18
(1,1266)	1:15:A:TYR:HE1	1:5:B:LYS:H	12	0.18
(1,1266)	1:15:A:TYR:HE2	1:5:B:LYS:H	12	0.18
(1,1259)	1:12:A:ILE:HD11	1:12:B:ILE:HA	17	0.18
(1,1259)	1:12:A:ILE:HD12	1:12:B:ILE:HA	17	0.18
(1,1259)	1:12:A:ILE:HD13	1:12:B:ILE:HA	17	0.18
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	5	0.18
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	5	0.18
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	5	0.18
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	5	0.18
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD11	12	0.18
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD12	12	0.18
(1,1235)	1:5:A:LYS:HA	1:19:B:ILE:HD13	12	0.18
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG12	9	0.18
(1,1234)	1:5:A:LYS:HA	1:19:B:ILE:HG13	9	0.18
(1,1181)	1:65:B:LEU:HD21	1:66:B:ALA:H	3	0.18
(1,1181)	1:65:B:LEU:HD22	1:66:B:ALA:H	3	0.18
(1,1181)	1:65:B:LEU:HD23	1:66:B:ALA:H	3	0.18
(1,1163)	1:62:B:GLY:H	1:63:B:GLN:H	10	0.18
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1150)	1:60:B:PHE:HB2	1:63:B:GLN:H	18	0.18
(1,1150)	1:60:B:PHE:HB3	1:63:B:GLN:H	18	0.18
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	4	0.18
(1,1009)	1:41:B:SER:HA	1:44:B:PHE:H	8	0.18
(1,957)	1:36:B:ALA:H	1:38:B:ASP:H	3	0.18
(1,880)	1:27:B:GLU:H	1:30:B:ALA:H	12	0.18
(1,834)	1:20:B:VAL:HA	1:23:B:LYS:HA	5	0.18
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD11	19	0.18
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD12	19	0.18
(1,580)	1:66:A:ALA:HA	1:69:A:LEU:HD13	19	0.18
(1,495)	1:54:A:ILE:HA	1:57:A:LYS:H	11	0.18
(1,474)	1:51:A:VAL:HA	1:55:A:LEU:H	3	0.18
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	17	0.18
(1,245)	1:22:A:LYS:HA	1:24:A:GLU:H	18	0.18
(1,224)	1:20:A:VAL:HA	1:23:A:LYS:H	17	0.18
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	2	0.18
(1,15)	1:4:A:SER:H	1:8:A:ILE:H	7	0.18
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	11	0.18
(1,4206)	1:343:B:GLU:H	1:344:B:ASN:H	17	0.17
(1,4199)	1:334:B:GLN:H	1:335:B:SER:H	7	0.17
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	7	0.17
(1,4124)	1:321:A:ARG:H	1:319:A:ALA:HB1	18	0.17
(1,4124)	1:321:A:ARG:H	1:319:A:ALA:HB2	18	0.17
(1,4124)	1:321:A:ARG:H	1:319:A:ALA:HB3	18	0.17
(1,4107)	1:342:A:ASN:H	1:343:A:GLU:H	14	0.17
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	2	0.17
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	12	0.17
(1,4095)	1:328:A:PHE:H	1:329:A:GLY:H	5	0.17
(1,4085)	1:316:A:ASN:H	1:317:A:ASN:H	12	0.17
(1,4078)	1:307:A:GLY:H	1:308:A:THR:H	20	0.17
(1,4077)	1:305:A:GLY:H	1:307:A:GLY:H	6	0.17
(1,4071)	1:300:A:GLU:H	1:301:A:GLY:H	5	0.17
(1,4055)	1:245:A:SER:H	1:246:A:ALA:H	3	0.17
(1,4044)	1:234:A:ARG:H	1:235:A:ASP:H	8	0.17
(1,4038)	1:227:B:LYS:HB2	1:228:B:THR:H	10	0.17
(1,4038)	1:227:B:LYS:HB3	1:228:B:THR:H	10	0.17
(1,4021)	1:224:B:ASN:H	1:225:B:LEU:H	20	0.17
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	17	0.17
(1,3828)	1:199:B:ILE:HA	1:201:B:GLY:H	19	0.17
(1,3792)	1:195:B:LYS:HB2	1:196:B:VAL:H	5	0.17
(1,3792)	1:195:B:LYS:HB3	1:196:B:VAL:H	5	0.17
(1,3721)	1:190:B:LEU:HA	1:194:B:LYS:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3689)	1:185:B:LYS:HA	1:188:B:GLU:H	13	0.17
(1,3610)	1:177:B:GLY:HA2	1:189:B:ALA:H	12	0.17
(1,3610)	1:177:B:GLY:HA3	1:189:B:ALA:H	12	0.17
(1,3595)	1:176:B:LEU:H	1:178:B:PHE:H	5	0.17
(1,3572)	1:173:B:TYR:HB2	1:196:B:VAL:H	12	0.17
(1,3572)	1:173:B:TYR:HB3	1:196:B:VAL:H	12	0.17
(1,3509)	1:169:B:TYR:HE1	1:172:B:GLY:H	8	0.17
(1,3509)	1:169:B:TYR:HE2	1:172:B:GLY:H	8	0.17
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	11	0.17
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	11	0.17
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	13	0.17
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	13	0.17
(1,3481)	1:164:B:SER:HA	1:166:B:ASP:H	7	0.17
(1,3396)	1:156:B:VAL:HA	1:176:B:LEU:HA	3	0.17
(1,3373)	1:153:B:ASP:HA	1:156:B:VAL:H	6	0.17
(1,3335)	1:150:B:LYS:HA	1:152:B:TYR:HA	8	0.17
(1,3312)	1:147:B:SER:HA	1:152:B:TYR:H	14	0.17
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB2	18	0.17
(1,3268)	1:143:B:ALA:HB1	1:175:B:ARG:HB3	18	0.17
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB2	18	0.17
(1,3268)	1:143:B:ALA:HB2	1:175:B:ARG:HB3	18	0.17
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB2	18	0.17
(1,3268)	1:143:B:ALA:HB3	1:175:B:ARG:HB3	18	0.17
(1,3262)	1:143:B:ALA:HB1	1:155:B:ALA:HA	8	0.17
(1,3262)	1:143:B:ALA:HB2	1:155:B:ALA:HA	8	0.17
(1,3262)	1:143:B:ALA:HB3	1:155:B:ALA:HA	8	0.17
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	9	0.17
(1,3214)	1:139:B:TYR:HD1	1:161:B:SER:HB2	4	0.17
(1,3214)	1:139:B:TYR:HD1	1:161:B:SER:HB3	4	0.17
(1,3214)	1:139:B:TYR:HD2	1:161:B:SER:HB2	4	0.17
(1,3214)	1:139:B:TYR:HD2	1:161:B:SER:HB3	4	0.17
(1,3190)	1:138:B:TYR:H	1:140:B:ALA:H	13	0.17
(1,3146)	1:132:B:LEU:HD21	1:134:B:THR:H	2	0.17
(1,3146)	1:132:B:LEU:HD22	1:134:B:THR:H	2	0.17
(1,3146)	1:132:B:LEU:HD23	1:134:B:THR:H	2	0.17
(1,3130)	1:129:B:ILE:HD11	1:142:B:ARG:HB2	20	0.17
(1,3130)	1:129:B:ILE:HD11	1:142:B:ARG:HB3	20	0.17
(1,3130)	1:129:B:ILE:HD12	1:142:B:ARG:HB2	20	0.17
(1,3130)	1:129:B:ILE:HD12	1:142:B:ARG:HB3	20	0.17
(1,3130)	1:129:B:ILE:HD13	1:142:B:ARG:HB2	20	0.17
(1,3130)	1:129:B:ILE:HD13	1:142:B:ARG:HB3	20	0.17
(1,3102)	1:128:B:ALA:H	1:131:B:VAL:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3082)	1:125:B:TYR:HE1	1:141:B:ASN:HB2	8	0.17
(1,3042)	1:122:B:ILE:HA	1:145:B:ALA:HB1	1	0.17
(1,3042)	1:122:B:ILE:HA	1:145:B:ALA:HB2	1	0.17
(1,3042)	1:122:B:ILE:HA	1:145:B:ALA:HB3	1	0.17
(1,2992)	1:118:B:TYR:HA	1:121:B:ALA:H	15	0.17
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE1	2	0.17
(1,2901)	1:110:B:ASN:HA	1:125:B:TYR:HE2	2	0.17
(1,2893)	1:109:B:GLY:HA2	1:121:B:ALA:H	10	0.17
(1,2893)	1:109:B:GLY:HA3	1:121:B:ALA:H	10	0.17
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG21	7	0.17
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG22	7	0.17
(1,2849)	1:105:B:LEU:HD11	1:131:B:VAL:HG23	7	0.17
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG21	7	0.17
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG22	7	0.17
(1,2849)	1:105:B:LEU:HD12	1:131:B:VAL:HG23	7	0.17
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG21	7	0.17
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG22	7	0.17
(1,2849)	1:105:B:LEU:HD13	1:131:B:VAL:HG23	7	0.17
(1,2842)	1:105:B:LEU:HA	1:109:B:GLY:H	18	0.17
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB1	8	0.17
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB2	8	0.17
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB3	8	0.17
(1,2789)	1:101:B:LYS:H	1:103:B:GLU:H	5	0.17
(1,2768)	1:98:B:THR:H	1:100:B:ALA:H	3	0.17
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	10	0.17
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	16	0.17
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	15	0.17
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	15	0.17
(1,2691)	1:220:A:GLU:HA	1:224:A:ASN:H	4	0.17
(1,2632)	1:213:A:GLU:HA	1:216:A:LYS:H	6	0.17
(1,2592)	1:208:A:MET:HA	1:211:A:ASP:H	4	0.17
(1,2571)	1:206:A:GLU:HA	1:209:A:LYS:HB2	13	0.17
(1,2571)	1:206:A:GLU:HA	1:209:A:LYS:HB3	13	0.17
(1,2534)	1:201:A:GLY:H	1:204:A:ALA:H	9	0.17
(1,2533)	1:201:A:GLY:H	1:203:A:ASN:H	14	0.17
(1,2512)	1:198:A:ASP:H	1:200:A:GLU:H	3	0.17
(1,2464)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	4	0.17
(1,2457)	1:193:A:TYR:HD1	1:211:A:ASP:HA	11	0.17
(1,2457)	1:193:A:TYR:HD2	1:211:A:ASP:HA	11	0.17
(1,2451)	1:193:A:TYR:HA	1:212:A:TYR:HA	16	0.17
(1,2416)	1:190:A:LEU:HA	1:212:A:TYR:HA	1	0.17
(1,2398)	1:188:A:GLU:HA	1:191:A:GLU:H	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2351)	1:181:A:TYR:H	1:189:A:ALA:HA	12	0.17
(1,2345)	1:180:A:LYS:HB2	1:189:A:ALA:H	6	0.17
(1,2345)	1:180:A:LYS:HB3	1:189:A:ALA:H	6	0.17
(1,2287)	1:175:A:ARG:HA	1:178:A:PHE:H	13	0.17
(1,2279)	1:174:A:SER:HA	1:193:A:TYR:HA	2	0.17
(1,2265)	1:173:A:TYR:HB2	1:195:A:LYS:HG2	16	0.17
(1,2265)	1:173:A:TYR:HB2	1:195:A:LYS:HG3	16	0.17
(1,2265)	1:173:A:TYR:HB3	1:195:A:LYS:HG2	16	0.17
(1,2265)	1:173:A:TYR:HB3	1:195:A:LYS:HG3	16	0.17
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD11	18	0.17
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD12	18	0.17
(1,2218)	1:170:A:PHE:HA	1:199:A:ILE:HD13	18	0.17
(1,2200)	1:169:A:TYR:HE1	1:171:A:ARG:H	15	0.17
(1,2200)	1:169:A:TYR:HE2	1:171:A:ARG:H	15	0.17
(1,2163)	1:163:A:ILE:HA	1:167:A:PRO:HA	3	0.17
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	3	0.17
(1,1998)	1:147:A:SER:H	1:155:A:ALA:HA	17	0.17
(1,1852)	1:135:A:ASN:HA	1:138:A:TYR:H	10	0.17
(1,1807)	1:129:A:ILE:H	1:132:A:LEU:H	3	0.17
(1,1761)	1:125:A:TYR:HA	1:129:A:ILE:H	8	0.17
(1,1752)	1:124:A:LYS:HA	1:127:A:GLU:H	17	0.17
(1,1667)	1:116:A:LYS:HA	1:118:A:TYR:HA	16	0.17
(1,1642)	1:113:A:MET:HE1	1:142:A:ARG:HA	7	0.17
(1,1642)	1:113:A:MET:HE2	1:142:A:ARG:HA	7	0.17
(1,1642)	1:113:A:MET:HE3	1:142:A:ARG:HA	7	0.17
(1,1627)	1:113:A:MET:H	1:121:A:ALA:HA	5	0.17
(1,1554)	1:106:A:LYS:HA	1:110:A:ASN:H	19	0.17
(1,1474)	1:99:A:LYS:HA	1:102:A:ALA:H	12	0.17
(1,1433)	1:93:A:GLU:HA	1:96:A:ALA:HA	7	0.17
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	2	0.17
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	2	0.17
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	2	0.17
(1,1384)	1:44:A:PHE:HA	1:25:B:ILE:HD11	4	0.17
(1,1357)	1:40:A:ILE:H	1:36:B:ALA:HB1	3	0.17
(1,1357)	1:40:A:ILE:H	1:36:B:ALA:HB2	3	0.17
(1,1357)	1:40:A:ILE:H	1:36:B:ALA:HB3	3	0.17
(1,1349)	1:39:A:CYS:HA	1:32:B:SER:HA	8	0.17
(1,1310)	1:25:A:ILE:HD11	1:43:B:ALA:HB1	10	0.17
(1,1310)	1:25:A:ILE:HD12	1:43:B:ALA:HB1	10	0.17
(1,1310)	1:25:A:ILE:HD13	1:43:B:ALA:HB1	10	0.17
(1,1279)	1:16:A:PHE:HE1	1:9:B:ALA:HA	8	0.17
(1,1279)	1:16:A:PHE:HE2	1:9:B:ALA:HA	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:15:A:TYR:HH	1:5:B:LYS:H	12	0.17
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE1	12	0.17
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE2	12	0.17
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG21	12	0.17
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG22	12	0.17
(1,1245)	1:8:A:ILE:HD11	1:68:B:ILE:HG23	12	0.17
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG21	12	0.17
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG22	12	0.17
(1,1245)	1:8:A:ILE:HD12	1:68:B:ILE:HG23	12	0.17
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG21	12	0.17
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG22	12	0.17
(1,1245)	1:8:A:ILE:HD13	1:68:B:ILE:HG23	12	0.17
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	9	0.17
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	2	0.17
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	2	0.17
(1,1125)	1:57:B:LYS:HB2	1:58:B:SER:H	15	0.17
(1,1125)	1:57:B:LYS:HB3	1:58:B:SER:H	15	0.17
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	7	0.17
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	19	0.17
(1,953)	1:35:B:VAL:HA	1:38:B:ASP:HA	18	0.17
(1,903)	1:30:B:ALA:H	1:33:B:LEU:H	2	0.17
(1,885)	1:27:B:GLU:HA	1:30:B:ALA:HA	3	0.17
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD21	19	0.17
(1,766)	1:15:B:TYR:HA	1:70:B:ASN:HD22	19	0.17
(1,728)	1:13:B:VAL:HA	1:37:B:MET:HB2	19	0.17
(1,728)	1:13:B:VAL:HA	1:37:B:MET:HB3	19	0.17
(1,626)	1:4:B:SER:HA	1:5:B:LYS:HA	17	0.17
(1,587)	1:68:A:ILE:H	1:69:A:LEU:HA	9	0.17
(1,587)	1:68:A:ILE:H	1:69:A:LEU:HA	13	0.17
(1,536)	1:60:A:PHE:HA	1:62:A:GLY:H	1	0.17
(1,536)	1:60:A:PHE:HA	1:62:A:GLY:H	6	0.17
(1,474)	1:51:A:VAL:HA	1:55:A:LEU:H	6	0.17
(1,325)	1:33:A:LEU:HA	1:37:A:MET:H	19	0.17
(1,284)	1:28:A:ASP:HA	1:32:A:SER:H	7	0.17
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	16	0.17
(1,277)	1:27:A:GLU:HA	1:31:A:ASP:H	15	0.17
(1,276)	1:27:A:GLU:HA	1:30:A:ALA:HA	15	0.17
(1,275)	1:27:A:GLU:HA	1:30:A:ALA:H	6	0.17
(1,264)	1:26:A:SER:H	1:29:A:GLY:H	9	0.17
(1,251)	1:23:A:LYS:HA	1:25:A:ILE:H	10	0.17
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB2	7	0.17
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB3	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:5:A:LYS:HA	1:9:A:ALA:H	3	0.17
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	12	0.17
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	16	0.17
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	17	0.17
(1,4205)	1:342:B:ASN:H	1:343:B:GLU:H	2	0.16
(1,4203)	1:338:B:GLU:H	1:339:B:THR:H	19	0.16
(1,4199)	1:334:B:GLN:H	1:335:B:SER:H	19	0.16
(1,4187)	1:322:B:ASN:H	1:323:B:MET:H	7	0.16
(1,4187)	1:322:B:ASN:H	1:323:B:MET:H	17	0.16
(1,4139)	1:231:B:GLU:H	1:232:B:GLN:H	17	0.16
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	18	0.16
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	19	0.16
(1,4073)	1:302:A:PHE:H	1:303:A:ALA:H	6	0.16
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	2	0.16
(1,4063)	1:255:A:LEU:H	1:256:A:LEU:H	2	0.16
(1,4062)	1:254:A:SER:H	1:255:A:LEU:H	2	0.16
(1,4045)	1:235:A:ASP:H	1:236:A:ALA:H	19	0.16
(1,4042)	1:232:A:GLN:H	1:233:A:SER:H	6	0.16
(1,4032)	1:226:B:GLU:HA	1:227:B:LYS:H	13	0.16
(1,3975)	1:218:B:LYS:H	1:221:B:GLN:H	19	0.16
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	13	0.16
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	13	0.16
(1,3946)	1:214:B:SER:HA	1:217:B:LYS:H	8	0.16
(1,3942)	1:214:B:SER:H	1:217:B:LYS:H	14	0.16
(1,3894)	1:208:B:MET:H	1:211:B:ASP:H	4	0.16
(1,3882)	1:207:B:ALA:H	1:210:B:ARG:H	16	0.16
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	9	0.16
(1,3769)	1:193:B:TYR:HD2	1:211:B:ASP:HA	14	0.16
(1,3738)	1:191:B:GLU:HA	1:195:B:LYS:H	18	0.16
(1,3689)	1:185:B:LYS:HA	1:188:B:GLU:H	19	0.16
(1,3686)	1:185:B:LYS:H	1:186:B:PRO:HA	14	0.16
(1,3654)	1:181:B:TYR:H	1:185:B:LYS:H	2	0.16
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	7	0.16
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	7	0.16
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	8	0.16
(1,3241)	1:141:B:ASN:HA	1:145:B:ALA:H	11	0.16
(1,3159)	1:135:B:ASN:HB2	1:138:B:TYR:H	4	0.16
(1,3159)	1:135:B:ASN:HB3	1:138:B:TYR:H	4	0.16
(1,3148)	1:134:B:THR:H	1:135:B:ASN:HA	19	0.16
(1,3126)	1:129:B:ILE:HD11	1:139:B:TYR:HA	9	0.16
(1,3126)	1:129:B:ILE:HD12	1:139:B:TYR:HA	9	0.16
(1,3126)	1:129:B:ILE:HD13	1:139:B:TYR:HA	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3075)	1:125:B:TYR:HB2	1:142:B:ARG:HA	5	0.16
(1,3075)	1:125:B:TYR:HB3	1:142:B:ARG:HA	5	0.16
(1,3067)	1:125:B:TYR:HA	1:129:B:ILE:H	11	0.16
(1,2991)	1:118:B:TYR:HA	1:120:B:LEU:H	9	0.16
(1,2980)	1:117:B:ASP:H	1:118:B:TYR:HA	10	0.16
(1,2980)	1:117:B:ASP:H	1:118:B:TYR:HA	20	0.16
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB1	18	0.16
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB2	18	0.16
(1,2950)	1:113:B:MET:HE1	1:144:B:ALA:HB3	18	0.16
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB1	18	0.16
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB2	18	0.16
(1,2950)	1:113:B:MET:HE2	1:144:B:ALA:HB3	18	0.16
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB1	18	0.16
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB2	18	0.16
(1,2950)	1:113:B:MET:HE3	1:144:B:ALA:HB3	18	0.16
(1,2824)	1:103:B:GLU:HA	1:106:B:LYS:H	10	0.16
(1,2816)	1:102:B:ALA:HB1	1:132:B:LEU:H	8	0.16
(1,2816)	1:102:B:ALA:HB2	1:132:B:LEU:H	8	0.16
(1,2816)	1:102:B:ALA:HB3	1:132:B:LEU:H	8	0.16
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB1	19	0.16
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB2	19	0.16
(1,2808)	1:102:B:ALA:HA	1:128:B:ALA:HB3	19	0.16
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD11	5	0.16
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD12	5	0.16
(1,2806)	1:102:B:ALA:HA	1:105:B:LEU:HD13	5	0.16
(1,2795)	1:101:B:LYS:HA	1:103:B:GLU:H	17	0.16
(1,2789)	1:101:B:LYS:H	1:103:B:GLU:H	15	0.16
(1,2753)	1:95:B:ASP:HA	1:99:B:LYS:H	9	0.16
(1,2745)	1:94:B:ASP:HA	1:96:B:ALA:H	18	0.16
(1,2729)	1:226:A:GLU:HG2	1:227:A:LYS:H	5	0.16
(1,2729)	1:226:A:GLU:HG3	1:227:A:LYS:H	5	0.16
(1,2648)	1:215:A:ALA:HA	1:217:A:LYS:H	3	0.16
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	20	0.16
(1,2588)	1:208:A:MET:H	1:211:A:ASP:H	15	0.16
(1,2570)	1:206:A:GLU:HA	1:209:A:LYS:H	14	0.16
(1,2501)	1:197:A:LEU:HA	1:199:A:ILE:H	18	0.16
(1,2469)	1:194:A:LYS:H	1:212:A:TYR:HA	20	0.16
(1,2463)	1:193:A:TYR:HE2	1:211:A:ASP:HA	9	0.16
(1,2320)	1:178:A:PHE:HA	1:182:A:ALA:H	18	0.16
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	9	0.16
(1,2277)	1:174:A:SER:HA	1:177:A:GLY:H	6	0.16
(1,2243)	1:171:A:ARG:HA	1:174:A:SER:H	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2231)	1:170:A:PHE:HE1	1:171:A:ARG:HA	9	0.16
(1,2231)	1:170:A:PHE:HE2	1:171:A:ARG:HA	9	0.16
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	2	0.16
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	2	0.16
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	3	0.16
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	3	0.16
(1,2163)	1:163:A:ILE:HA	1:167:A:PRO:HA	7	0.16
(1,2061)	1:152:A:TYR:HD2	1:183:A:GLN:HG2	13	0.16
(1,2055)	1:152:A:TYR:HB2	1:183:A:GLN:H	10	0.16
(1,2055)	1:152:A:TYR:HB3	1:183:A:GLN:H	10	0.16
(1,1962)	1:143:A:ALA:HB1	1:175:A:ARG:HB2	11	0.16
(1,1962)	1:143:A:ALA:HB1	1:175:A:ARG:HB3	11	0.16
(1,1962)	1:143:A:ALA:HB2	1:175:A:ARG:HB2	11	0.16
(1,1962)	1:143:A:ALA:HB2	1:175:A:ARG:HB3	11	0.16
(1,1962)	1:143:A:ALA:HB3	1:175:A:ARG:HB2	11	0.16
(1,1962)	1:143:A:ALA:HB3	1:175:A:ARG:HB3	11	0.16
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	19	0.16
(1,1951)	1:143:A:ALA:HA	1:155:A:ALA:HA	15	0.16
(1,1946)	1:143:A:ALA:H	1:155:A:ALA:HA	5	0.16
(1,1898)	1:139:A:TYR:HA	1:142:A:ARG:H	11	0.16
(1,1818)	1:129:A:ILE:HD11	1:138:A:TYR:HD2	1	0.16
(1,1818)	1:129:A:ILE:HD12	1:138:A:TYR:HD2	1	0.16
(1,1818)	1:129:A:ILE:HD13	1:138:A:TYR:HD2	1	0.16
(1,1796)	1:128:A:ALA:H	1:131:A:VAL:H	3	0.16
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD2	20	0.16
(1,1764)	1:125:A:TYR:HA	1:142:A:ARG:HD3	20	0.16
(1,1713)	1:120:A:LEU:HA	1:123:A:ASN:H	14	0.16
(1,1689)	1:118:A:TYR:HA	1:145:A:ALA:HA	14	0.16
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	6	0.16
(1,1645)	1:113:A:MET:HE1	1:145:A:ALA:H	11	0.16
(1,1645)	1:113:A:MET:HE2	1:145:A:ALA:H	11	0.16
(1,1645)	1:113:A:MET:HE3	1:145:A:ALA:H	11	0.16
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	8	0.16
(1,1535)	1:105:A:LEU:HA	1:108:A:GLN:H	13	0.16
(1,1493)	1:102:A:ALA:H	1:104:A:ASP:H	1	0.16
(1,1424)	1:69:A:LEU:HD11	1:2:B:SER:H	13	0.16
(1,1424)	1:69:A:LEU:HD12	1:2:B:SER:H	13	0.16
(1,1424)	1:69:A:LEU:HD13	1:2:B:SER:H	13	0.16
(1,1416)	1:68:A:ILE:HA	1:2:B:SER:HA	7	0.16
(1,1398)	1:44:A:PHE:HE1	1:33:B:LEU:HD11	20	0.16
(1,1398)	1:44:A:PHE:HE2	1:33:B:LEU:HD11	20	0.16
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	6	0.16
(1,1395)	1:44:A:PHE:HE1	1:25:B:ILE:HD13	11	0.16
(1,1395)	1:44:A:PHE:HE2	1:25:B:ILE:HD13	11	0.16
(1,1345)	1:36:A:ALA:HB1	1:40:B:ILE:HA	17	0.16
(1,1345)	1:36:A:ALA:HB2	1:40:B:ILE:HA	17	0.16
(1,1345)	1:36:A:ALA:HB3	1:40:B:ILE:HA	17	0.16
(1,1340)	1:36:A:ALA:HA	1:39:B:CYS:H	1	0.16
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE2	16	0.16
(1,1305)	1:25:A:ILE:HG12	1:5:B:LYS:HE3	16	0.16
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE2	16	0.16
(1,1305)	1:25:A:ILE:HG13	1:5:B:LYS:HE3	16	0.16
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG21	15	0.16
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG22	15	0.16
(1,1224)	1:2:A:SER:HA	1:68:B:ILE:HG23	15	0.16
(1,1207)	1:69:B:LEU:HA	1:71:B:SER:H	17	0.16
(1,1172)	1:64:B:HIS:H	1:65:B:LEU:H	19	0.16
(1,1163)	1:62:B:GLY:H	1:63:B:GLN:H	3	0.16
(1,1148)	1:60:B:PHE:HB2	1:61:B:LYS:HA	19	0.16
(1,1148)	1:60:B:PHE:HB3	1:61:B:LYS:HA	19	0.16
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	11	0.16
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	19	0.16
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	19	0.16
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	2	0.16
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	14	0.16
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD11	11	0.16
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD12	11	0.16
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD13	11	0.16
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD11	11	0.16
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD12	11	0.16
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD13	11	0.16
(1,988)	1:39:B:CYS:HA	1:42:B:GLU:H	6	0.16
(1,988)	1:39:B:CYS:HA	1:42:B:GLU:H	15	0.16
(1,852)	1:22:B:LYS:H	1:24:B:GLU:H	1	0.16
(1,836)	1:20:B:VAL:HA	1:30:B:ALA:HA	13	0.16
(1,732)	1:13:B:VAL:HG11	1:37:B:MET:HB2	3	0.16
(1,732)	1:13:B:VAL:HG11	1:37:B:MET:HB3	3	0.16
(1,732)	1:13:B:VAL:HG12	1:37:B:MET:HB2	3	0.16
(1,732)	1:13:B:VAL:HG12	1:37:B:MET:HB3	3	0.16
(1,732)	1:13:B:VAL:HG13	1:37:B:MET:HB2	3	0.16
(1,732)	1:13:B:VAL:HG13	1:37:B:MET:HB3	3	0.16
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	1	0.16
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:9:B:ALA:HA	1:13:B:VAL:H	4	0.16
(1,635)	1:5:B:LYS:HA	1:9:B:ALA:H	12	0.16
(1,624)	1:4:B:SER:H	1:8:B:ILE:H	1	0.16
(1,603)	1:70:A:ASN:HA	1:72:A:ALA:H	9	0.16
(1,587)	1:68:A:ILE:H	1:69:A:LEU:HA	16	0.16
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE21	3	0.16
(1,545)	1:60:A:PHE:HB2	1:63:A:GLN:HE22	3	0.16
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE21	3	0.16
(1,545)	1:60:A:PHE:HB3	1:63:A:GLN:HE22	3	0.16
(1,524)	1:58:A:SER:HB2	1:60:A:PHE:H	10	0.16
(1,524)	1:58:A:SER:HB3	1:60:A:PHE:H	10	0.16
(1,495)	1:54:A:ILE:HA	1:57:A:LYS:H	5	0.16
(1,474)	1:51:A:VAL:HA	1:55:A:LEU:H	12	0.16
(1,458)	1:48:A:ARG:HA	1:50:A:ALA:H	19	0.16
(1,451)	1:47:A:GLU:HB2	1:48:A:ARG:H	4	0.16
(1,451)	1:47:A:GLU:HB3	1:48:A:ARG:H	4	0.16
(1,445)	1:47:A:GLU:H	1:50:A:ALA:H	17	0.16
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	6	0.16
(1,401)	1:41:A:SER:HA	1:45:A:GLY:H	7	0.16
(1,286)	1:29:A:GLY:H	1:31:A:ASP:H	6	0.16
(1,239)	1:21:A:GLU:HB2	1:22:A:LYS:H	15	0.16
(1,239)	1:21:A:GLU:HB3	1:22:A:LYS:H	15	0.16
(1,226)	1:20:A:VAL:HA	1:24:A:GLU:H	1	0.16
(1,205)	1:18:A:SER:H	1:21:A:GLU:H	17	0.16
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD21	15	0.15
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD22	15	0.15
(1,4216)	1:248:B:GLY:H	1:249:B:LEU:HD23	15	0.15
(1,4199)	1:334:B:GLN:H	1:335:B:SER:H	3	0.15
(1,4199)	1:334:B:GLN:H	1:335:B:SER:H	18	0.15
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	20	0.15
(1,4189)	1:324:B:ALA:H	1:325:B:GLY:H	16	0.15
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	11	0.15
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	19	0.15
(1,4164)	1:258:B:GLY:H	1:259:B:GLY:H	17	0.15
(1,4149)	1:241:B:SER:H	1:242:B:GLN:H	9	0.15
(1,4139)	1:231:B:GLU:H	1:232:B:GLN:H	7	0.15
(1,4092)	1:325:A:GLY:H	1:326:A:ASN:H	19	0.15
(1,4091)	1:324:A:ALA:H	1:325:A:GLY:H	4	0.15
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	12	0.15
(1,4072)	1:301:A:GLY:H	1:302:A:PHE:H	10	0.15
(1,4065)	1:257:A:GLY:H	1:258:A:GLY:H	2	0.15
(1,4027)	1:225:B:LEU:H	1:226:B:GLU:H	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	7	0.15
(1,3921)	1:211:B:ASP:HA	1:215:B:ALA:H	2	0.15
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	13	0.15
(1,3828)	1:199:B:ILE:HA	1:201:B:GLY:H	11	0.15
(1,3807)	1:197:B:LEU:HA	1:199:B:ILE:H	1	0.15
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	17	0.15
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	17	0.15
(1,3722)	1:190:B:LEU:HA	1:212:B:TYR:HA	19	0.15
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	7	0.15
(1,3677)	1:182:B:ALA:HA	1:184:B:GLY:H	13	0.15
(1,3572)	1:173:B:TYR:HB2	1:196:B:VAL:H	4	0.15
(1,3572)	1:173:B:TYR:HB3	1:196:B:VAL:H	4	0.15
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD11	1	0.15
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD12	1	0.15
(1,3516)	1:170:B:PHE:H	1:199:B:ILE:HD13	1	0.15
(1,3507)	1:169:B:TYR:HE1	1:171:B:ARG:HB2	11	0.15
(1,3507)	1:169:B:TYR:HE1	1:171:B:ARG:HB3	11	0.15
(1,3507)	1:169:B:TYR:HE2	1:171:B:ARG:HB2	11	0.15
(1,3507)	1:169:B:TYR:HE2	1:171:B:ARG:HB3	11	0.15
(1,3506)	1:169:B:TYR:HE1	1:171:B:ARG:H	6	0.15
(1,3506)	1:169:B:TYR:HE2	1:171:B:ARG:H	6	0.15
(1,3437)	1:160:B:GLU:H	1:163:B:ILE:H	3	0.15
(1,3420)	1:158:B:ASP:HA	1:162:B:ALA:H	4	0.15
(1,3335)	1:150:B:LYS:HA	1:152:B:TYR:HA	7	0.15
(1,3300)	1:146:B:HIS:HB2	1:155:B:ALA:HB1	8	0.15
(1,3300)	1:146:B:HIS:HB2	1:155:B:ALA:HB2	8	0.15
(1,3300)	1:146:B:HIS:HB2	1:155:B:ALA:HB3	8	0.15
(1,3300)	1:146:B:HIS:HB3	1:155:B:ALA:HB1	8	0.15
(1,3300)	1:146:B:HIS:HB3	1:155:B:ALA:HB2	8	0.15
(1,3300)	1:146:B:HIS:HB3	1:155:B:ALA:HB3	8	0.15
(1,3204)	1:139:B:TYR:HA	1:142:B:ARG:H	7	0.15
(1,3098)	1:127:B:GLU:HA	1:130:B:LYS:H	8	0.15
(1,2976)	1:116:B:LYS:HA	1:118:B:TYR:HE1	1	0.15
(1,2972)	1:116:B:LYS:HA	1:118:B:TYR:H	9	0.15
(1,2854)	1:106:B:LYS:H	1:128:B:ALA:HA	18	0.15
(1,2833)	1:104:B:ASP:HA	1:107:B:MET:H	17	0.15
(1,2819)	1:103:B:GLU:H	1:105:B:LEU:H	5	0.15
(1,2799)	1:102:B:ALA:H	1:104:B:ASP:H	11	0.15
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	8	0.15
(1,2795)	1:101:B:LYS:HA	1:103:B:GLU:H	19	0.15
(1,2749)	1:95:B:ASP:HA	1:96:B:ALA:HA	20	0.15
(1,2703)	1:222:A:SER:H	1:225:A:LEU:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2659)	1:217:A:LYS:H	1:219:A:VAL:H	3	0.15
(1,2641)	1:214:A:SER:HA	1:218:A:LYS:H	11	0.15
(1,2576)	1:207:A:ALA:H	1:210:A:ARG:H	12	0.15
(1,2562)	1:205:A:THR:HG21	1:208:A:MET:HG2	7	0.15
(1,2562)	1:205:A:THR:HG21	1:208:A:MET:HG3	7	0.15
(1,2562)	1:205:A:THR:HG22	1:208:A:MET:HG2	7	0.15
(1,2562)	1:205:A:THR:HG22	1:208:A:MET:HG3	7	0.15
(1,2562)	1:205:A:THR:HG23	1:208:A:MET:HG2	7	0.15
(1,2562)	1:205:A:THR:HG23	1:208:A:MET:HG3	7	0.15
(1,2484)	1:195:A:LYS:HA	1:198:A:ASP:H	4	0.15
(1,2464)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	11	0.15
(1,2463)	1:193:A:TYR:HE1	1:211:A:ASP:HA	2	0.15
(1,2419)	1:190:A:LEU:HD11	1:212:A:TYR:HA	7	0.15
(1,2419)	1:190:A:LEU:HD12	1:212:A:TYR:HA	7	0.15
(1,2419)	1:190:A:LEU:HD13	1:212:A:TYR:HA	7	0.15
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG21	17	0.15
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG22	17	0.15
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG23	17	0.15
(1,2383)	1:185:A:LYS:HA	1:188:A:GLU:H	20	0.15
(1,2359)	1:181:A:TYR:HA	1:189:A:ALA:H	12	0.15
(1,2342)	1:180:A:LYS:HB2	1:185:A:LYS:H	14	0.15
(1,2342)	1:180:A:LYS:HB3	1:185:A:LYS:H	14	0.15
(1,2277)	1:174:A:SER:HA	1:177:A:GLY:H	12	0.15
(1,2214)	1:170:A:PHE:HA	1:173:A:TYR:H	9	0.15
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	3	0.15
(1,2137)	1:160:A:GLU:HA	1:163:A:ILE:HD11	6	0.15
(1,2137)	1:160:A:GLU:HA	1:163:A:ILE:HD12	6	0.15
(1,2137)	1:160:A:GLU:HA	1:163:A:ILE:HD13	6	0.15
(1,2123)	1:159:A:ALA:HA	1:176:A:LEU:H	6	0.15
(1,2105)	1:157:A:LYS:HA	1:160:A:GLU:H	2	0.15
(1,1973)	1:144:A:ALA:HB1	1:175:A:ARG:HE	12	0.15
(1,1973)	1:144:A:ALA:HB2	1:175:A:ARG:HE	12	0.15
(1,1973)	1:144:A:ALA:HB3	1:175:A:ARG:HE	12	0.15
(1,1953)	1:143:A:ALA:HA	1:158:A:ASP:H	10	0.15
(1,1889)	1:138:A:TYR:HA	1:141:A:ASN:H	11	0.15
(1,1865)	1:136:A:ALA:HA	1:166:A:ASP:H	16	0.15
(1,1852)	1:135:A:ASN:HA	1:138:A:TYR:H	13	0.15
(1,1813)	1:129:A:ILE:HA	1:133:A:PRO:HA	1	0.15
(1,1813)	1:129:A:ILE:HA	1:133:A:PRO:HA	10	0.15
(1,1785)	1:126:A:THR:HA	1:130:A:LYS:H	9	0.15
(1,1767)	1:125:A:TYR:HB2	1:139:A:TYR:H	15	0.15
(1,1767)	1:125:A:TYR:HB3	1:139:A:TYR:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:125:A:TYR:H	1:128:A:ALA:H	14	0.15
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD1	8	0.15
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD2	8	0.15
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD1	8	0.15
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD2	8	0.15
(1,1667)	1:116:A:LYS:HA	1:118:A:TYR:HA	10	0.15
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD21	9	0.15
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD22	9	0.15
(1,1614)	1:112:A:ALA:HA	1:120:A:LEU:HD23	9	0.15
(1,1535)	1:105:A:LEU:HA	1:108:A:GLN:H	4	0.15
(1,1530)	1:105:A:LEU:H	1:107:A:MET:H	1	0.15
(1,1519)	1:103:A:GLU:HA	1:107:A:MET:H	8	0.15
(1,1507)	1:102:A:ALA:HB1	1:128:A:ALA:HA	11	0.15
(1,1507)	1:102:A:ALA:HB2	1:128:A:ALA:HA	11	0.15
(1,1507)	1:102:A:ALA:HB3	1:128:A:ALA:HA	11	0.15
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB2	9	0.15
(1,1369)	1:42:A:GLU:HB2	1:32:B:SER:HB3	9	0.15
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB2	9	0.15
(1,1369)	1:42:A:GLU:HB3	1:32:B:SER:HB3	9	0.15
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	14	0.15
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	18	0.15
(1,1283)	1:16:A:PHE:HE1	1:12:B:ILE:HB	8	0.15
(1,1283)	1:16:A:PHE:HE2	1:12:B:ILE:HB	8	0.15
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB2	2	0.15
(1,1275)	1:15:A:TYR:HH	1:5:B:LYS:HB3	2	0.15
(1,1182)	1:65:B:LEU:HD21	1:71:B:SER:H	8	0.15
(1,1182)	1:65:B:LEU:HD22	1:71:B:SER:H	8	0.15
(1,1182)	1:65:B:LEU:HD23	1:71:B:SER:H	8	0.15
(1,1179)	1:65:B:LEU:HA	1:67:B:ASP:H	20	0.15
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	17	0.15
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	17	0.15
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	17	0.15
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	17	0.15
(1,1147)	1:60:B:PHE:HB2	1:61:B:LYS:H	5	0.15
(1,1147)	1:60:B:PHE:HB3	1:61:B:LYS:H	5	0.15
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	2	0.15
(1,1114)	1:55:B:LEU:HD11	1:71:B:SER:HA	12	0.15
(1,1114)	1:55:B:LEU:HD12	1:71:B:SER:HA	12	0.15
(1,1114)	1:55:B:LEU:HD13	1:71:B:SER:HA	12	0.15
(1,1009)	1:41:B:SER:HA	1:44:B:PHE:H	20	0.15
(1,989)	1:39:B:CYS:HA	1:42:B:GLU:HA	10	0.15
(1,988)	1:39:B:CYS:HA	1:42:B:GLU:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:28:B:ASP:HA	1:32:B:SER:H	8	0.15
(1,836)	1:20:B:VAL:HA	1:30:B:ALA:HA	3	0.15
(1,781)	1:16:B:PHE:HA	1:18:B:SER:HB2	7	0.15
(1,781)	1:16:B:PHE:HA	1:18:B:SER:HB3	7	0.15
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD11	9	0.15
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD12	9	0.15
(1,701)	1:11:B:LEU:HA	1:55:B:LEU:HD13	9	0.15
(1,685)	1:10:B:ALA:HA	1:48:B:ARG:HA	13	0.15
(1,635)	1:5:B:LYS:HA	1:9:B:ALA:H	5	0.15
(1,635)	1:5:B:LYS:HA	1:9:B:ALA:H	15	0.15
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	4	0.15
(1,598)	1:69:A:LEU:HA	1:71:A:SER:H	18	0.15
(1,512)	1:56:A:GLY:HA2	1:58:A:SER:H	11	0.15
(1,512)	1:56:A:GLY:HA3	1:58:A:SER:H	11	0.15
(1,458)	1:48:A:ARG:HA	1:50:A:ALA:H	18	0.15
(1,431)	1:45:A:GLY:H	1:46:A:PHE:HD1	13	0.15
(1,381)	1:39:A:CYS:HA	1:43:A:ALA:H	18	0.15
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	19	0.15
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	6	0.15
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	9	0.15
(1,59)	1:9:A:ALA:HA	1:12:A:ILE:HD11	19	0.15
(1,59)	1:9:A:ALA:HA	1:12:A:ILE:HD12	19	0.15
(1,59)	1:9:A:ALA:HA	1:12:A:ILE:HD13	19	0.15
(1,21)	1:5:A:LYS:H	1:8:A:ILE:H	17	0.15
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	5	0.15
(1,4153)	1:245:B:SER:H	1:246:B:ALA:H	3	0.14
(1,4147)	1:239:B:ASP:H	1:240:B:ALA:H	10	0.14
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	5	0.14
(1,4101)	1:334:A:GLN:H	1:335:A:SER:H	15	0.14
(1,4098)	1:331:A:ALA:H	1:332:A:GLY:H	15	0.14
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	16	0.14
(1,4077)	1:305:A:GLY:H	1:307:A:GLY:H	3	0.14
(1,4070)	1:299:A:ALA:H	1:300:A:GLU:H	20	0.14
(1,4063)	1:255:A:LEU:H	1:256:A:LEU:H	6	0.14
(1,4048)	1:238:A:VAL:H	1:239:A:ASP:H	20	0.14
(1,4042)	1:232:A:GLN:H	1:233:A:SER:H	17	0.14
(1,3979)	1:218:B:LYS:HA	1:221:B:GLN:H	4	0.14
(1,3970)	1:217:B:LYS:HA	1:220:B:GLU:H	5	0.14
(1,3954)	1:215:B:ALA:HA	1:217:B:LYS:H	4	0.14
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	10	0.14
(1,3822)	1:198:B:ASP:HA	1:200:B:GLU:H	1	0.14
(1,3763)	1:193:B:TYR:HD1	1:211:B:ASP:HA	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3763)	1:193:B:TYR:HD2	1:211:B:ASP:HA	3	0.14
(1,3756)	1:193:B:TYR:HA	1:197:B:LEU:H	5	0.14
(1,3727)	1:190:B:LEU:HD11	1:216:B:LYS:H	3	0.14
(1,3727)	1:190:B:LEU:HD12	1:216:B:LYS:H	3	0.14
(1,3727)	1:190:B:LEU:HD13	1:216:B:LYS:H	3	0.14
(1,3645)	1:180:B:LYS:HA	1:183:B:GLN:H	11	0.14
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	7	0.14
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB2	11	0.14
(1,3570)	1:173:B:TYR:HB2	1:195:B:LYS:HB3	11	0.14
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB2	11	0.14
(1,3570)	1:173:B:TYR:HB3	1:195:B:LYS:HB3	11	0.14
(1,3549)	1:171:B:ARG:HA	1:174:B:SER:H	6	0.14
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	11	0.14
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	11	0.14
(1,3481)	1:164:B:SER:HA	1:166:B:ASP:H	20	0.14
(1,3452)	1:161:B:SER:HA	1:165:B:ILE:H	15	0.14
(1,3452)	1:161:B:SER:HA	1:165:B:ILE:H	20	0.14
(1,3377)	1:154:B:GLN:H	1:157:B:LYS:H	8	0.14
(1,3335)	1:150:B:LYS:HA	1:152:B:TYR:HA	12	0.14
(1,3205)	1:139:B:TYR:HA	1:143:B:ALA:H	2	0.14
(1,3158)	1:135:B:ASN:HA	1:138:B:TYR:H	19	0.14
(1,3120)	1:129:B:ILE:HA	1:135:B:ASN:H	19	0.14
(1,3106)	1:128:B:ALA:HA	1:131:B:VAL:H	10	0.14
(1,3075)	1:125:B:TYR:HB2	1:142:B:ARG:HA	12	0.14
(1,3075)	1:125:B:TYR:HB3	1:142:B:ARG:HA	12	0.14
(1,3073)	1:125:B:TYR:HB2	1:139:B:TYR:H	13	0.14
(1,3073)	1:125:B:TYR:HB3	1:139:B:TYR:H	13	0.14
(1,2979)	1:117:B:ASP:H	1:118:B:TYR:H	11	0.14
(1,2979)	1:117:B:ASP:H	1:118:B:TYR:H	20	0.14
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	2	0.14
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	2	0.14
(1,2941)	1:113:B:MET:HA	1:118:B:TYR:HA	3	0.14
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB2	6	0.14
(1,2883)	1:109:B:GLY:H	1:124:B:LYS:HB3	6	0.14
(1,2877)	1:108:B:GLN:HA	1:110:B:ASN:H	7	0.14
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	14	0.14
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	14	0.14
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	14	0.14
(1,2805)	1:102:B:ALA:HA	1:105:B:LEU:H	7	0.14
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	15	0.14
(1,2754)	1:95:B:ASP:HB2	1:99:B:LYS:H	17	0.14
(1,2754)	1:95:B:ASP:HB3	1:99:B:LYS:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2752)	1:95:B:ASP:HA	1:98:B:THR:H	17	0.14
(1,2719)	1:224:A:ASN:HA	1:226:A:GLU:H	7	0.14
(1,2674)	1:218:A:LYS:HA	1:222:A:SER:H	16	0.14
(1,2666)	1:217:A:LYS:HG2	1:218:A:LYS:H	3	0.14
(1,2666)	1:217:A:LYS:HG3	1:218:A:LYS:H	3	0.14
(1,2648)	1:215:A:ALA:HA	1:217:A:LYS:H	5	0.14
(1,2640)	1:214:A:SER:HA	1:217:A:LYS:H	18	0.14
(1,2583)	1:207:A:ALA:HA	1:211:A:ASP:H	19	0.14
(1,2581)	1:207:A:ALA:HA	1:210:A:ARG:HB2	7	0.14
(1,2581)	1:207:A:ALA:HA	1:210:A:ARG:HB3	7	0.14
(1,2562)	1:205:A:THR:HG21	1:208:A:MET:HG2	19	0.14
(1,2562)	1:205:A:THR:HG21	1:208:A:MET:HG3	19	0.14
(1,2562)	1:205:A:THR:HG22	1:208:A:MET:HG2	19	0.14
(1,2562)	1:205:A:THR:HG22	1:208:A:MET:HG3	19	0.14
(1,2562)	1:205:A:THR:HG23	1:208:A:MET:HG2	19	0.14
(1,2562)	1:205:A:THR:HG23	1:208:A:MET:HG3	19	0.14
(1,2529)	1:200:A:GLU:HB2	1:204:A:ALA:HA	4	0.14
(1,2529)	1:200:A:GLU:HB3	1:204:A:ALA:HA	4	0.14
(1,2529)	1:200:A:GLU:HB2	1:204:A:ALA:HA	14	0.14
(1,2529)	1:200:A:GLU:HB3	1:204:A:ALA:HA	14	0.14
(1,2457)	1:193:A:TYR:HD1	1:211:A:ASP:HA	8	0.14
(1,2457)	1:193:A:TYR:HD2	1:211:A:ASP:HA	8	0.14
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG21	11	0.14
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG22	11	0.14
(1,2392)	1:187:A:GLU:HA	1:219:A:VAL:HG23	11	0.14
(1,2343)	1:180:A:LYS:HB2	1:188:A:GLU:H	12	0.14
(1,2343)	1:180:A:LYS:HB3	1:188:A:GLU:H	12	0.14
(1,2205)	1:169:A:TYR:HD1	1:171:A:ARG:H	17	0.14
(1,2201)	1:169:A:TYR:HE1	1:171:A:ARG:HB2	14	0.14
(1,2201)	1:169:A:TYR:HE1	1:171:A:ARG:HB3	14	0.14
(1,2201)	1:169:A:TYR:HE2	1:171:A:ARG:HB2	14	0.14
(1,2201)	1:169:A:TYR:HE2	1:171:A:ARG:HB3	14	0.14
(1,2197)	1:169:A:TYR:HD1	1:171:A:ARG:H	5	0.14
(1,2197)	1:169:A:TYR:HD2	1:171:A:ARG:H	5	0.14
(1,2176)	1:164:A:SER:HA	1:167:A:PRO:HA	11	0.14
(1,2147)	1:161:A:SER:HA	1:165:A:ILE:HD11	8	0.14
(1,2147)	1:161:A:SER:HA	1:165:A:ILE:HD12	8	0.14
(1,2147)	1:161:A:SER:HA	1:165:A:ILE:HD13	8	0.14
(1,2067)	1:153:A:ASP:HA	1:156:A:VAL:H	10	0.14
(1,2061)	1:152:A:TYR:HD2	1:183:A:GLN:HG2	16	0.14
(1,2032)	1:150:A:LYS:HB2	1:152:A:TYR:HE1	3	0.14
(1,2032)	1:150:A:LYS:HB2	1:152:A:TYR:HE2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2032)	1:150:A:LYS:HB3	1:152:A:TYR:HE1	3	0.14
(1,2032)	1:150:A:LYS:HB3	1:152:A:TYR:HE2	3	0.14
(1,2005)	1:147:A:SER:HA	1:151:A:GLU:H	5	0.14
(1,1768)	1:125:A:TYR:HB2	1:142:A:ARG:H	15	0.14
(1,1768)	1:125:A:TYR:HB3	1:142:A:ARG:H	15	0.14
(1,1678)	1:117:A:ASP:HA	1:120:A:LEU:H	2	0.14
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE1	20	0.14
(1,1669)	1:116:A:LYS:HA	1:118:A:TYR:HE2	20	0.14
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	2	0.14
(1,1522)	1:104:A:ASP:H	1:107:A:MET:H	15	0.14
(1,1517)	1:103:A:GLU:HA	1:105:A:LEU:H	6	0.14
(1,1514)	1:103:A:GLU:H	1:106:A:LYS:H	5	0.14
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG11	9	0.14
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG12	9	0.14
(1,1468)	1:98:A:THR:HA	1:131:A:VAL:HG13	9	0.14
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB2	17	0.14
(1,1445)	1:95:A:ASP:HA	1:97:A:GLU:HB3	17	0.14
(1,1425)	1:69:A:LEU:HD11	1:2:B:SER:HA	8	0.14
(1,1425)	1:69:A:LEU:HD12	1:2:B:SER:HA	8	0.14
(1,1425)	1:69:A:LEU:HD13	1:2:B:SER:HA	8	0.14
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	8	0.14
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	8	0.14
(1,1407)	1:63:A:GLN:HA	1:63:B:GLN:HA	10	0.14
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	11	0.14
(1,1344)	1:36:A:ALA:HB1	1:40:B:ILE:H	16	0.14
(1,1344)	1:36:A:ALA:HB2	1:40:B:ILE:H	16	0.14
(1,1344)	1:36:A:ALA:HB3	1:40:B:ILE:H	16	0.14
(1,1321)	1:32:A:SER:HB2	1:43:B:ALA:H	6	0.14
(1,1321)	1:32:A:SER:HB3	1:43:B:ALA:H	6	0.14
(1,1306)	1:25:A:ILE:HG12	1:43:B:ALA:HB1	8	0.14
(1,1306)	1:25:A:ILE:HG13	1:43:B:ALA:HB1	8	0.14
(1,1278)	1:16:A:PHE:HA	1:44:B:PHE:HZ	1	0.14
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE1	20	0.14
(1,1246)	1:9:A:ALA:HA	1:16:B:PHE:HE2	20	0.14
(1,1229)	1:2:A:SER:HB2	1:69:B:LEU:H	19	0.14
(1,1229)	1:2:A:SER:HB3	1:69:B:LEU:H	19	0.14
(1,1202)	1:69:B:LEU:H	1:70:B:ASN:H	10	0.14
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	7	0.14
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	17	0.14
(1,1179)	1:65:B:LEU:HA	1:67:B:ASP:H	10	0.14
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	16	0.14
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	14	0.14
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	5	0.14
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	5	0.14
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	5	0.14
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	5	0.14
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	14	0.14
(1,1118)	1:56:B:GLY:H	1:58:B:SER:H	16	0.14
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	6	0.14
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	6	0.14
(1,1093)	1:52:B:SER:HA	1:56:B:GLY:H	19	0.14
(1,1083)	1:51:B:VAL:HA	1:55:B:LEU:H	13	0.14
(1,1067)	1:48:B:ARG:HA	1:50:B:ALA:H	17	0.14
(1,854)	1:22:B:LYS:HA	1:24:B:GLU:H	15	0.14
(1,852)	1:22:B:LYS:H	1:24:B:GLU:H	20	0.14
(1,826)	1:19:B:ILE:HA	1:21:B:GLU:H	8	0.14
(1,628)	1:5:B:LYS:H	1:6:B:GLU:H	8	0.14
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	5	0.14
(1,567)	1:65:A:LEU:H	1:67:A:ASP:H	10	0.14
(1,560)	1:63:A:GLN:HA	1:65:A:LEU:H	12	0.14
(1,537)	1:60:A:PHE:HA	1:63:A:GLN:H	2	0.14
(1,401)	1:41:A:SER:HA	1:45:A:GLY:H	11	0.14
(1,383)	1:40:A:ILE:H	1:42:A:GLU:H	3	0.14
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	17	0.14
(1,379)	1:39:A:CYS:HA	1:42:A:GLU:H	20	0.14
(1,362)	1:37:A:MET:HA	1:40:A:ILE:H	9	0.14
(1,336)	1:34:A:ASN:HA	1:38:A:ASP:H	12	0.14
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	1	0.14
(1,155)	1:15:A:TYR:HA	1:19:A:ILE:H	15	0.14
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	14	0.14
(1,4191)	1:326:B:ASN:H	1:327:B:LEU:H	4	0.13
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	14	0.13
(1,4075)	1:304:A:SER:H	1:305:A:GLY:H	20	0.13
(1,4071)	1:300:A:GLU:H	1:301:A:GLY:H	1	0.13
(1,4066)	1:258:A:GLY:H	1:259:A:GLY:H	4	0.13
(1,4054)	1:244:A:ALA:H	1:245:A:SER:H	3	0.13
(1,4045)	1:235:A:ASP:H	1:236:A:ALA:H	6	0.13
(1,4009)	1:222:B:SER:H	1:225:B:LEU:H	3	0.13
(1,3808)	1:197:B:LEU:HA	1:200:B:GLU:H	12	0.13
(1,3791)	1:195:B:LYS:HA	1:199:B:ILE:H	10	0.13
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	10	0.13
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	10	0.13
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG21	13	0.13
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG22	13	0.13
(1,3586)	1:174:B:SER:HA	1:196:B:VAL:HG23	13	0.13
(1,3551)	1:171:B:ARG:HA	1:175:B:ARG:H	12	0.13
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	5	0.13
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	5	0.13
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	12	0.13
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	12	0.13
(1,3452)	1:161:B:SER:HA	1:165:B:ILE:H	8	0.13
(1,3354)	1:152:B:TYR:HA	1:155:B:ALA:H	14	0.13
(1,3315)	1:147:B:SER:HA	1:179:B:ALA:HA	2	0.13
(1,3225)	1:140:B:ALA:H	1:162:B:ALA:HA	12	0.13
(1,3205)	1:139:B:TYR:HA	1:143:B:ALA:H	4	0.13
(1,3186)	1:137:B:ILE:HA	1:140:B:ALA:H	1	0.13
(1,3108)	1:128:B:ALA:HA	1:132:B:LEU:H	5	0.13
(1,3091)	1:126:B:THR:HA	1:130:B:LYS:H	3	0.13
(1,3002)	1:118:B:TYR:HB2	1:148:B:SER:HB2	6	0.13
(1,3002)	1:118:B:TYR:HB2	1:148:B:SER:HB3	6	0.13
(1,3002)	1:118:B:TYR:HB3	1:148:B:SER:HB2	6	0.13
(1,3002)	1:118:B:TYR:HB3	1:148:B:SER:HB3	6	0.13
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD1	6	0.13
(1,2974)	1:116:B:LYS:HA	1:118:B:TYR:HD2	6	0.13
(1,2939)	1:113:B:MET:HA	1:116:B:LYS:HA	16	0.13
(1,2825)	1:103:B:GLU:HA	1:107:B:MET:H	10	0.13
(1,2819)	1:103:B:GLU:H	1:105:B:LEU:H	19	0.13
(1,2742)	1:94:B:ASP:H	1:96:B:ALA:H	9	0.13
(1,2726)	1:226:A:GLU:HA	1:227:A:LYS:H	5	0.13
(1,2642)	1:214:A:SER:HB2	1:215:A:ALA:H	8	0.13
(1,2642)	1:214:A:SER:HB3	1:215:A:ALA:H	8	0.13
(1,2555)	1:205:A:THR:H	1:209:A:LYS:H	10	0.13
(1,2550)	1:204:A:ALA:HA	1:208:A:MET:HE1	9	0.13
(1,2550)	1:204:A:ALA:HA	1:208:A:MET:HE2	9	0.13
(1,2550)	1:204:A:ALA:HA	1:208:A:MET:HE3	9	0.13
(1,2522)	1:199:A:ILE:HA	1:201:A:GLY:H	13	0.13
(1,2501)	1:197:A:LEU:HA	1:199:A:ILE:H	12	0.13
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	5	0.13
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	5	0.13
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB2	5	0.13
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	5	0.13
(1,2432)	1:191:A:GLU:HA	1:195:A:LYS:H	14	0.13
(1,2418)	1:190:A:LEU:HA	1:216:A:LYS:H	13	0.13
(1,2345)	1:180:A:LYS:HB2	1:189:A:ALA:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2345)	1:180:A:LYS:HB3	1:189:A:ALA:H	12	0.13
(1,2278)	1:174:A:SER:HA	1:178:A:PHE:H	6	0.13
(1,2245)	1:171:A:ARG:HA	1:175:A:ARG:H	8	0.13
(1,2163)	1:163:A:ILE:HA	1:167:A:PRO:HA	20	0.13
(1,2033)	1:150:A:LYS:HB2	1:152:A:TYR:HE2	3	0.13
(1,2004)	1:147:A:SER:HA	1:150:A:LYS:HA	9	0.13
(1,1985)	1:146:A:HIS:H	1:155:A:ALA:HA	5	0.13
(1,1919)	1:140:A:ALA:H	1:162:A:ALA:HA	14	0.13
(1,1812)	1:129:A:ILE:HA	1:132:A:LEU:H	1	0.13
(1,1785)	1:126:A:THR:HA	1:130:A:LYS:H	11	0.13
(1,1587)	1:109:A:GLY:HA2	1:121:A:ALA:H	3	0.13
(1,1587)	1:109:A:GLY:HA3	1:121:A:ALA:H	3	0.13
(1,1580)	1:109:A:GLY:H	1:125:A:TYR:HE1	14	0.13
(1,1552)	1:106:A:LYS:HA	1:108:A:GLN:H	17	0.13
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB1	14	0.13
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB2	14	0.13
(1,1549)	1:106:A:LYS:H	1:128:A:ALA:HB3	14	0.13
(1,1519)	1:103:A:GLU:HA	1:107:A:MET:H	10	0.13
(1,1446)	1:95:A:ASP:HA	1:98:A:THR:H	2	0.13
(1,1424)	1:69:A:LEU:HD11	1:2:B:SER:H	18	0.13
(1,1424)	1:69:A:LEU:HD12	1:2:B:SER:H	18	0.13
(1,1424)	1:69:A:LEU:HD13	1:2:B:SER:H	18	0.13
(1,1414)	1:67:A:ASP:HB2	1:63:B:GLN:H	14	0.13
(1,1414)	1:67:A:ASP:HB3	1:63:B:GLN:H	14	0.13
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	2	0.13
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	2	0.13
(1,1353)	1:39:A:CYS:HB2	1:36:B:ALA:H	7	0.13
(1,1353)	1:39:A:CYS:HB3	1:36:B:ALA:H	7	0.13
(1,1347)	1:39:A:CYS:H	1:36:B:ALA:HA	10	0.13
(1,1325)	1:33:A:LEU:HA	1:40:B:ILE:HA	2	0.13
(1,1318)	1:32:A:SER:HB2	1:39:B:CYS:HA	20	0.13
(1,1318)	1:32:A:SER:HB3	1:39:B:CYS:HA	20	0.13
(1,1298)	1:16:A:PHE:HE1	1:40:B:ILE:HD12	2	0.13
(1,1298)	1:16:A:PHE:HE2	1:40:B:ILE:HD12	2	0.13
(1,1221)	1:2:A:SER:HA	1:67:B:ASP:HA	7	0.13
(1,1219)	1:2:A:SER:H	1:69:B:LEU:H	12	0.13
(1,1191)	1:67:B:ASP:H	1:68:B:ILE:H	12	0.13
(1,1188)	1:66:B:ALA:HA	1:69:B:LEU:HA	12	0.13
(1,1184)	1:66:B:ALA:H	1:68:B:ILE:H	20	0.13
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	20	0.13
(1,1165)	1:62:B:GLY:H	1:64:B:HIS:H	3	0.13
(1,1133)	1:58:B:SER:HB2	1:60:B:PHE:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1133)	1:58:B:SER:HB3	1:60:B:PHE:H	10	0.13
(1,1133)	1:58:B:SER:HB2	1:60:B:PHE:H	14	0.13
(1,1133)	1:58:B:SER:HB3	1:60:B:PHE:H	14	0.13
(1,1125)	1:57:B:LYS:HB2	1:58:B:SER:H	8	0.13
(1,1125)	1:57:B:LYS:HB3	1:58:B:SER:H	8	0.13
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB1	14	0.13
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB2	14	0.13
(1,1055)	1:47:B:GLU:H	1:50:B:ALA:HB3	14	0.13
(1,1039)	1:45:B:GLY:H	1:46:B:PHE:H	16	0.13
(1,953)	1:35:B:VAL:HA	1:38:B:ASP:HA	16	0.13
(1,896)	1:29:B:GLY:H	1:32:B:SER:H	9	0.13
(1,889)	1:28:B:ASP:H	1:31:B:ASP:H	19	0.13
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	12	0.13
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	15	0.13
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD21	11	0.13
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD22	11	0.13
(1,650)	1:7:B:GLU:HA	1:55:B:LEU:HD23	11	0.13
(1,625)	1:4:B:SER:HA	1:5:B:LYS:H	5	0.13
(1,572)	1:65:A:LEU:HD21	1:66:A:ALA:H	11	0.13
(1,572)	1:65:A:LEU:HD22	1:66:A:ALA:H	11	0.13
(1,572)	1:65:A:LEU:HD23	1:66:A:ALA:H	11	0.13
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	1	0.13
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	19	0.13
(1,567)	1:65:A:LEU:H	1:67:A:ASP:H	6	0.13
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB2	8	0.13
(1,496)	1:54:A:ILE:HA	1:57:A:LYS:HB3	8	0.13
(1,484)	1:52:A:SER:HA	1:56:A:GLY:H	5	0.13
(1,482)	1:52:A:SER:HA	1:55:A:LEU:H	11	0.13
(1,458)	1:48:A:ARG:HA	1:50:A:ALA:H	1	0.13
(1,431)	1:45:A:GLY:H	1:46:A:PHE:HD1	3	0.13
(1,402)	1:41:A:SER:HA	1:46:A:PHE:H	12	0.13
(1,362)	1:37:A:MET:HA	1:40:A:ILE:H	12	0.13
(1,247)	1:23:A:LYS:H	1:24:A:GLU:H	13	0.13
(1,225)	1:20:A:VAL:HA	1:23:A:LYS:HA	4	0.13
(1,220)	1:20:A:VAL:H	1:23:A:LYS:H	14	0.13
(1,210)	1:18:A:SER:HA	1:21:A:GLU:HA	16	0.13
(1,201)	1:17:A:SER:HA	1:21:A:GLU:H	10	0.13
(1,167)	1:16:A:PHE:H	1:18:A:SER:H	18	0.13
(1,76)	1:10:A:ALA:HA	1:48:A:ARG:HA	2	0.13
(1,36)	1:7:A:GLU:H	1:10:A:ALA:H	17	0.13
(1,21)	1:5:A:LYS:H	1:8:A:ILE:H	3	0.13
(1,21)	1:5:A:LYS:H	1:8:A:ILE:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:2:A:SER:H	1:3:A:ALA:HA	20	0.13
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	6	0.12
(1,4183)	1:316:B:ASN:H	1:317:B:ASN:H	12	0.12
(1,4152)	1:244:B:ALA:H	1:245:B:SER:H	2	0.12
(1,4147)	1:239:B:ASP:H	1:240:B:ALA:H	2	0.12
(1,4093)	1:326:A:ASN:H	1:327:A:LEU:H	17	0.12
(1,4092)	1:325:A:GLY:H	1:326:A:ASN:H	18	0.12
(1,4090)	1:323:A:MET:H	1:324:A:ALA:H	20	0.12
(1,4064)	1:256:A:LEU:H	1:257:A:GLY:H	19	0.12
(1,3997)	1:220:B:GLU:HA	1:224:B:ASN:H	9	0.12
(1,3970)	1:217:B:LYS:HA	1:220:B:GLU:H	6	0.12
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	7	0.12
(1,3947)	1:214:B:SER:HA	1:218:B:LYS:H	4	0.12
(1,3941)	1:214:B:SER:H	1:216:B:LYS:H	4	0.12
(1,3939)	1:213:B:GLU:HA	1:217:B:LYS:H	3	0.12
(1,3886)	1:207:B:ALA:HA	1:210:B:ARG:H	6	0.12
(1,3872)	1:206:B:GLU:H	1:209:B:LYS:H	7	0.12
(1,3861)	1:205:B:THR:H	1:209:B:LYS:H	17	0.12
(1,3807)	1:197:B:LEU:HA	1:199:B:ILE:H	7	0.12
(1,3770)	1:193:B:TYR:HE2	1:211:B:ASP:HB3	8	0.12
(1,3769)	1:193:B:TYR:HE2	1:211:B:ASP:HA	8	0.12
(1,3759)	1:193:B:TYR:HB2	1:212:B:TYR:HA	7	0.12
(1,3759)	1:193:B:TYR:HB3	1:212:B:TYR:HA	7	0.12
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG21	20	0.12
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG22	20	0.12
(1,3717)	1:190:B:LEU:H	1:219:B:VAL:HG23	20	0.12
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	4	0.12
(1,3677)	1:182:B:ALA:HA	1:184:B:GLY:H	3	0.12
(1,3668)	1:181:B:TYR:HD1	1:218:B:LYS:HB2	9	0.12
(1,3668)	1:181:B:TYR:HD1	1:218:B:LYS:HB3	9	0.12
(1,3668)	1:181:B:TYR:HD2	1:218:B:LYS:HB2	9	0.12
(1,3668)	1:181:B:TYR:HD2	1:218:B:LYS:HB3	9	0.12
(1,3664)	1:181:B:TYR:HA	1:186:B:PRO:HA	5	0.12
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB1	17	0.12
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB2	17	0.12
(1,3658)	1:181:B:TYR:H	1:189:B:ALA:HB3	17	0.12
(1,3584)	1:174:B:SER:HA	1:178:B:PHE:H	7	0.12
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG2	1	0.12
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG3	1	0.12
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG2	1	0.12
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG3	1	0.12
(1,3569)	1:173:B:TYR:HB2	1:195:B:LYS:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3569)	1:173:B:TYR:HB3	1:195:B:LYS:H	11	0.12
(1,3511)	1:169:B:TYR:HD1	1:171:B:ARG:H	14	0.12
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	4	0.12
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	4	0.12
(1,3482)	1:164:B:SER:HA	1:167:B:PRO:HA	3	0.12
(1,3475)	1:163:B:ILE:HD11	1:176:B:LEU:HB2	12	0.12
(1,3475)	1:163:B:ILE:HD11	1:176:B:LEU:HB3	12	0.12
(1,3475)	1:163:B:ILE:HD12	1:176:B:LEU:HB2	12	0.12
(1,3475)	1:163:B:ILE:HD12	1:176:B:LEU:HB3	12	0.12
(1,3475)	1:163:B:ILE:HD13	1:176:B:LEU:HB2	12	0.12
(1,3475)	1:163:B:ILE:HD13	1:176:B:LEU:HB3	12	0.12
(1,3411)	1:157:B:LYS:HA	1:160:B:GLU:H	5	0.12
(1,3396)	1:156:B:VAL:HA	1:176:B:LEU:HA	13	0.12
(1,3334)	1:150:B:LYS:HA	1:152:B:TYR:H	7	0.12
(1,3310)	1:147:B:SER:HA	1:150:B:LYS:HA	9	0.12
(1,3257)	1:143:B:ALA:HA	1:155:B:ALA:HA	13	0.12
(1,3001)	1:118:B:TYR:HB2	1:145:B:ALA:HB3	20	0.12
(1,3001)	1:118:B:TYR:HB3	1:145:B:ALA:HB3	20	0.12
(1,2932)	1:113:B:MET:H	1:121:B:ALA:H	4	0.12
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE1	16	0.12
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE2	16	0.12
(1,2829)	1:104:B:ASP:H	1:107:B:MET:HE3	16	0.12
(1,2800)	1:102:B:ALA:H	1:105:B:LEU:H	19	0.12
(1,2747)	1:95:B:ASP:H	1:96:B:ALA:HA	2	0.12
(1,2610)	1:211:A:ASP:H	1:214:A:SER:H	18	0.12
(1,2602)	1:210:A:ARG:H	1:213:A:GLU:H	11	0.12
(1,2580)	1:207:A:ALA:HA	1:210:A:ARG:H	5	0.12
(1,2580)	1:207:A:ALA:HA	1:210:A:ARG:H	19	0.12
(1,2570)	1:206:A:GLU:HA	1:209:A:LYS:H	11	0.12
(1,2463)	1:193:A:TYR:HE2	1:211:A:ASP:HA	6	0.12
(1,2380)	1:185:A:LYS:H	1:186:A:PRO:HA	16	0.12
(1,2206)	1:169:A:TYR:HE2	1:171:A:ARG:HB3	6	0.12
(1,2201)	1:169:A:TYR:HE1	1:171:A:ARG:HB2	7	0.12
(1,2201)	1:169:A:TYR:HE1	1:171:A:ARG:HB3	7	0.12
(1,2201)	1:169:A:TYR:HE2	1:171:A:ARG:HB2	7	0.12
(1,2201)	1:169:A:TYR:HE2	1:171:A:ARG:HB3	7	0.12
(1,2106)	1:157:A:LYS:HA	1:161:A:SER:H	8	0.12
(1,2090)	1:156:A:VAL:HA	1:176:A:LEU:HA	10	0.12
(1,2039)	1:151:A:GLU:H	1:152:A:TYR:HA	3	0.12
(1,2039)	1:151:A:GLU:H	1:152:A:TYR:HA	11	0.12
(1,1962)	1:143:A:ALA:HB1	1:175:A:ARG:HB2	5	0.12
(1,1962)	1:143:A:ALA:HB1	1:175:A:ARG:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1962)	1:143:A:ALA:HB2	1:175:A:ARG:HB2	5	0.12
(1,1962)	1:143:A:ALA:HB2	1:175:A:ARG:HB3	5	0.12
(1,1962)	1:143:A:ALA:HB3	1:175:A:ARG:HB2	5	0.12
(1,1962)	1:143:A:ALA:HB3	1:175:A:ARG:HB3	5	0.12
(1,1853)	1:135:A:ASN:HB2	1:138:A:TYR:H	18	0.12
(1,1853)	1:135:A:ASN:HB3	1:138:A:TYR:H	18	0.12
(1,1802)	1:128:A:ALA:HA	1:132:A:LEU:H	9	0.12
(1,1721)	1:121:A:ALA:HA	1:125:A:TYR:H	1	0.12
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD1	16	0.12
(1,1671)	1:116:A:LYS:HB2	1:118:A:TYR:HD2	16	0.12
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD1	16	0.12
(1,1671)	1:116:A:LYS:HB3	1:118:A:TYR:HD2	16	0.12
(1,1666)	1:116:A:LYS:HA	1:118:A:TYR:H	16	0.12
(1,1641)	1:113:A:MET:HE1	1:141:A:ASN:HA	20	0.12
(1,1641)	1:113:A:MET:HE2	1:141:A:ASN:HA	20	0.12
(1,1641)	1:113:A:MET:HE3	1:141:A:ASN:HA	20	0.12
(1,1593)	1:110:A:ASN:HA	1:113:A:MET:H	7	0.12
(1,1579)	1:109:A:GLY:H	1:125:A:TYR:HD1	12	0.12
(1,1547)	1:106:A:LYS:H	1:109:A:GLY:H	20	0.12
(1,1538)	1:105:A:LEU:HD11	1:127:A:GLU:HA	14	0.12
(1,1538)	1:105:A:LEU:HD12	1:127:A:GLU:HA	14	0.12
(1,1538)	1:105:A:LEU:HD13	1:127:A:GLU:HA	14	0.12
(1,1535)	1:105:A:LEU:HA	1:108:A:GLN:H	17	0.12
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB1	15	0.12
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB2	15	0.12
(1,1434)	1:93:A:GLU:HA	1:96:A:ALA:HB3	15	0.12
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	14	0.12
(1,1314)	1:29:A:GLY:HA2	1:43:B:ALA:H	16	0.12
(1,1314)	1:29:A:GLY:HA3	1:43:B:ALA:H	16	0.12
(1,1289)	1:16:A:PHE:HE1	1:12:B:ILE:HD12	9	0.12
(1,1289)	1:16:A:PHE:HE2	1:12:B:ILE:HD12	9	0.12
(1,1279)	1:16:A:PHE:HE1	1:9:B:ALA:HA	11	0.12
(1,1279)	1:16:A:PHE:HE2	1:9:B:ALA:HA	11	0.12
(1,1239)	1:8:A:ILE:HG21	1:12:B:ILE:HA	11	0.12
(1,1239)	1:8:A:ILE:HG22	1:12:B:ILE:HA	11	0.12
(1,1239)	1:8:A:ILE:HG23	1:12:B:ILE:HA	11	0.12
(1,1181)	1:65:B:LEU:HD21	1:66:B:ALA:H	12	0.12
(1,1181)	1:65:B:LEU:HD22	1:66:B:ALA:H	12	0.12
(1,1181)	1:65:B:LEU:HD23	1:66:B:ALA:H	12	0.12
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	4	0.12
(1,1162)	1:61:B:LYS:HG2	1:62:B:GLY:H	3	0.12
(1,1162)	1:61:B:LYS:HG3	1:62:B:GLY:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1159)	1:61:B:LYS:H	1:63:B:GLN:H	1	0.12
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG2	18	0.12
(1,1153)	1:60:B:PHE:HB2	1:63:B:GLN:HG3	18	0.12
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG2	18	0.12
(1,1153)	1:60:B:PHE:HB3	1:63:B:GLN:HG3	18	0.12
(1,1133)	1:58:B:SER:HB2	1:60:B:PHE:H	8	0.12
(1,1133)	1:58:B:SER:HB3	1:60:B:PHE:H	8	0.12
(1,1130)	1:58:B:SER:HA	1:60:B:PHE:H	4	0.12
(1,1113)	1:55:B:LEU:HA	1:58:B:SER:H	5	0.12
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD11	7	0.12
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD12	7	0.12
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD13	7	0.12
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD11	7	0.12
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD12	7	0.12
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD13	7	0.12
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD11	20	0.12
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD12	20	0.12
(1,1049)	1:46:B:PHE:HB2	1:54:B:ILE:HD13	20	0.12
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD11	20	0.12
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD12	20	0.12
(1,1049)	1:46:B:PHE:HB3	1:54:B:ILE:HD13	20	0.12
(1,1032)	1:44:B:PHE:H	1:46:B:PHE:H	9	0.12
(1,1009)	1:41:B:SER:HA	1:44:B:PHE:H	4	0.12
(1,984)	1:39:B:CYS:H	1:42:B:GLU:H	1	0.12
(1,953)	1:35:B:VAL:HA	1:38:B:ASP:HA	13	0.12
(1,948)	1:35:B:VAL:H	1:38:B:ASP:H	18	0.12
(1,909)	1:30:B:ALA:HA	1:34:B:ASN:H	5	0.12
(1,776)	1:16:B:PHE:H	1:18:B:SER:H	3	0.12
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG11	12	0.12
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG12	12	0.12
(1,746)	1:14:B:ASN:H	1:51:B:VAL:HG13	12	0.12
(1,685)	1:10:B:ALA:HA	1:48:B:ARG:HA	19	0.12
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD11	20	0.12
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD12	20	0.12
(1,663)	1:9:B:ALA:H	1:12:B:ILE:HD13	20	0.12
(1,605)	1:71:A:SER:H	1:72:A:ALA:HA	17	0.12
(1,599)	1:70:A:ASN:H	1:71:A:SER:H	13	0.12
(1,599)	1:70:A:ASN:H	1:71:A:SER:H	17	0.12
(1,587)	1:68:A:ILE:H	1:69:A:LEU:HA	6	0.12
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	9	0.12
(1,571)	1:65:A:LEU:HA	1:71:A:SER:H	5	0.12
(1,556)	1:62:A:GLY:H	1:64:A:HIS:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:60:A:PHE:HB2	1:63:A:GLN:HG2	10	0.12
(1,544)	1:60:A:PHE:HB2	1:63:A:GLN:HG3	10	0.12
(1,544)	1:60:A:PHE:HB3	1:63:A:GLN:HG2	10	0.12
(1,544)	1:60:A:PHE:HB3	1:63:A:GLN:HG3	10	0.12
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD11	7	0.12
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD12	7	0.12
(1,440)	1:46:A:PHE:HB2	1:54:A:ILE:HD13	7	0.12
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD11	7	0.12
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD12	7	0.12
(1,440)	1:46:A:PHE:HB3	1:54:A:ILE:HD13	7	0.12
(1,380)	1:39:A:CYS:HA	1:42:A:GLU:HA	5	0.12
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD2	11	0.12
(1,365)	1:37:A:MET:HA	1:48:A:ARG:HD3	11	0.12
(1,339)	1:35:A:VAL:H	1:38:A:ASP:H	8	0.12
(1,310)	1:31:A:ASP:HA	1:35:A:VAL:H	10	0.12
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	2	0.12
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	19	0.12
(1,171)	1:16:A:PHE:HA	1:18:A:SER:H	9	0.12
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB2	8	0.12
(1,156)	1:15:A:TYR:HA	1:70:A:ASN:HB3	8	0.12
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB2	15	0.12
(1,154)	1:15:A:TYR:HA	1:18:A:SER:HB3	15	0.12
(1,25)	1:5:A:LYS:HA	1:8:A:ILE:H	17	0.12
(1,4171)	1:302:B:PHE:H	1:303:B:ALA:H	10	0.11
(1,4170)	1:301:B:GLY:H	1:302:B:PHE:H	14	0.11
(1,4150)	1:242:B:GLN:H	1:243:B:GLY:H	6	0.11
(1,4022)	1:224:B:ASN:H	1:226:B:GLU:H	9	0.11
(1,4000)	1:221:B:GLN:H	1:224:B:ASN:H	15	0.11
(1,4000)	1:221:B:GLN:H	1:224:B:ASN:H	19	0.11
(1,3972)	1:217:B:LYS:HG2	1:218:B:LYS:H	5	0.11
(1,3972)	1:217:B:LYS:HG3	1:218:B:LYS:H	5	0.11
(1,3904)	1:209:B:LYS:HA	1:211:B:ASP:H	6	0.11
(1,3898)	1:208:B:MET:HA	1:211:B:ASP:H	14	0.11
(1,3889)	1:207:B:ALA:HA	1:211:B:ASP:H	19	0.11
(1,3879)	1:206:B:GLU:HB2	1:207:B:ALA:H	14	0.11
(1,3879)	1:206:B:GLU:HB3	1:207:B:ALA:H	14	0.11
(1,3835)	1:200:B:GLU:HB2	1:204:B:ALA:HA	2	0.11
(1,3835)	1:200:B:GLU:HB3	1:204:B:ALA:HA	2	0.11
(1,3825)	1:199:B:ILE:H	1:201:B:GLY:H	19	0.11
(1,3791)	1:195:B:LYS:HA	1:199:B:ILE:H	16	0.11
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD2	1	0.11
(1,3672)	1:181:B:TYR:HE1	1:218:B:LYS:HD3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD2	1	0.11
(1,3672)	1:181:B:TYR:HE2	1:218:B:LYS:HD3	1	0.11
(1,3585)	1:174:B:SER:HA	1:193:B:TYR:HA	8	0.11
(1,3573)	1:173:B:TYR:HB2	1:196:B:VAL:HA	1	0.11
(1,3573)	1:173:B:TYR:HB3	1:196:B:VAL:HA	1	0.11
(1,3542)	1:170:B:PHE:HD2	1:171:B:ARG:HD2	1	0.11
(1,3537)	1:170:B:PHE:HE1	1:171:B:ARG:HA	16	0.11
(1,3537)	1:170:B:PHE:HE2	1:171:B:ARG:HA	16	0.11
(1,3521)	1:170:B:PHE:HA	1:174:B:SER:H	14	0.11
(1,3512)	1:169:B:TYR:HE1	1:171:B:ARG:HB2	14	0.11
(1,3503)	1:169:B:TYR:HD1	1:171:B:ARG:H	9	0.11
(1,3503)	1:169:B:TYR:HD2	1:171:B:ARG:H	9	0.11
(1,3429)	1:159:B:ALA:HA	1:176:B:LEU:H	10	0.11
(1,3406)	1:157:B:LYS:H	1:159:B:ALA:H	3	0.11
(1,3400)	1:156:B:VAL:HG11	1:160:B:GLU:H	11	0.11
(1,3400)	1:156:B:VAL:HG12	1:160:B:GLU:H	11	0.11
(1,3400)	1:156:B:VAL:HG13	1:160:B:GLU:H	11	0.11
(1,3377)	1:154:B:GLN:H	1:157:B:LYS:H	11	0.11
(1,3361)	1:152:B:TYR:HB2	1:183:B:GLN:H	19	0.11
(1,3361)	1:152:B:TYR:HB3	1:183:B:GLN:H	19	0.11
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	4	0.11
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	15	0.11
(1,3345)	1:151:B:GLU:H	1:152:B:TYR:HA	16	0.11
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE1	18	0.11
(1,3338)	1:150:B:LYS:HB2	1:152:B:TYR:HE2	18	0.11
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE1	18	0.11
(1,3338)	1:150:B:LYS:HB3	1:152:B:TYR:HE2	18	0.11
(1,3314)	1:147:B:SER:HA	1:155:B:ALA:HB1	3	0.11
(1,3314)	1:147:B:SER:HA	1:155:B:ALA:HB2	3	0.11
(1,3314)	1:147:B:SER:HA	1:155:B:ALA:HB3	3	0.11
(1,3182)	1:137:B:ILE:H	1:169:B:TYR:HE2	12	0.11
(1,3171)	1:136:B:ALA:HA	1:166:B:ASP:H	8	0.11
(1,3157)	1:135:B:ASN:HA	1:137:B:ILE:H	6	0.11
(1,3135)	1:130:B:LYS:HA	1:132:B:LEU:H	20	0.11
(1,3089)	1:126:B:THR:HA	1:129:B:ILE:H	8	0.11
(1,3089)	1:126:B:THR:HA	1:129:B:ILE:H	17	0.11
(1,3054)	1:124:B:LYS:H	1:127:B:GLU:H	12	0.11
(1,2980)	1:117:B:ASP:H	1:118:B:TYR:HA	1	0.11
(1,2969)	1:116:B:LYS:H	1:118:B:TYR:HE1	1	0.11
(1,2899)	1:110:B:ASN:HA	1:113:B:MET:H	8	0.11
(1,2899)	1:110:B:ASN:HA	1:113:B:MET:H	12	0.11
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	9	0.11
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	9	0.11
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	4	0.11
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	4	0.11
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	4	0.11
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG11	3	0.11
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG12	3	0.11
(1,2801)	1:102:B:ALA:H	1:131:B:VAL:HG13	3	0.11
(1,2800)	1:102:B:ALA:H	1:105:B:LEU:H	18	0.11
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	10	0.11
(1,2797)	1:101:B:LYS:HA	1:105:B:LEU:H	12	0.11
(1,2785)	1:100:B:ALA:HA	1:101:B:LYS:HA	5	0.11
(1,2780)	1:99:B:LYS:HA	1:102:B:ALA:H	11	0.11
(1,2768)	1:98:B:THR:H	1:100:B:ALA:H	18	0.11
(1,2716)	1:224:A:ASN:H	1:226:A:GLU:H	9	0.11
(1,2633)	1:213:A:GLU:HA	1:217:A:LYS:H	12	0.11
(1,2627)	1:213:A:GLU:H	1:215:A:ALA:H	18	0.11
(1,2613)	1:211:A:ASP:HA	1:213:A:GLU:H	3	0.11
(1,2517)	1:198:A:ASP:HA	1:201:A:GLY:H	12	0.11
(1,2502)	1:197:A:LEU:HA	1:200:A:GLU:H	6	0.11
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB2	6	0.11
(1,2462)	1:193:A:TYR:HE1	1:211:A:ASP:HB3	6	0.11
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB2	6	0.11
(1,2462)	1:193:A:TYR:HE2	1:211:A:ASP:HB3	6	0.11
(1,2450)	1:193:A:TYR:HA	1:197:A:LEU:H	19	0.11
(1,2390)	1:187:A:GLU:HA	1:190:A:LEU:H	15	0.11
(1,2359)	1:181:A:TYR:HA	1:189:A:ALA:H	18	0.11
(1,2349)	1:181:A:TYR:H	1:186:A:PRO:HA	11	0.11
(1,2339)	1:180:A:LYS:HA	1:183:A:GLN:H	3	0.11
(1,2293)	1:176:A:LEU:HA	1:180:A:LYS:H	18	0.11
(1,2245)	1:171:A:ARG:HA	1:175:A:ARG:H	7	0.11
(1,2231)	1:170:A:PHE:HE1	1:171:A:ARG:HA	2	0.11
(1,2231)	1:170:A:PHE:HE2	1:171:A:ARG:HA	2	0.11
(1,2076)	1:154:A:GLN:HA	1:158:A:ASP:H	1	0.11
(1,2009)	1:147:A:SER:HA	1:179:A:ALA:HA	9	0.11
(1,1985)	1:146:A:HIS:H	1:155:A:ALA:HA	9	0.11
(1,1919)	1:140:A:ALA:H	1:162:A:ALA:HA	12	0.11
(1,1894)	1:139:A:TYR:H	1:162:A:ALA:HA	16	0.11
(1,1829)	1:130:A:LYS:HA	1:132:A:LEU:H	4	0.11
(1,1826)	1:130:A:LYS:H	1:132:A:LEU:H	1	0.11
(1,1712)	1:120:A:LEU:HA	1:122:A:ILE:H	14	0.11
(1,1695)	1:118:A:TYR:HB2	1:145:A:ALA:HB3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1695)	1:118:A:TYR:HB3	1:145:A:ALA:HB3	2	0.11
(1,1670)	1:116:A:LYS:HA	1:118:A:TYR:HE1	18	0.11
(1,1633)	1:113:A:MET:HA	1:116:A:LYS:HA	9	0.11
(1,1517)	1:103:A:GLU:HA	1:105:A:LEU:H	11	0.11
(1,1501)	1:102:A:ALA:HA	1:128:A:ALA:HA	12	0.11
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG12	11	0.11
(1,1382)	1:44:A:PHE:HA	1:25:B:ILE:HG13	11	0.11
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB2	20	0.11
(1,1368)	1:42:A:GLU:H	1:32:B:SER:HB3	20	0.11
(1,1358)	1:40:A:ILE:HA	1:33:B:LEU:HA	15	0.11
(1,1348)	1:39:A:CYS:H	1:36:B:ALA:HB1	3	0.11
(1,1348)	1:39:A:CYS:H	1:36:B:ALA:HB2	3	0.11
(1,1348)	1:39:A:CYS:H	1:36:B:ALA:HB3	3	0.11
(1,1316)	1:32:A:SER:HA	1:39:B:CYS:HA	13	0.11
(1,1315)	1:32:A:SER:H	1:43:B:ALA:HA	6	0.11
(1,1314)	1:29:A:GLY:HA2	1:43:B:ALA:H	19	0.11
(1,1314)	1:29:A:GLY:HA3	1:43:B:ALA:H	19	0.11
(1,1294)	1:16:A:PHE:HE1	1:40:B:ILE:HG22	14	0.11
(1,1294)	1:16:A:PHE:HE2	1:40:B:ILE:HG22	14	0.11
(1,1282)	1:16:A:PHE:HE1	1:9:B:ALA:HB2	3	0.11
(1,1282)	1:16:A:PHE:HE2	1:9:B:ALA:HB2	3	0.11
(1,1282)	1:16:A:PHE:HE1	1:9:B:ALA:HB2	18	0.11
(1,1282)	1:16:A:PHE:HE2	1:9:B:ALA:HB2	18	0.11
(1,1281)	1:16:A:PHE:HE1	1:9:B:ALA:HB1	1	0.11
(1,1281)	1:16:A:PHE:HE2	1:9:B:ALA:HB1	1	0.11
(1,1279)	1:16:A:PHE:HE1	1:9:B:ALA:HA	13	0.11
(1,1279)	1:16:A:PHE:HE2	1:9:B:ALA:HA	13	0.11
(1,1274)	1:15:A:TYR:HH	1:5:B:LYS:HA	13	0.11
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE1	11	0.11
(1,1242)	1:8:A:ILE:HG12	1:15:B:TYR:HE2	11	0.11
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE1	11	0.11
(1,1242)	1:8:A:ILE:HG13	1:15:B:TYR:HE2	11	0.11
(1,1227)	1:2:A:SER:HB2	1:15:B:TYR:HE1	19	0.11
(1,1227)	1:2:A:SER:HB2	1:15:B:TYR:HE2	19	0.11
(1,1227)	1:2:A:SER:HB3	1:15:B:TYR:HE1	19	0.11
(1,1227)	1:2:A:SER:HB3	1:15:B:TYR:HE2	19	0.11
(1,1212)	1:70:B:ASN:HA	1:72:B:ALA:H	13	0.11
(1,1196)	1:68:B:ILE:H	1:69:B:LEU:HA	10	0.11
(1,1187)	1:66:B:ALA:HA	1:68:B:ILE:H	14	0.11
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	1	0.11
(1,1176)	1:65:B:LEU:H	1:67:B:ASP:H	11	0.11
(1,1157)	1:60:B:PHE:HD1	1:61:B:LYS:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1157)	1:60:B:PHE:HD2	1:61:B:LYS:H	9	0.11
(1,1157)	1:60:B:PHE:HD1	1:61:B:LYS:H	19	0.11
(1,1157)	1:60:B:PHE:HD2	1:61:B:LYS:H	19	0.11
(1,1127)	1:58:B:SER:H	1:59:B:GLU:HA	16	0.11
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB2	2	0.11
(1,1105)	1:54:B:ILE:HA	1:57:B:LYS:HB3	2	0.11
(1,1075)	1:50:B:ALA:H	1:51:B:VAL:H	4	0.11
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD2	15	0.11
(1,974)	1:37:B:MET:HA	1:48:B:ARG:HD3	15	0.11
(1,900)	1:29:B:GLY:HA2	1:32:B:SER:H	2	0.11
(1,900)	1:29:B:GLY:HA3	1:32:B:SER:H	2	0.11
(1,686)	1:10:B:ALA:HA	1:51:B:VAL:HA	10	0.11
(1,653)	1:8:B:ILE:H	1:11:B:LEU:H	17	0.11
(1,635)	1:5:B:LYS:HA	1:9:B:ALA:H	4	0.11
(1,633)	1:5:B:LYS:HA	1:7:B:GLU:H	6	0.11
(1,587)	1:68:A:ILE:H	1:69:A:LEU:HA	14	0.11
(1,575)	1:66:A:ALA:H	1:68:A:ILE:H	3	0.11
(1,503)	1:55:A:LEU:HA	1:57:A:LYS:H	15	0.11
(1,462)	1:49:A:GLU:H	1:51:A:VAL:H	7	0.11
(1,375)	1:39:A:CYS:H	1:42:A:GLU:H	16	0.11
(1,283)	1:28:A:ASP:HA	1:31:A:ASP:H	13	0.11
(1,248)	1:23:A:LYS:H	1:25:A:ILE:H	5	0.11
(1,239)	1:21:A:GLU:HB2	1:22:A:LYS:H	16	0.11
(1,239)	1:21:A:GLU:HB3	1:22:A:LYS:H	16	0.11
(1,171)	1:16:A:PHE:HA	1:18:A:SER:H	19	0.11
(1,161)	1:15:A:TYR:HB3	1:16:A:PHE:HD1	11	0.11
(1,153)	1:15:A:TYR:HA	1:18:A:SER:H	15	0.11
(1,26)	1:5:A:LYS:HA	1:9:A:ALA:H	11	0.11
(1,25)	1:5:A:LYS:HA	1:8:A:ILE:H	15	0.11
(1,1)	1:2:A:SER:H	1:3:A:ALA:H	8	0.11
(1,4166)	1:260:B:LEU:H	1:261:B:GLY:H	5	0.1
(1,4068)	1:260:A:LEU:H	1:261:A:GLY:H	5	0.1
(1,4040)	1:228:A:THR:H	1:229:A:VAL:H	20	0.1
(1,3955)	1:215:B:ALA:HA	1:218:B:LYS:H	5	0.1
(1,3933)	1:213:B:GLU:H	1:215:B:ALA:H	20	0.1
(1,3834)	1:200:B:GLU:HB2	1:204:B:ALA:H	16	0.1
(1,3834)	1:200:B:GLU:HB3	1:204:B:ALA:H	16	0.1
(1,3765)	1:193:B:TYR:HD1	1:212:B:TYR:H	19	0.1
(1,3765)	1:193:B:TYR:HD2	1:212:B:TYR:H	19	0.1
(1,3696)	1:187:B:GLU:HA	1:190:B:LEU:H	9	0.1
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG2	11	0.1
(1,3571)	1:173:B:TYR:HB2	1:195:B:LYS:HG3	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG2	11	0.1
(1,3571)	1:173:B:TYR:HB3	1:195:B:LYS:HG3	11	0.1
(1,3502)	1:169:B:TYR:HD1	1:170:B:PHE:H	3	0.1
(1,3502)	1:169:B:TYR:HD2	1:170:B:PHE:H	3	0.1
(1,3400)	1:156:B:VAL:HG11	1:160:B:GLU:H	13	0.1
(1,3400)	1:156:B:VAL:HG12	1:160:B:GLU:H	13	0.1
(1,3400)	1:156:B:VAL:HG13	1:160:B:GLU:H	13	0.1
(1,3357)	1:152:B:TYR:HA	1:156:B:VAL:H	20	0.1
(1,3325)	1:149:B:LEU:H	1:151:B:GLU:H	2	0.1
(1,3311)	1:147:B:SER:HA	1:151:B:GLU:H	14	0.1
(1,3241)	1:141:B:ASN:HA	1:145:B:ALA:H	9	0.1
(1,3219)	1:139:B:TYR:HE1	1:161:B:SER:HB2	1	0.1
(1,3219)	1:139:B:TYR:HE1	1:161:B:SER:HB3	1	0.1
(1,3219)	1:139:B:TYR:HE2	1:161:B:SER:HB2	1	0.1
(1,3219)	1:139:B:TYR:HE2	1:161:B:SER:HB3	1	0.1
(1,3119)	1:129:B:ILE:HA	1:133:B:PRO:HA	14	0.1
(1,3106)	1:128:B:ALA:HA	1:131:B:VAL:H	7	0.1
(1,3091)	1:126:B:THR:HA	1:130:B:LYS:H	2	0.1
(1,3072)	1:125:B:TYR:HB2	1:141:B:ASN:HB2	7	0.1
(1,3072)	1:125:B:TYR:HB2	1:141:B:ASN:HB3	7	0.1
(1,3072)	1:125:B:TYR:HB3	1:141:B:ASN:HB2	7	0.1
(1,3072)	1:125:B:TYR:HB3	1:141:B:ASN:HB3	7	0.1
(1,2872)	1:107:B:MET:HA	1:111:B:LYS:H	13	0.1
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB1	12	0.1
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB2	12	0.1
(1,2855)	1:106:B:LYS:H	1:128:B:ALA:HB3	12	0.1
(1,2848)	1:105:B:LEU:HD11	1:131:B:VAL:H	19	0.1
(1,2848)	1:105:B:LEU:HD12	1:131:B:VAL:H	19	0.1
(1,2848)	1:105:B:LEU:HD13	1:131:B:VAL:H	19	0.1
(1,2698)	1:221:A:GLN:HA	1:224:A:ASN:HB2	6	0.1
(1,2698)	1:221:A:GLN:HA	1:224:A:ASN:HB3	6	0.1
(1,2632)	1:213:A:GLU:HA	1:216:A:LYS:H	3	0.1
(1,2607)	1:210:A:ARG:HA	1:214:A:SER:H	17	0.1
(1,2552)	1:205:A:THR:H	1:208:A:MET:H	3	0.1
(1,2552)	1:205:A:THR:H	1:208:A:MET:H	17	0.1
(1,2528)	1:200:A:GLU:HB2	1:204:A:ALA:H	17	0.1
(1,2528)	1:200:A:GLU:HB3	1:204:A:ALA:H	17	0.1
(1,2408)	1:190:A:LEU:H	1:192:A:ALA:H	3	0.1
(1,2320)	1:178:A:PHE:HA	1:182:A:ALA:H	2	0.1
(1,2261)	1:173:A:TYR:HA	1:192:A:ALA:HA	17	0.1
(1,2029)	1:150:A:LYS:HA	1:152:A:TYR:HA	11	0.1
(1,1973)	1:144:A:ALA:HB1	1:175:A:ARG:HE	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1973)	1:144:A:ALA:HB2	1:175:A:ARG:HE	7	0.1
(1,1973)	1:144:A:ALA:HB3	1:175:A:ARG:HE	7	0.1
(1,1793)	1:127:A:GLU:HA	1:131:A:VAL:H	18	0.1
(1,1742)	1:123:A:ASN:H	1:126:A:THR:H	14	0.1
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE1	7	0.1
(1,1672)	1:116:A:LYS:HB2	1:118:A:TYR:HE2	7	0.1
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE1	7	0.1
(1,1672)	1:116:A:LYS:HB3	1:118:A:TYR:HE2	7	0.1
(1,1536)	1:105:A:LEU:HA	1:109:A:GLY:H	3	0.1
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE1	3	0.1
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE2	3	0.1
(1,1523)	1:104:A:ASP:H	1:107:A:MET:HE3	3	0.1
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB2	6	0.1
(1,1426)	1:69:A:LEU:HD11	1:2:B:SER:HB3	6	0.1
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB2	6	0.1
(1,1426)	1:69:A:LEU:HD12	1:2:B:SER:HB3	6	0.1
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB2	6	0.1
(1,1426)	1:69:A:LEU:HD13	1:2:B:SER:HB3	6	0.1
(1,1356)	1:40:A:ILE:H	1:36:B:ALA:HA	13	0.1
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB2	13	0.1
(1,1335)	1:35:A:VAL:HG21	1:39:B:CYS:HB3	13	0.1
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB2	13	0.1
(1,1335)	1:35:A:VAL:HG22	1:39:B:CYS:HB3	13	0.1
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB2	13	0.1
(1,1335)	1:35:A:VAL:HG23	1:39:B:CYS:HB3	13	0.1
(1,1266)	1:15:A:TYR:HE1	1:5:B:LYS:H	15	0.1
(1,1266)	1:15:A:TYR:HE2	1:5:B:LYS:H	15	0.1
(1,1158)	1:61:B:LYS:H	1:62:B:GLY:H	12	0.1
(1,1138)	1:59:B:GLU:HA	1:64:B:HIS:HA	19	0.1
(1,1106)	1:54:B:ILE:HA	1:57:B:LYS:HG2	20	0.1
(1,1106)	1:54:B:ILE:HA	1:57:B:LYS:HG3	20	0.1
(1,1058)	1:47:B:GLU:HA	1:49:B:GLU:H	1	0.1
(1,945)	1:34:B:ASN:HA	1:38:B:ASP:H	15	0.1
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE1	12	0.1
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE2	12	0.1
(1,944)	1:34:B:ASN:HA	1:37:B:MET:HE3	12	0.1
(1,852)	1:22:B:LYS:H	1:24:B:GLU:H	13	0.1
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	9	0.1
(1,819)	1:18:B:SER:HA	1:21:B:GLU:HA	16	0.1
(1,710)	1:11:B:LEU:HD21	1:68:B:ILE:HD11	5	0.1
(1,710)	1:11:B:LEU:HD21	1:68:B:ILE:HD12	5	0.1
(1,710)	1:11:B:LEU:HD21	1:68:B:ILE:HD13	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:11:B:LEU:HD22	1:68:B:ILE:HD11	5	0.1
(1,710)	1:11:B:LEU:HD22	1:68:B:ILE:HD12	5	0.1
(1,710)	1:11:B:LEU:HD22	1:68:B:ILE:HD13	5	0.1
(1,710)	1:11:B:LEU:HD23	1:68:B:ILE:HD11	5	0.1
(1,710)	1:11:B:LEU:HD23	1:68:B:ILE:HD12	5	0.1
(1,710)	1:11:B:LEU:HD23	1:68:B:ILE:HD13	5	0.1
(1,518)	1:58:A:SER:H	1:59:A:GLU:HA	2	0.1
(1,505)	1:55:A:LEU:HD11	1:71:A:SER:HA	18	0.1
(1,505)	1:55:A:LEU:HD12	1:71:A:SER:HA	18	0.1
(1,505)	1:55:A:LEU:HD13	1:71:A:SER:HA	18	0.1
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB1	17	0.1
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB2	17	0.1
(1,446)	1:47:A:GLU:H	1:50:A:ALA:HB3	17	0.1
(1,336)	1:34:A:ASN:HA	1:38:A:ASP:H	11	0.1
(1,276)	1:27:A:GLU:HA	1:30:A:ALA:HA	16	0.1
(1,275)	1:27:A:GLU:HA	1:30:A:ALA:H	5	0.1
(1,248)	1:23:A:LYS:H	1:25:A:ILE:H	8	0.1
(1,26)	1:5:A:LYS:HA	1:9:A:ALA:H	4	0.1

10 Dihedral-angle violation analysis

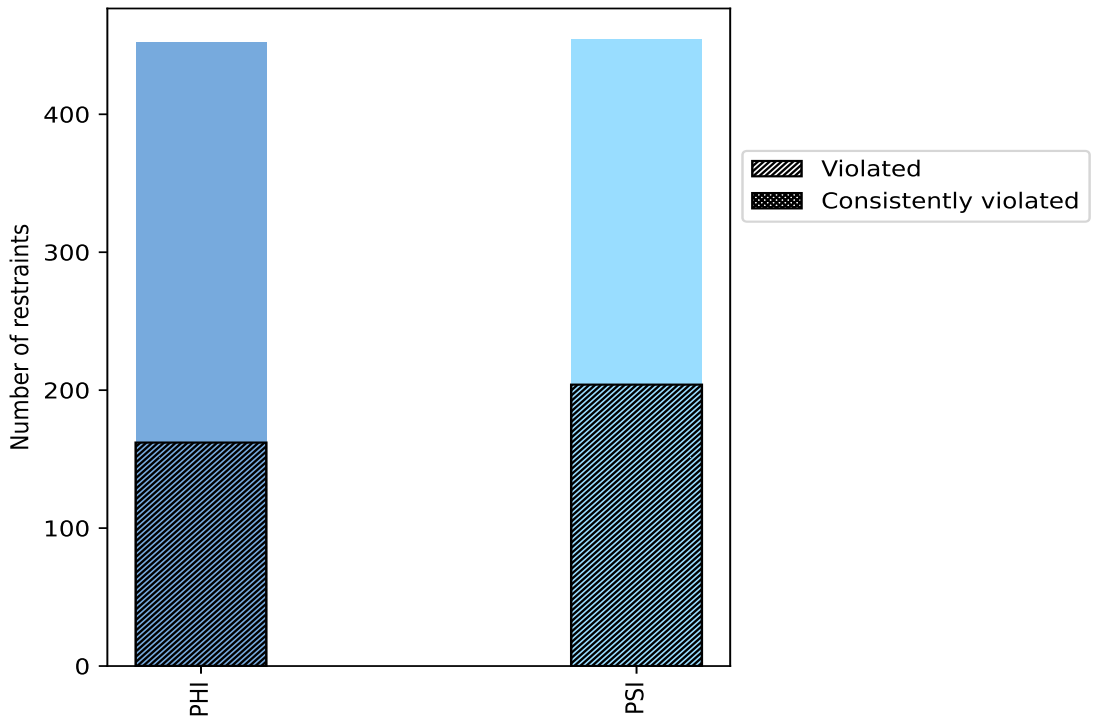
10.1 Summary of dihedral-angle violations

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	452	49.9	162	35.8	17.9	0	0.0	0.0
PSI	454	50.1	204	44.9	22.5	0	0.0	0.0
Total	906	100.0	366	40.4	40.4	0	0.0	0.0

[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



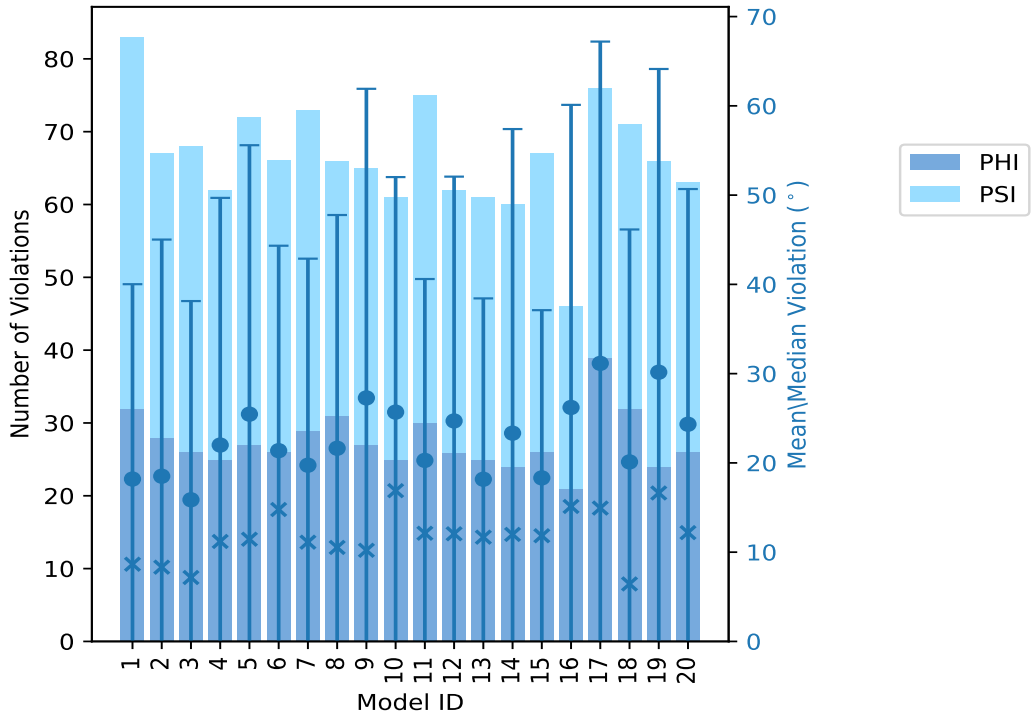
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	32	51	83	18.19	105.31	21.83	8.65
2	28	39	67	18.51	147.69	26.51	8.32
3	26	42	68	15.87	103.7	22.26	7.16
4	25	37	62	22.0	125.71	27.69	11.2
5	27	45	72	25.46	130.35	30.13	11.45
6	26	40	66	21.37	107.33	22.96	14.78
7	29	44	73	19.74	139.37	23.14	11.12
8	31	35	66	21.64	122.92	26.13	10.53
9	27	38	65	27.28	130.49	34.63	10.21
10	25	36	61	25.69	101.57	26.33	16.89
11	30	45	75	20.28	95.01	20.32	12.12
12	26	36	62	24.7	122.36	27.37	12.06
13	25	36	61	18.17	79.62	20.26	11.68
14	24	36	60	23.33	141.85	34.07	11.99
15	26	41	67	18.32	83.35	18.79	11.84
16	21	25	46	26.21	146.15	33.9	15.12
17	39	37	76	31.15	127.57	36.05	14.94
18	32	39	71	20.11	122.17	26.04	6.44
19	24	42	66	30.16	147.4	33.97	16.63
20	26	37	63	24.33	97.97	26.35	12.19

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]	%
63	73	136	1	5.0
29	31	60	2	10.0
19	15	34	3	15.0
11	18	29	4	20.0
6	16	22	5	25.0
6	13	19	6	30.0
6	11	17	7	35.0
5	6	11	8	40.0
7	4	11	9	45.0
4	4	8	10	50.0
1	6	7	11	55.0

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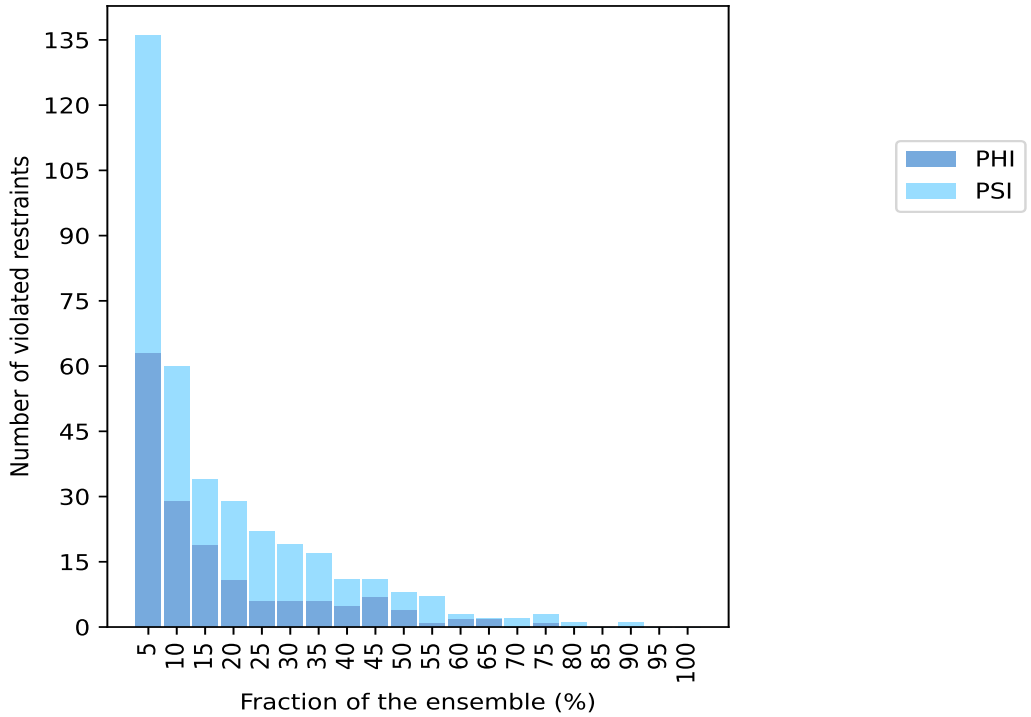
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
2	1	3	12	60.0
2	0	2	13	65.0
0	2	2	14	70.0
1	2	3	15	75.0
0	1	1	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

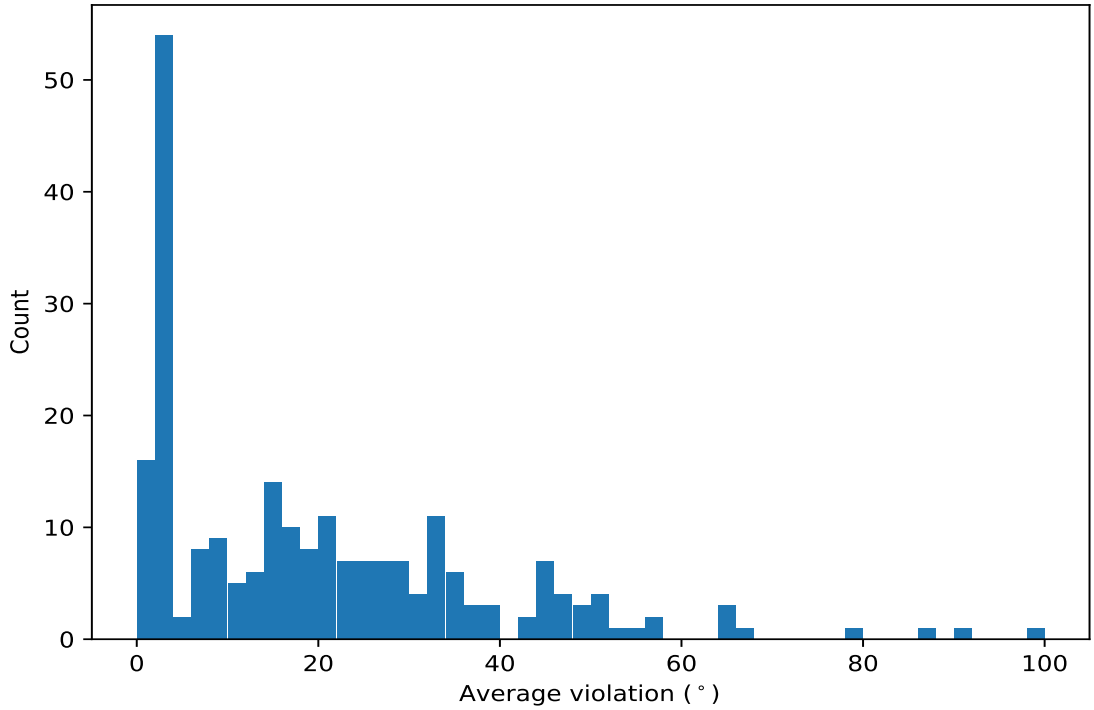


10.4 Most violated dihedral-angle restraints in the ensemble

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
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	18	39.84	45.02	16.63
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	16	37.61	13.84	34.11
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	15	50.86	20.04	47.87
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	15	50.51	44.14	28.05
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	15	38.5	20.26	32.99
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	14	48.06	38.33	30.87
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	14	33.46	16.43	30.33
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	13	25.07	10.83	23.83
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	13	14.83	10.51	12.48
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	12	34.97	23.93	31.98
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	12	31.78	35.76	22.8
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	12	23.68	12.49	21.45
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	11	55.08	32.31	70.61
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	11	51.58	29.18	42.82
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	11	31.45	44.56	13.05
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	11	27.29	21.68	27.27
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	11	21.72	11.73	19.72
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	11	16.41	21.5	10.49
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	11	2.86	1.43	2.63
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	10	45.09	20.52	45.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	10	33.38	32.43	19.0
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	10	29.18	24.5	26.79
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	10	26.02	12.86	25.91
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	10	24.45	25.3	14.64
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	10	15.67	6.67	14.64
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	10	7.16	5.77	5.57
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	10	3.44	1.73	3.01
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	9	99.28	33.68	119.81
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	9	38.72	28.26	52.99
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	9	37.9	16.8	38.91
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	9	33.67	22.52	35.63
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	9	25.01	20.42	12.78
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	9	22.36	19.68	17.1
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	9	21.01	12.31	21.72
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	9	20.11	7.72	20.01
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	9	15.33	6.12	13.31
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	9	3.64	0.99	3.67
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	9	2.41	0.74	2.7
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	8	45.32	35.83	38.76
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	8	33.35	40.59	10.38
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	8	30.91	32.96	22.1
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	8	27.08	25.77	15.1
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	8	25.32	7.64	24.74
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	8	21.5	26.67	10.81
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	8	10.61	6.18	11.54
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	8	6.83	4.22	5.91
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	8	4.07	2.29	4.23
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	8	3.95	1.37	3.94
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	8	2.98	2.09	2.44
(1,147)	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	1:5:B:LYS:N	7	65.87	50.55	101.56
(1,897)	1:331:B:ALA:C	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	7	52.94	38.16	47.26
(1,558)	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	1:97:B:GLU:N	7	51.74	25.68	45.48
(1,145)	1:3:B:ALA:N	1:3:B:ALA:CA	1:3:B:ALA:C	1:4:B:SER:N	7	49.09	16.11	52.06
(1,256)	1:58:B:SER:C	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	7	46.79	49.99	15.0
(1,557)	1:95:B:ASP:C	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	7	44.32	31.14	48.36
(1,255)	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	1:59:B:GLU:N	7	43.23	32.41	35.43
(1,811)	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1:225:B:LEU:N	7	36.54	38.29	17.51
(1,896)	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1:328:B:PHE:N	7	29.66	26.39	12.0
(1,892)	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	1:320:B:LEU:N	7	27.97	31.37	19.37
(1,874)	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	1:295:B:ILE:N	7	27.14	27.69	12.43
(1,187)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ILE:N	7	24.7	11.56	27.88
(1,562)	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	1:99:B:LYS:N	7	14.88	15.56	7.37
(1,771)	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	1:205:B:THR:N	7	11.96	6.48	10.04
(1,823)	1:271:A:GLN:C	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	7	3.8	1.76	3.81
(1,287)	1:94:A:ASP:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	7	2.55	1.16	2.6
(1,121)	1:61:A:LYS:C	1:62:A:GLY:N	1:62:A:GLY:CA	1:62:A:GLY:C	7	2.47	1.03	2.17
(1,148)	1:4:B:SER:C	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	6	66.58	24.97	70.85
(1,146)	1:3:B:ALA:C	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	6	34.03	12.16	38.29
(1,866)	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	1:238:B:VAL:N	6	32.64	42.73	14.27
(1,568)	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	1:102:B:ALA:N	6	32.04	36.75	13.91
(1,600)	1:117:B:ASP:N	1:117:B:ASP:CA	1:117:B:ASP:C	1:118:B:TYR:N	6	28.0	11.18	29.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,765)	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	1:202:B:ASP:N	6	27.72	18.25	22.04
(1,884)	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	1:314:B:LEU:N	6	20.43	16.78	17.73
(1,901)	1:333:B:ALA:C	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	6	15.01	10.53	13.04
(1,253)	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	1:58:B:SER:N	6	12.52	2.21	12.0
(1,576)	1:105:B:LEU:N	1:105:B:LEU:CA	1:105:B:LEU:C	1:106:B:LYS:N	6	12.0	10.04	7.84
(1,734)	1:185:B:LYS:N	1:185:B:LYS:CA	1:185:B:LYS:C	1:186:B:PRO:N	6	9.44	5.94	8.6
(1,237)	1:49:B:GLU:N	1:49:B:GLU:CA	1:49:B:GLU:C	1:50:B:ALA:N	6	9.42	5.49	8.9
(1,882)	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	1:313:B:ASP:N	6	8.78	5.14	8.46
(1,632)	1:133:B:PRO:C	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	6	8.2	4.67	7.04
(1,138)	1:70:A:ASN:N	1:70:A:ASN:CA	1:70:A:ASN:C	1:71:A:SER:N	6	3.84	1.6	4.05
(1,550)	1:227:A:LYS:C	1:228:A:THR:N	1:228:A:THR:CA	1:228:A:THR:C	6	3.38	1.74	2.96
(1,285)	1:93:A:GLU:C	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	6	3.36	1.32	2.61
(1,140)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:ALA:N	6	3.28	1.79	2.84
(1,365)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	6	2.54	0.85	2.12
(1,265)	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	1:64:B:HIS:N	5	34.2	45.47	13.44
(1,889)	1:316:B:ASN:C	1:317:B:ASN:N	1:317:B:ASN:CA	1:317:B:ASN:C	5	33.17	10.09	31.4
(1,876)	1:295:B:ILE:N	1:295:B:ILE:CA	1:295:B:ILE:C	1:296:B:ARG:N	5	28.74	32.96	3.18
(1,894)	1:320:B:LEU:N	1:320:B:LEU:CA	1:320:B:LEU:C	1:321:B:ARG:N	5	27.54	35.15	14.97
(1,601)	1:117:B:ASP:C	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	5	23.36	9.79	27.35
(1,551)	1:92:B:PRO:C	1:93:B:GLU:N	1:93:B:GLU:CA	1:93:B:GLU:C	5	23.03	16.52	23.14
(1,899)	1:332:B:GLY:C	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	5	19.96	9.93	14.5
(1,763)	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	1:201:B:GLY:N	5	18.96	12.95	12.91
(1,887)	1:314:B:LEU:C	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	5	18.19	9.86	11.68
(1,735)	1:186:B:PRO:N	1:186:B:PRO:CA	1:186:B:PRO:C	1:187:B:GLU:N	5	17.72	12.01	19.4
(1,870)	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	1:274:B:GLN:N	5	17.7	9.68	14.17
(1,277)	1:69:B:LEU:N	1:69:B:LEU:CA	1:69:B:LEU:C	1:70:B:ASN:N	5	16.64	16.71	11.52
(1,249)	1:55:B:LEU:N	1:55:B:LEU:CA	1:55:B:LEU:C	1:56:B:GLY:N	5	12.25	3.21	10.6
(1,257)	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	1:60:B:PHE:N	5	11.7	8.52	6.43
(1,665)	1:150:B:LYS:N	1:150:B:LYS:CA	1:150:B:LYS:C	1:151:B:GLU:N	5	6.76	5.33	5.2
(1,284)	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	1:94:A:ASP:N	5	3.03	1.03	3.09
(1,541)	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	1:224:A:ASN:N	5	3.03	1.24	2.89
(1,854)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:ALA:N	5	2.42	0.59	2.07
(1,862)	1:337:A:ASP:N	1:337:A:ASP:CA	1:337:A:ASP:C	1:338:A:GLU:N	5	2.41	2.11	1.51
(1,840)	1:313:A:ASP:N	1:313:A:ASP:CA	1:313:A:ASP:C	1:314:A:LEU:N	5	2.13	0.52	1.93
(1,124)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:HIS:N	5	2.05	1.17	1.42
(1,855)	1:332:A:GLY:C	1:333:A:ALA:N	1:333:A:ALA:CA	1:333:A:ALA:C	5	1.71	0.57	1.35
(1,873)	1:293:B:PRO:C	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	4	64.31	39.53	70.51
(1,269)	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	1:66:B:ALA:N	4	47.12	29.37	53.99
(1,251)	1:56:B:GLY:N	1:56:B:GLY:CA	1:56:B:GLY:C	1:57:B:LYS:N	4	45.34	21.16	52.98
(1,805)	1:221:B:GLN:N	1:221:B:GLN:CA	1:221:B:GLN:C	1:222:B:SER:N	4	35.31	38.12	16.3
(1,865)	1:236:B:ALA:C	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	4	32.88	10.75	27.98
(1,702)	1:169:B:TYR:N	1:169:B:TYR:CA	1:169:B:TYR:C	1:170:B:PHE:N	4	31.71	42.84	10.04
(1,769)	1:203:B:ASN:N	1:203:B:ASN:CA	1:203:B:ASN:C	1:204:B:ALA:N	4	29.02	26.99	24.32
(1,150)	1:5:B:LYS:C	1:6:B:GLU:N	1:6:B:GLU:CA	1:6:B:GLU:C	4	24.18	22.14	18.76
(1,764)	1:200:B:GLU:C	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	4	21.97	9.81	21.66
(1,871)	1:273:B:ALA:C	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	4	21.82	10.95	23.56
(1,895)	1:326:B:ASN:C	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	4	20.78	15.28	18.26
(1,149)	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	1:6:B:GLU:N	4	19.22	2.95	17.92
(1,560)	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	1:98:B:THR:N	4	18.56	11.91	17.48
(1,275)	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	1:69:B:LEU:N	4	17.9	12.41	17.18
(1,602)	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	1:119:B:GLU:N	4	16.99	3.95	17.52

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,762)	1:199:B:ILE:C	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	4	16.71	9.66	17.67
(1,635)	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	1:136:B:ALA:N	4	15.82	11.46	9.7
(1,809)	1:223:B:LEU:N	1:223:B:LEU:CA	1:223:B:LEU:C	1:224:B:ASN:N	4	11.32	7.17	10.0
(1,631)	1:133:B:PRO:N	1:133:B:PRO:CA	1:133:B:PRO:C	1:134:B:THR:N	4	9.56	7.56	5.44
(1,244)	1:52:B:SER:C	1:53:B:GLY:N	1:53:B:GLY:CA	1:53:B:GLY:C	4	6.3	5.62	4.78
(1,629)	1:131:B:VAL:C	1:132:B:LEU:N	1:132:B:LEU:CA	1:132:B:LEU:C	4	3.38	3.46	1.53
(1,288)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:ALA:N	4	3.0	0.61	3.17
(1,132)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:ILE:N	4	2.97	0.49	2.76
(1,286)	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	1:95:A:ASP:N	4	2.7	1.21	2.36
(1,835)	1:310:A:ASN:C	1:311:A:LEU:N	1:311:A:LEU:CA	1:311:A:LEU:C	4	2.44	1.24	2.18
(1,822)	1:237:A:ASP:N	1:237:A:ASP:CA	1:237:A:ASP:C	1:238:A:VAL:N	4	2.35	0.47	2.52
(1,844)	1:315:A:MET:N	1:315:A:MET:CA	1:315:A:MET:C	1:316:A:ASN:N	4	2.18	1.1	1.6
(1,850)	1:320:A:LEU:N	1:320:A:LEU:CA	1:320:A:LEU:C	1:321:A:ARG:N	4	2.0	0.41	2.12
(1,544)	1:224:A:ASN:C	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	4	1.77	0.4	1.83
(1,559)	1:96:B:ALA:C	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	3	57.62	24.7	58.58
(1,869)	1:272:B:ALA:C	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	3	57.45	36.17	71.01
(1,806)	1:221:B:GLN:C	1:222:B:SER:N	1:222:B:SER:CA	1:222:B:SER:C	3	48.17	38.07	26.37
(1,801)	1:219:B:VAL:N	1:219:B:VAL:CA	1:219:B:VAL:C	1:220:B:GLU:N	3	47.21	37.93	23.57
(1,567)	1:100:B:ALA:C	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	3	45.27	30.27	49.76
(1,571)	1:102:B:ALA:C	1:103:B:GLU:N	1:103:B:GLU:CA	1:103:B:GLU:C	3	44.52	28.59	46.04
(1,731)	1:183:B:GLN:C	1:184:B:GLY:N	1:184:B:GLY:CA	1:184:B:GLY:C	3	33.5	22.14	38.51
(1,252)	1:56:B:GLY:C	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	3	33.02	22.59	46.03
(1,803)	1:220:B:GLU:N	1:220:B:GLU:CA	1:220:B:GLU:C	1:221:B:GLN:N	3	29.26	12.11	29.64
(1,797)	1:217:B:LYS:N	1:217:B:LYS:CA	1:217:B:LYS:C	1:218:B:LYS:N	3	28.96	14.03	19.41
(1,883)	1:312:B:SER:C	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	3	24.06	25.8	10.65
(1,603)	1:118:B:TYR:C	1:119:B:GLU:N	1:119:B:GLU:CA	1:119:B:GLU:C	3	23.29	10.48	30.07
(1,798)	1:217:B:LYS:C	1:218:B:LYS:N	1:218:B:LYS:CA	1:218:B:LYS:C	3	20.36	18.6	14.19
(1,881)	1:311:B:LEU:C	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	3	19.96	7.46	23.84
(1,767)	1:202:B:ASP:N	1:202:B:ASP:CA	1:202:B:ASP:C	1:203:B:ASN:N	3	17.93	9.03	23.74
(1,761)	1:199:B:ILE:N	1:199:B:ILE:CA	1:199:B:ILE:C	1:200:B:GLU:N	3	17.3	14.45	10.59
(1,636)	1:135:B:ASN:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	3	15.69	14.36	10.47
(1,732)	1:184:B:GLY:N	1:184:B:GLY:CA	1:184:B:GLY:C	1:185:B:LYS:N	3	15.45	11.79	13.61
(1,268)	1:64:B:HIS:C	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	3	13.37	12.11	5.5
(1,800)	1:218:B:LYS:C	1:219:B:VAL:N	1:219:B:VAL:CA	1:219:B:VAL:C	3	9.19	5.69	11.26
(1,785)	1:211:B:ASP:N	1:211:B:ASP:CA	1:211:B:ASP:C	1:212:B:TYR:N	3	9.13	5.05	7.62
(1,872)	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	1:275:B:LYS:N	3	6.07	3.56	4.6
(1,807)	1:222:B:SER:N	1:222:B:SER:CA	1:222:B:SER:C	1:223:B:LEU:N	3	6.05	2.69	5.77
(1,300)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:ALA:N	3	3.68	1.79	3.37
(1,546)	1:225:A:LEU:C	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	3	3.12	0.23	3.24
(1,845)	1:316:A:ASN:C	1:317:A:ASN:N	1:317:A:ASN:CA	1:317:A:ASN:C	3	2.76	0.95	3.11
(1,141)	1:71:A:SER:C	1:72:A:ALA:N	1:72:A:ALA:CA	1:72:A:ALA:C	3	2.62	0.72	2.19
(1,290)	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	1:97:A:GLU:N	3	2.42	0.98	2.25
(1,842)	1:314:A:LEU:N	1:314:A:LEU:CA	1:314:A:LEU:C	1:315:A:MET:N	3	2.3	1.19	1.65
(1,540)	1:222:A:SER:C	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	3	2.28	0.48	2.44
(1,46)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ILE:N	3	2.07	1.22	1.38
(1,832)	1:295:A:ILE:N	1:295:A:ILE:CA	1:295:A:ILE:C	1:296:A:ARG:N	3	1.93	0.55	1.62
(1,503)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:THR:N	3	1.91	0.72	1.75
(1,47)	1:24:A:GLU:C	1:25:A:ILE:N	1:25:A:ILE:CA	1:25:A:ILE:C	3	1.78	0.4	1.94
(1,192)	1:26:B:SER:C	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	2	90.8	4.22	90.8
(1,569)	1:101:B:LYS:C	1:102:B:ALA:N	1:102:B:ALA:CA	1:102:B:ALA:C	2	86.28	0.96	86.28
(1,228)	1:44:B:PHE:C	1:45:B:GLY:N	1:45:B:GLY:CA	1:45:B:GLY:C	2	78.56	67.59	78.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,227)	1:44:B:PHE:N	1:44:B:PHE:CA	1:44:B:PHE:C	1:45:B:GLY:N	2	65.31	60.63	65.31
(1,802)	1:219:B:VAL:C	1:220:B:GLU:N	1:220:B:GLU:CA	1:220:B:GLU:C	2	46.84	36.84	46.84
(1,572)	1:103:B:GLU:N	1:103:B:GLU:CA	1:103:B:GLU:C	1:104:B:ASP:N	2	44.88	13.38	44.88
(1,570)	1:102:B:ALA:N	1:102:B:ALA:CA	1:102:B:ALA:C	1:103:B:GLU:N	2	43.88	30.36	43.88
(1,738)	1:187:B:GLU:C	1:188:B:GLU:N	1:188:B:GLU:CA	1:188:B:GLU:C	2	34.24	2.46	34.24
(1,264)	1:62:B:GLY:C	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	2	34.11	25.7	34.11
(1,766)	1:201:B:GLY:C	1:202:B:ASP:N	1:202:B:ASP:CA	1:202:B:ASP:C	2	32.08	24.92	32.08
(1,239)	1:50:B:ALA:N	1:50:B:ALA:CA	1:50:B:ALA:C	1:51:B:VAL:N	2	23.91	15.5	23.91
(1,792)	1:214:B:SER:C	1:215:B:ALA:N	1:215:B:ALA:CA	1:215:B:ALA:C	2	22.14	19.18	22.14
(1,191)	1:26:B:SER:N	1:26:B:SER:CA	1:26:B:SER:C	1:27:B:GLU:N	2	21.56	9.44	21.56
(1,193)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:ASP:N	2	20.18	1.75	20.18
(1,902)	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	1:335:B:SER:N	2	19.15	7.17	19.15
(1,891)	1:318:B:PRO:C	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	2	18.4	16.08	18.4
(1,240)	1:50:B:ALA:C	1:51:B:VAL:N	1:51:B:VAL:CA	1:51:B:VAL:C	2	16.9	3.31	16.9
(1,565)	1:99:B:LYS:C	1:100:B:ALA:N	1:100:B:ALA:CA	1:100:B:ALA:C	2	15.9	0.34	15.9
(1,810)	1:223:B:LEU:C	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	2	15.85	4.99	15.85
(1,905)	1:336:B:THR:C	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	2	15.31	0.72	15.31
(1,804)	1:220:B:GLU:C	1:221:B:GLN:N	1:221:B:GLN:CA	1:221:B:GLN:C	2	15.08	1.77	15.08
(1,230)	1:45:B:GLY:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	2	14.92	6.45	14.92
(1,760)	1:198:B:ASP:C	1:199:B:ILE:N	1:199:B:ILE:CA	1:199:B:ILE:C	2	14.09	6.8	14.09
(1,739)	1:188:B:GLU:N	1:188:B:GLU:CA	1:188:B:GLU:C	1:189:B:ALA:N	2	12.98	2.39	12.98
(1,245)	1:53:B:GLY:N	1:53:B:GLY:CA	1:53:B:GLY:C	1:54:B:ILE:N	2	12.86	8.04	12.86
(1,642)	1:138:B:TYR:C	1:139:B:TYR:N	1:139:B:TYR:CA	1:139:B:TYR:C	2	11.91	1.76	11.91
(1,757)	1:197:B:LEU:N	1:197:B:LEU:CA	1:197:B:LEU:C	1:198:B:ASP:N	2	8.85	4.0	8.85
(1,278)	1:69:B:LEU:C	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	2	8.22	6.78	8.22
(1,243)	1:52:B:SER:N	1:52:B:SER:CA	1:52:B:SER:C	1:53:B:GLY:N	2	7.43	0.98	7.43
(1,669)	1:152:B:TYR:N	1:152:B:TYR:CA	1:152:B:TYR:C	1:153:B:ASP:N	2	6.24	4.66	6.24
(1,824)	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	1:273:A:ALA:N	2	4.26	3.12	4.26
(1,532)	1:218:A:LYS:C	1:219:A:VAL:N	1:219:A:VAL:CA	1:219:A:VAL:C	2	3.94	1.57	3.94
(1,238)	1:49:B:GLU:C	1:50:B:ALA:N	1:50:B:ALA:CA	1:50:B:ALA:C	2	3.82	0.5	3.82
(1,428)	1:165:A:ILE:C	1:166:A:ASP:N	1:166:A:ASP:CA	1:166:A:ASP:C	2	3.59	1.02	3.59
(1,367)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ALA:N	2	3.56	0.01	3.56
(1,517)	1:211:A:ASP:N	1:211:A:ASP:CA	1:211:A:ASP:C	1:212:A:TYR:N	2	3.1	0.88	3.1
(1,828)	1:274:A:GLN:N	1:274:A:GLN:CA	1:274:A:GLN:C	1:275:A:LYS:N	2	3.02	0.02	3.02
(1,294)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:LYS:N	2	2.88	0.31	2.88
(1,851)	1:326:A:ASN:C	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	2	2.82	0.88	2.82
(1,820)	1:236:A:ALA:N	1:236:A:ALA:CA	1:236:A:ALA:C	1:237:A:ASP:N	2	2.77	0.53	2.77
(1,291)	1:96:A:ALA:C	1:97:A:GLU:N	1:97:A:GLU:CA	1:97:A:GLU:C	2	2.7	1.01	2.7
(1,364)	1:133:A:PRO:C	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	2	2.49	1.26	2.49
(1,263)	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	1:63:B:GLN:N	2	2.42	0.9	2.42
(1,494)	1:199:A:ILE:C	1:200:A:GLU:N	1:200:A:GLU:CA	1:200:A:GLU:C	2	2.38	0.22	2.38
(1,841)	1:313:A:ASP:C	1:314:A:LEU:N	1:314:A:LEU:CA	1:314:A:LEU:C	2	2.37	0.64	2.37
(1,497)	1:201:A:GLY:N	1:201:A:GLY:CA	1:201:A:GLY:C	1:202:A:ASP:N	2	2.2	1.15	2.2
(1,501)	1:203:A:ASN:N	1:203:A:ASN:CA	1:203:A:ASN:C	1:204:A:ALA:N	2	2.16	1.12	2.16
(1,538)	1:221:A:GLN:C	1:222:A:SER:N	1:222:A:SER:CA	1:222:A:SER:C	2	2.14	1.02	2.14
(1,283)	1:92:A:PRO:C	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	2	2.04	0.08	2.04
(1,848)	1:319:A:ALA:N	1:319:A:ALA:CA	1:319:A:ALA:C	1:320:A:LEU:N	2	1.94	0.57	1.94
(1,397)	1:150:A:LYS:N	1:150:A:LYS:CA	1:150:A:LYS:C	1:151:A:GLU:N	2	1.91	0.06	1.91
(1,533)	1:219:A:VAL:N	1:219:A:VAL:CA	1:219:A:VAL:C	1:220:A:GLU:N	2	1.86	0.48	1.86
(1,830)	1:294:A:SER:N	1:294:A:SER:CA	1:294:A:SER:C	1:295:A:ILE:N	2	1.85	0.27	1.85
(1,118)	1:60:A:PHE:N	1:60:A:PHE:CA	1:60:A:PHE:C	1:61:A:LYS:N	2	1.73	0.07	1.73

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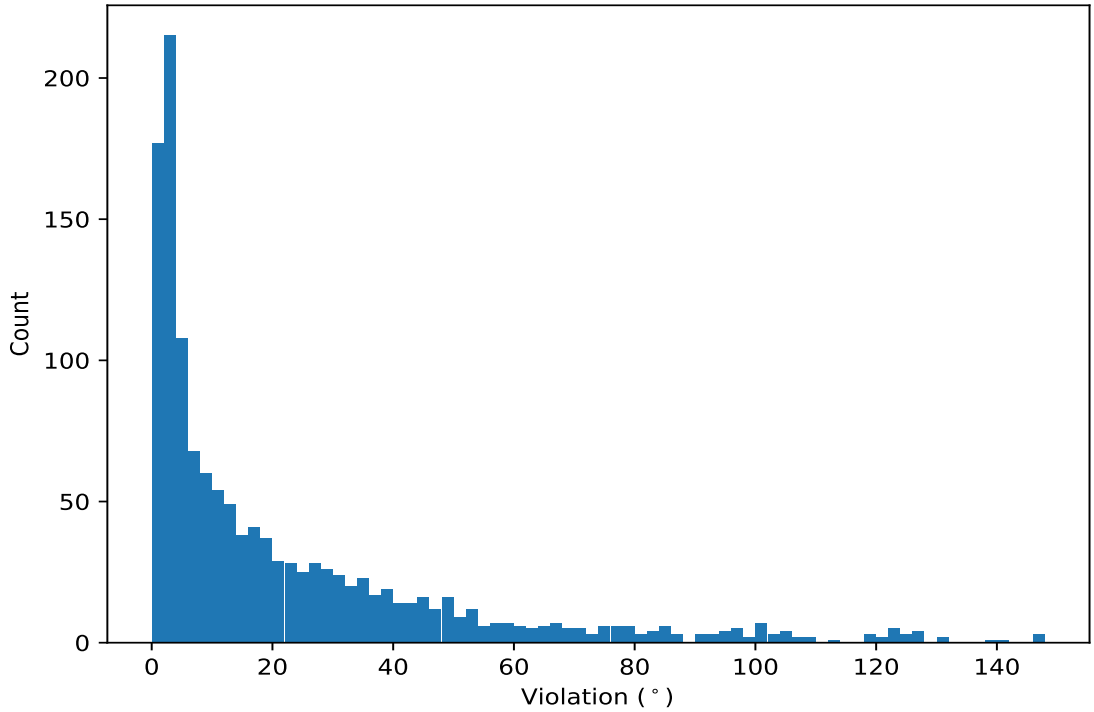
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,537)	1:221:A:GLN:N	1:221:A:GLN:CA	1:221:A:GLN:C	1:222:A:SER:N	2	1.6	0.0	1.6
(1,829)	1:293:A:PRO:C	1:294:A:SER:N	1:294:A:SER:CA	1:294:A:SER:C	2	1.44	0.37	1.44
(1,826)	1:273:A:ALA:N	1:273:A:ALA:CA	1:273:A:ALA:C	1:274:A:GLN:N	2	1.43	0.42	1.43
(1,96)	1:49:A:GLU:N	1:49:A:GLU:CA	1:49:A:GLU:C	1:50:A:ALA:N	2	1.36	0.07	1.36
(1,697)	1:166:B:ASP:N	1:166:B:ASP:CA	1:166:B:ASP:C	1:167:B:PRO:N	2	1.34	0.26	1.34
(1,467)	1:186:A:PRO:N	1:186:A:PRO:CA	1:186:A:PRO:C	1:187:A:GLU:N	2	1.27	0.24	1.27

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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 (°)
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	2	147.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	19	147.4
(1,228)	1:44:B:PHE:C	1:45:B:GLY:N	1:45:B:GLY:CA	1:45:B:GLY:C	16	146.15
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	14	141.85
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	7	139.37
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	9	130.49
(1,256)	1:58:B:SER:C	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	5	130.35
(1,866)	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	1:238:B:VAL:N	17	127.57
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	9	126.61
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	19	126.49
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	2	126.46
(1,227)	1:44:B:PHE:N	1:44:B:PHE:CA	1:44:B:PHE:C	1:45:B:GLY:N	16	125.94
(1,897)	1:331:B:ALA:C	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	4	125.71
(1,265)	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	1:64:B:HIS:N	14	124.57
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	17	123.45
(1,147)	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	1:5:B:LYS:N	8	122.92
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	12	122.36
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	5	122.24
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	18	122.17
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	16	121.34
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	19	120.42
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	14	119.81
(1,256)	1:58:B:SER:C	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	17	119.17
(1,255)	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	1:59:B:GLU:N	5	118.31
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	9	112.08
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	18	109.86
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	17	109.32
(1,147)	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	1:5:B:LYS:N	6	107.33
(1,811)	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1:225:B:LEU:N	17	107.06
(1,702)	1:169:B:TYR:N	1:169:B:TYR:CA	1:169:B:TYR:C	1:170:B:PHE:N	19	105.56
(1,147)	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	1:5:B:LYS:N	1	105.31
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	4	105.22
(1,568)	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	1:102:B:ALA:N	12	104.72
(1,873)	1:293:B:PRO:C	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	16	103.75
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	3	103.7
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	17	102.48
(1,266)	1:63:B:GLN:C	1:64:B:HIS:N	1:64:B:HIS:CA	1:64:B:HIS:C	14	101.98
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	17	101.8
(1,806)	1:221:B:GLN:C	1:222:B:SER:N	1:222:B:SER:CA	1:222:B:SER:C	9	101.7
(1,873)	1:293:B:PRO:C	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	10	101.57
(1,147)	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	1:5:B:LYS:N	17	101.56
(1,805)	1:221:B:GLN:N	1:221:B:GLN:CA	1:221:B:GLN:C	1:222:B:SER:N	9	101.02
(1,801)	1:219:B:VAL:N	1:219:B:VAL:CA	1:219:B:VAL:C	1:220:B:GLU:N	3	100.74
(1,892)	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	1:320:B:LEU:N	10	99.76
(1,558)	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	1:97:B:GLU:N	9	99.37
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	20	97.97
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	4	97.9
(1,894)	1:320:B:LEU:N	1:320:B:LEU:CA	1:320:B:LEU:C	1:321:B:ARG:N	14	97.07
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	6	96.98
(1,148)	1:4:B:SER:C	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	17	96.24
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	8	95.54
(1,664)	1:149:B:LEU:C	1:150:B:LYS:N	1:150:B:LYS:CA	1:150:B:LYS:C	10	95.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,192)	1:26:B:SER:C	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	11	95.01
(1,270)	1:65:B:LEU:C	1:66:B:ALA:N	1:66:B:ALA:CA	1:66:B:ALA:C	17	94.26
(1,703)	1:169:B:TYR:C	1:170:B:PHE:N	1:170:B:PHE:CA	1:170:B:PHE:C	19	93.55
(1,869)	1:272:B:ALA:C	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	17	93.38
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	10	92.96
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	14	91.47
(1,148)	1:4:B:SER:C	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	8	90.71
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	18	90.29
(1,559)	1:96:B:ALA:C	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	9	87.39
(1,569)	1:101:B:LYS:C	1:102:B:ALA:N	1:102:B:ALA:CA	1:102:B:ALA:C	19	87.24
(1,192)	1:26:B:SER:C	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	20	86.58
(1,557)	1:95:B:ASP:C	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	20	85.92
(1,569)	1:101:B:LYS:C	1:102:B:ALA:N	1:102:B:ALA:CA	1:102:B:ALA:C	12	85.32
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	9	84.91
(1,557)	1:95:B:ASP:C	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	14	84.85
(1,897)	1:331:B:ALA:C	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1	84.6
(1,874)	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	1:295:B:ILE:N	3	84.5
(1,802)	1:219:B:VAL:C	1:220:B:GLU:N	1:220:B:GLU:CA	1:220:B:GLU:C	3	83.69
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	15	83.35
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	5	82.34
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	12	82.28
(1,876)	1:295:B:ILE:N	1:295:B:ILE:CA	1:295:B:ILE:C	1:296:B:ARG:N	4	81.59
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	5	80.9
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	17	80.31
(1,567)	1:100:B:ALA:C	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	5	79.89
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	13	79.62
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	7	79.35
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	20	78.88
(1,571)	1:102:B:ALA:C	1:103:B:GLU:N	1:103:B:GLU:CA	1:103:B:GLU:C	4	78.75
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	11	78.19
(1,269)	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	1:66:B:ALA:N	10	77.56
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	13	77.49
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	10	77.31
(1,558)	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	1:97:B:GLU:N	20	76.72
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	11	76.54
(1,774)	1:205:B:THR:C	1:206:B:GLU:N	1:206:B:GLU:CA	1:206:B:GLU:C	8	76.26
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	18	75.7
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	18	75.37
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	12	75.11
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	5	74.5
(1,570)	1:102:B:ALA:N	1:102:B:ALA:CA	1:102:B:ALA:C	1:103:B:GLU:N	4	74.25
(1,148)	1:4:B:SER:C	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	1	74.1
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	12	73.42
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	9	72.43
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	20	72.08
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	13	71.79
(1,869)	1:272:B:ALA:C	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	1	71.01
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	18	70.99
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	6	70.72
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	2	70.61
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	12	69.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	5	69.84
(1,269)	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	1:66:B:ALA:N	19	69.45
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	8	68.8
(1,811)	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1:225:B:LEU:N	20	68.43
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	17	67.69
(1,148)	1:4:B:SER:C	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	6	67.61
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	15	67.23
(1,145)	1:3:B:ALA:N	1:3:B:ALA:CA	1:3:B:ALA:C	1:4:B:SER:N	6	66.86
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	9	66.5
(1,896)	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1:328:B:PHE:N	20	66.44
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	19	66.24
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	13	65.61
(1,765)	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	1:202:B:ASP:N	7	65.59
(1,770)	1:203:B:ASN:C	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	4	65.48
(1,564)	1:99:B:LYS:N	1:99:B:LYS:CA	1:99:B:LYS:C	1:100:B:ALA:N	9	65.41
(1,769)	1:203:B:ASN:N	1:203:B:ASN:CA	1:203:B:ASN:C	1:204:B:ALA:N	4	65.18
(1,251)	1:56:B:GLY:N	1:56:B:GLY:CA	1:56:B:GLY:C	1:57:B:LYS:N	17	64.31
(1,145)	1:3:B:ALA:N	1:3:B:ALA:CA	1:3:B:ALA:C	1:4:B:SER:N	15	63.3
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	1	62.96
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	19	62.8
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	14	62.67
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	17	62.08
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	2	61.94
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	19	61.86
(1,251)	1:56:B:GLY:N	1:56:B:GLY:CA	1:56:B:GLY:C	1:57:B:LYS:N	1	61.46
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	20	61.21
(1,896)	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1:328:B:PHE:N	8	60.99
(1,883)	1:312:B:SER:C	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	16	60.15
(1,264)	1:62:B:GLY:C	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	7	59.81
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	19	59.7
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	13	59.05
(1,559)	1:96:B:ALA:C	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	19	58.58
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1	58.48
(1,572)	1:103:B:GLU:N	1:103:B:GLU:CA	1:103:B:GLU:C	1:104:B:ASP:N	11	58.26
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	11	58.04
(1,731)	1:183:B:GLN:C	1:184:B:GLY:N	1:184:B:GLY:CA	1:184:B:GLY:C	15	57.76
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	20	57.55
(1,150)	1:5:B:LYS:C	1:6:B:GLU:N	1:6:B:GLU:CA	1:6:B:GLU:C	17	57.43
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	5	57.1
(1,766)	1:201:B:GLY:C	1:202:B:ASP:N	1:202:B:ASP:CA	1:202:B:ASP:C	10	56.99
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	9	56.44
(1,811)	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1:225:B:LEU:N	9	56.04
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	15	55.87
(1,897)	1:331:B:ALA:C	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	8	55.62
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	8	55.43
(1,557)	1:95:B:ASP:C	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	19	55.36
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	7	54.76
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	19	54.75
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	11	53.87
(1,558)	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	1:97:B:GLU:N	19	53.69
(1,876)	1:295:B:ILE:N	1:295:B:ILE:CA	1:295:B:ILE:C	1:296:B:ARG:N	2	53.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,145)	1:3:B:ALA:N	1:3:B:ALA:CA	1:3:B:ALA:C	1:4:B:SER:N	12	53.62
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	9	53.61
(1,561)	1:97:B:GLU:C	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	19	53.55
(1,568)	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	1:102:B:ALA:N	5	53.45
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	7	53.4
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	11	53.07
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	6	52.99
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	8	52.64
(1,145)	1:3:B:ALA:N	1:3:B:ALA:CA	1:3:B:ALA:C	1:4:B:SER:N	18	52.06
(1,252)	1:56:B:GLY:C	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	1	51.79
(1,896)	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1:328:B:PHE:N	3	51.36
(1,889)	1:316:B:ASN:C	1:317:B:ASN:N	1:317:B:ASN:CA	1:317:B:ASN:C	8	51.32
(1,865)	1:236:B:ALA:C	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	17	51.14
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	2	51.06
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	13	50.67
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	14	50.56
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	2	50.16
(1,145)	1:3:B:ALA:N	1:3:B:ALA:CA	1:3:B:ALA:C	1:4:B:SER:N	16	50.05
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	8	49.98
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	20	49.96
(1,567)	1:100:B:ALA:C	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	19	49.76
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	15	49.67
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	7	49.55
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	7	49.49
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	12	49.45
(1,277)	1:69:B:LEU:N	1:69:B:LEU:CA	1:69:B:LEU:C	1:70:B:ASN:N	17	49.42
(1,146)	1:3:B:ALA:C	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	18	49.4
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	17	49.15
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	17	49.05
(1,797)	1:217:B:LYS:N	1:217:B:LYS:CA	1:217:B:LYS:C	1:218:B:LYS:N	12	48.79
(1,235)	1:48:B:ARG:N	1:48:B:ARG:CA	1:48:B:ARG:C	1:49:B:GLU:N	1	48.44
(1,557)	1:95:B:ASP:C	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	2	48.36
(1,874)	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	1:295:B:ILE:N	10	48.21
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	9	48.16
(1,267)	1:64:B:HIS:N	1:64:B:HIS:CA	1:64:B:HIS:C	1:65:B:LEU:N	19	47.95
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	10	47.87
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	18	47.85
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	19	47.85
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	5	47.59
(1,148)	1:4:B:SER:C	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	10	47.28
(1,897)	1:331:B:ALA:C	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	6	47.26
(1,893)	1:319:B:ALA:C	1:320:B:LEU:N	1:320:B:LEU:CA	1:320:B:LEU:C	10	47.02
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	2	46.44
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	11	46.26
(1,571)	1:102:B:ALA:C	1:103:B:GLU:N	1:103:B:GLU:CA	1:103:B:GLU:C	6	46.04
(1,252)	1:56:B:GLY:C	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	5	46.03
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	5	45.66
(1,798)	1:217:B:LYS:C	1:218:B:LYS:N	1:218:B:LYS:CA	1:218:B:LYS:C	11	45.6
(1,558)	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	1:97:B:GLU:N	12	45.48
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	6	45.33
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	7	45.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,255)	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	1:59:B:GLU:N	7	45.09
(1,562)	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	1:99:B:LYS:N	19	45.08
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	10	44.96
(1,884)	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	1:314:B:LEU:N	1	44.94
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	11	44.94
(1,769)	1:203:B:ASN:N	1:203:B:ASN:CA	1:203:B:ASN:C	1:204:B:ALA:N	16	44.89
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	16	44.78
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	15	44.71
(1,251)	1:56:B:GLY:N	1:56:B:GLY:CA	1:56:B:GLY:C	1:57:B:LYS:N	5	44.49
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	5	44.48
(1,600)	1:117:B:ASP:N	1:117:B:ASP:CA	1:117:B:ASP:C	1:118:B:TYR:N	15	44.02
(1,803)	1:220:B:GLU:N	1:220:B:GLU:CA	1:220:B:GLU:C	1:221:B:GLN:N	12	43.9
(1,145)	1:3:B:ALA:N	1:3:B:ALA:CA	1:3:B:ALA:C	1:4:B:SER:N	13	43.86
(1,187)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ILE:N	20	43.85
(1,895)	1:326:B:ASN:C	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	20	43.67
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	19	43.6
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	5	43.33
(1,663)	1:149:B:LEU:N	1:149:B:LEU:CA	1:149:B:LEU:C	1:150:B:LYS:N	10	42.99
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	1	42.82
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	18	42.36
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	15	42.21
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	10	42.2
(1,276)	1:68:B:ILE:C	1:69:B:LEU:N	1:69:B:LEU:CA	1:69:B:LEU:C	11	42.08
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	8	42.06
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	1	42.02
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	8	41.94
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	12	41.91
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	20	41.81
(1,551)	1:92:B:PRO:C	1:93:B:GLU:N	1:93:B:GLU:CA	1:93:B:GLU:C	9	41.73
(1,146)	1:3:B:ALA:C	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	16	41.65
(1,573)	1:103:B:GLU:C	1:104:B:ASP:N	1:104:B:ASP:CA	1:104:B:ASP:C	11	41.59
(1,792)	1:214:B:SER:C	1:215:B:ALA:N	1:215:B:ALA:CA	1:215:B:ALA:C	5	41.32
(1,551)	1:92:B:PRO:C	1:93:B:GLU:N	1:93:B:GLU:CA	1:93:B:GLU:C	20	41.05
(1,146)	1:3:B:ALA:C	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	12	40.6
(1,875)	1:294:B:SER:C	1:295:B:ILE:N	1:295:B:ILE:CA	1:295:B:ILE:C	3	40.44
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	6	40.38
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	7	40.28
(1,763)	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	1:201:B:GLY:N	7	40.26
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	15	40.23
(1,808)	1:222:B:SER:C	1:223:B:LEU:N	1:223:B:LEU:CA	1:223:B:LEU:C	5	39.7
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	7	39.47
(1,873)	1:293:B:PRO:C	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	5	39.45
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	12	39.45
(1,239)	1:50:B:ALA:N	1:50:B:ALA:CA	1:50:B:ALA:C	1:51:B:VAL:N	1	39.41
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	19	39.13
(1,778)	1:207:B:ALA:C	1:208:B:MET:N	1:208:B:MET:CA	1:208:B:MET:C	11	38.97
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	18	38.92
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	14	38.91
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	13	38.83
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	8	38.78
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	12	38.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	1	38.56
(1,269)	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	1:66:B:ALA:N	17	38.53
(1,731)	1:183:B:GLN:C	1:184:B:GLY:N	1:184:B:GLY:CA	1:184:B:GLY:C	13	38.51
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	10	38.49
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	6	38.22
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	10	38.05
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	6	38.03
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	8	37.96
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	20	37.71
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	2	37.69
(1,236)	1:48:B:ARG:C	1:49:B:GLU:N	1:49:B:GLU:CA	1:49:B:GLU:C	1	37.62
(1,255)	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	1:59:B:GLU:N	6	37.48
(1,761)	1:199:B:ILE:N	1:199:B:ILE:CA	1:199:B:ILE:C	1:200:B:GLU:N	10	37.38
(1,735)	1:186:B:PRO:N	1:186:B:PRO:CA	1:186:B:PRO:C	1:187:B:GLU:N	11	37.31
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	16	37.29
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	1	37.24
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	20	36.82
(1,600)	1:117:B:ASP:N	1:117:B:ASP:CA	1:117:B:ASP:C	1:118:B:TYR:N	10	36.78
(1,738)	1:187:B:GLU:C	1:188:B:GLU:N	1:188:B:GLU:CA	1:188:B:GLU:C	11	36.7
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	12	36.62
(1,558)	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	1:97:B:GLU:N	18	36.58
(1,730)	1:183:B:GLN:N	1:183:B:GLN:CA	1:183:B:GLN:C	1:184:B:GLY:N	15	36.39
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	20	36.1
(1,601)	1:117:B:ASP:C	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	15	36.01
(1,146)	1:3:B:ALA:C	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	15	35.98
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	17	35.68
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	4	35.63
(1,635)	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	1:136:B:ALA:N	6	35.59
(1,884)	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	1:314:B:LEU:N	14	35.43
(1,255)	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	1:59:B:GLU:N	4	35.43
(1,897)	1:331:B:ALA:C	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	5	35.38
(1,887)	1:314:B:LEU:C	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	11	35.33
(1,871)	1:273:B:ALA:C	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	18	35.29
(1,636)	1:135:B:ASN:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	6	35.29
(1,764)	1:200:B:GLU:C	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	6	35.09
(1,889)	1:316:B:ASN:C	1:317:B:ASN:N	1:317:B:ASN:CA	1:317:B:ASN:C	11	35.07
(1,892)	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	1:320:B:LEU:N	7	35.0
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	20	34.83
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	12	34.79
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	11	34.64
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	9	34.59
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	9	34.56
(1,891)	1:318:B:PRO:C	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	8	34.48
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	6	34.47
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	17	34.44
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	18	34.34
(1,899)	1:332:B:GLY:C	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	19	34.28
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	13	33.96
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	18	33.86
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	11	33.83
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	5	33.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	6	33.78
(1,560)	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	1:98:B:THR:N	15	33.6
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	1	33.46
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	5	33.27
(1,901)	1:333:B:ALA:C	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	9	33.21
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	15	33.16
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	5	32.99
(1,275)	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	1:69:B:LEU:N	17	32.97
(1,256)	1:58:B:SER:C	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	20	32.92
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	7	32.63
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	18	32.56
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	17	32.53
(1,870)	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	1:274:B:GLN:N	5	32.25
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	4	32.11
(1,562)	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	1:99:B:LYS:N	3	32.07
(1,187)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ILE:N	3	32.0
(1,738)	1:187:B:GLU:C	1:188:B:GLU:N	1:188:B:GLU:CA	1:188:B:GLU:C	3	31.78
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	5	31.73
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	16	31.71
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	13	31.57
(1,572)	1:103:B:GLU:N	1:103:B:GLU:CA	1:103:B:GLU:C	1:104:B:ASP:N	19	31.49
(1,889)	1:316:B:ASN:C	1:317:B:ASN:N	1:317:B:ASN:CA	1:317:B:ASN:C	12	31.4
(1,603)	1:118:B:TYR:C	1:119:B:GLU:N	1:119:B:GLU:CA	1:119:B:GLU:C	7	31.32
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	4	31.21
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	4	31.16
(1,191)	1:26:B:SER:N	1:26:B:SER:CA	1:26:B:SER:C	1:27:B:GLU:N	20	31.0
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	10	30.94
(1,150)	1:5:B:LYS:C	1:6:B:GLU:N	1:6:B:GLU:CA	1:6:B:GLU:C	1	30.91
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	15	30.82
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	13	30.75
(1,732)	1:184:B:GLY:N	1:184:B:GLY:CA	1:184:B:GLY:C	1:185:B:LYS:N	13	30.73
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	3	30.55
(1,268)	1:64:B:HIS:C	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	19	30.48
(1,765)	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	1:202:B:ASP:N	4	30.26
(1,865)	1:236:B:ALA:C	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	14	30.19
(1,187)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ILE:N	7	30.11
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	12	30.09
(1,603)	1:118:B:TYR:C	1:119:B:GLU:N	1:119:B:GLU:CA	1:119:B:GLU:C	15	30.07
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	10	30.03
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	12	30.01
(1,600)	1:117:B:ASP:N	1:117:B:ASP:CA	1:117:B:ASP:C	1:118:B:TYR:N	7	29.98
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	5	29.97
(1,255)	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	1:59:B:GLU:N	2	29.92
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	6	29.9
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	2	29.89
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	18	29.85
(1,773)	1:205:B:THR:N	1:205:B:THR:CA	1:205:B:THR:C	1:206:B:GLU:N	7	29.75
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	8	29.71
(1,803)	1:220:B:GLU:N	1:220:B:GLU:CA	1:220:B:GLU:C	1:221:B:GLN:N	13	29.64
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	4	29.59
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	4	29.55

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,558)	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	1:97:B:GLU:N	2	29.5
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	18	29.45
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	20	29.41
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	12	29.37
(1,899)	1:332:B:GLY:C	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	15	29.17
(1,884)	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	1:314:B:LEU:N	7	29.07
(1,601)	1:117:B:ASP:C	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	3	29.05
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	16	28.8
(1,762)	1:199:B:ILE:C	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	7	28.62
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	2	28.52
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	4	28.49
(1,600)	1:117:B:ASP:N	1:117:B:ASP:CA	1:117:B:ASP:C	1:118:B:TYR:N	3	28.34
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	14	28.15
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	18	28.11
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	16	28.05
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	3	27.93
(1,255)	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	1:59:B:GLU:N	20	27.88
(1,187)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ILE:N	6	27.88
(1,874)	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	1:295:B:ILE:N	16	27.84
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	8	27.37
(1,601)	1:117:B:ASP:C	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	7	27.35
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	8	27.32
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	16	27.27
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	15	27.26
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	1	27.25
(1,275)	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	1:69:B:LEU:N	11	27.23
(1,892)	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	1:320:B:LEU:N	2	27.2
(1,765)	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	1:202:B:ASP:N	10	27.13
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	13	27.11
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	6	27.08
(1,576)	1:105:B:LEU:N	1:105:B:LEU:CA	1:105:B:LEU:C	1:106:B:LYS:N	6	26.98
(1,764)	1:200:B:GLU:C	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	18	26.96
(1,559)	1:96:B:ALA:C	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	2	26.9
(1,560)	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	1:98:B:THR:N	2	26.77
(1,881)	1:311:B:LEU:C	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	14	26.51
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	13	26.47
(1,806)	1:221:B:GLN:C	1:222:B:SER:N	1:222:B:SER:CA	1:222:B:SER:C	5	26.37
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	10	26.37
(1,777)	1:207:B:ALA:N	1:207:B:ALA:CA	1:207:B:ALA:C	1:208:B:MET:N	11	26.35
(1,902)	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	1:335:B:SER:N	5	26.32
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	7	26.31
(1,763)	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	1:201:B:GLY:N	6	26.21
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	8	26.13
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	18	25.89
(1,865)	1:236:B:ALA:C	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	18	25.78
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	11	25.73
(1,889)	1:316:B:ASN:C	1:317:B:ASN:N	1:317:B:ASN:CA	1:317:B:ASN:C	10	25.69
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	17	25.68
(1,870)	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	1:274:B:GLN:N	9	25.6
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	20	25.46
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	10	25.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	4	25.24
(1,775)	1:206:B:GLU:N	1:206:B:GLU:CA	1:206:B:GLU:C	1:207:B:ALA:N	8	25.11
(1,871)	1:273:B:ALA:C	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	11	25.03
(1,799)	1:218:B:LYS:N	1:218:B:LYS:CA	1:218:B:LYS:C	1:219:B:VAL:N	11	25.01
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1	24.9
(1,767)	1:202:B:ASP:N	1:202:B:ASP:CA	1:202:B:ASP:C	1:203:B:ASN:N	16	24.87
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	12	24.8
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	3	24.79
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	20	24.63
(1,280)	1:70:B:ASN:C	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	4	24.62
(1,895)	1:326:B:ASN:C	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1	24.56
(1,576)	1:105:B:LEU:N	1:105:B:LEU:CA	1:105:B:LEU:C	1:106:B:LYS:N	19	24.48
(1,865)	1:236:B:ALA:C	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	11	24.42
(1,149)	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	1:6:B:GLU:N	1	24.26
(1,627)	1:130:B:LYS:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	7	24.14
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	13	24.08
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	18	24.05
(1,771)	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	1:205:B:THR:N	13	23.94
(1,881)	1:311:B:LEU:C	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	16	23.84
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	13	23.83
(1,767)	1:202:B:ASP:N	1:202:B:ASP:CA	1:202:B:ASP:C	1:203:B:ASN:N	7	23.74
(1,257)	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	1:60:B:PHE:N	17	23.7
(1,801)	1:219:B:VAL:N	1:219:B:VAL:CA	1:219:B:VAL:C	1:220:B:GLU:N	11	23.57
(1,148)	1:4:B:SER:C	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	5	23.57
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	6	23.36
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	6	23.33
(1,887)	1:314:B:LEU:C	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	14	23.28
(1,146)	1:3:B:ALA:C	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	13	23.26
(1,551)	1:92:B:PRO:C	1:93:B:GLU:N	1:93:B:GLU:CA	1:93:B:GLU:C	11	23.14
(1,250)	1:55:B:LEU:C	1:56:B:GLY:N	1:56:B:GLY:CA	1:56:B:GLY:C	7	23.11
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	9	22.85
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	7	22.75
(1,631)	1:133:B:PRO:N	1:133:B:PRO:CA	1:133:B:PRO:C	1:134:B:THR:N	1	22.64
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	5	22.62
(1,784)	1:210:B:ARG:C	1:211:B:ASP:N	1:211:B:ASP:CA	1:211:B:ASP:C	18	22.44
(1,809)	1:223:B:LEU:N	1:223:B:LEU:CA	1:223:B:LEU:C	1:224:B:ASN:N	5	22.39
(1,889)	1:316:B:ASN:C	1:317:B:ASN:N	1:317:B:ASN:CA	1:317:B:ASN:C	19	22.37
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	14	22.31
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	19	22.23
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	17	22.22
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	6	22.11
(1,871)	1:273:B:ALA:C	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	14	22.09
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	14	22.05
(1,762)	1:199:B:ILE:C	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	4	22.04
(1,901)	1:333:B:ALA:C	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	13	22.0
(1,193)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:ASP:N	20	21.93
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	10	21.92
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	19	21.91
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	19	21.85
(1,866)	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	1:238:B:VAL:N	14	21.84
(1,602)	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	1:119:B:GLU:N	3	21.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	16	21.72
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	1	21.7
(1,735)	1:186:B:PRO:N	1:186:B:PRO:CA	1:186:B:PRO:C	1:187:B:GLU:N	3	21.68
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	16	21.66
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	13	21.63
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	11	21.56
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	6	21.53
(1,230)	1:45:B:GLY:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	15	21.37
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	2	21.33
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	13	21.2
(1,734)	1:185:B:LYS:N	1:185:B:LYS:CA	1:185:B:LYS:C	1:186:B:PRO:N	1	21.14
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	1	21.05
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	7	21.03
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	6	20.93
(1,245)	1:53:B:GLY:N	1:53:B:GLY:CA	1:53:B:GLY:C	1:54:B:ILE:N	17	20.9
(1,760)	1:198:B:ASP:C	1:199:B:ILE:N	1:199:B:ILE:CA	1:199:B:ILE:C	10	20.89
(1,810)	1:223:B:LEU:C	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	20	20.84
(1,558)	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	1:97:B:GLU:N	8	20.83
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	5	20.72
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	8	20.42
(1,237)	1:49:B:GLU:N	1:49:B:GLU:CA	1:49:B:GLU:C	1:50:B:ALA:N	1	20.23
(1,240)	1:50:B:ALA:C	1:51:B:VAL:N	1:51:B:VAL:CA	1:51:B:VAL:C	1	20.21
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	18	20.01
(1,257)	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	1:60:B:PHE:N	9	19.98
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1	19.96
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	12	19.93
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	17	19.89
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	13	19.8
(1,733)	1:184:B:GLY:C	1:185:B:LYS:N	1:185:B:LYS:CA	1:185:B:LYS:C	1	19.74
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	9	19.72
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	16	19.64
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	20	19.58
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	17	19.57
(1,279)	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	1:71:B:SER:N	4	19.47
(1,797)	1:217:B:LYS:N	1:217:B:LYS:CA	1:217:B:LYS:C	1:218:B:LYS:N	11	19.41
(1,735)	1:186:B:PRO:N	1:186:B:PRO:CA	1:186:B:PRO:C	1:187:B:GLU:N	7	19.4
(1,892)	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	1:320:B:LEU:N	14	19.37
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	16	19.27
(1,771)	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	1:205:B:THR:N	19	19.22
(1,600)	1:117:B:ASP:N	1:117:B:ASP:CA	1:117:B:ASP:C	1:118:B:TYR:N	20	19.2
(1,602)	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	1:119:B:GLU:N	15	19.09
(1,196)	1:28:B:ASP:C	1:29:B:GLY:N	1:29:B:GLY:CA	1:29:B:GLY:C	10	19.07
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	20	19.01
(1,176)	1:18:B:SER:C	1:19:B:ILE:N	1:19:B:ILE:CA	1:19:B:ILE:C	8	18.94
(1,265)	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	1:64:B:HIS:N	4	18.91
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	2	18.79
(1,797)	1:217:B:LYS:N	1:217:B:LYS:CA	1:217:B:LYS:C	1:218:B:LYS:N	5	18.67
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	18	18.61
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	3	18.6
(1,175)	1:18:B:SER:N	1:18:B:SER:CA	1:18:B:SER:C	1:19:B:ILE:N	8	18.5
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	15	18.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,193)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:ASP:N	11	18.42
(1,780)	1:208:B:MET:C	1:209:B:LYS:N	1:209:B:LYS:CA	1:209:B:LYS:C	6	18.25
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	17	18.2
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	9	18.2
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	12	18.2
(1,187)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ILE:N	1	18.2
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	3	18.15
(1,149)	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	1:6:B:GLU:N	10	18.13
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	11	18.12
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	10	17.86
(1,805)	1:221:B:GLN:N	1:221:B:GLN:CA	1:221:B:GLN:C	1:222:B:SER:N	17	17.83
(1,568)	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	1:102:B:ALA:N	15	17.76
(1,149)	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	1:6:B:GLU:N	5	17.71
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	13	17.7
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	2	17.65
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	6	17.64
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	17	17.58
(1,811)	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1:225:B:LEU:N	13	17.51
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	14	17.45
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	19	17.35
(1,801)	1:219:B:VAL:N	1:219:B:VAL:CA	1:219:B:VAL:C	1:220:B:GLU:N	15	17.33
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	16	17.25
(1,665)	1:150:B:LYS:N	1:150:B:LYS:CA	1:150:B:LYS:C	1:151:B:GLU:N	10	17.19
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	7	17.1
(1,554)	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	1:95:B:ASP:N	11	17.08
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	15	17.03
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	3	16.98
(1,249)	1:55:B:LEU:N	1:55:B:LEU:CA	1:55:B:LEU:C	1:56:B:GLY:N	18	16.97
(1,765)	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	1:202:B:ASP:N	1	16.94
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	19	16.93
(1,728)	1:182:B:ALA:N	1:182:B:ALA:CA	1:182:B:ALA:C	1:183:B:GLN:N	10	16.89
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	9	16.88
(1,901)	1:333:B:ALA:C	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	8	16.87
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	12	16.86
(1,804)	1:220:B:GLU:C	1:221:B:GLN:N	1:221:B:GLN:CA	1:221:B:GLN:C	6	16.85
(1,557)	1:95:B:ASP:C	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	18	16.79
(1,149)	1:5:B:LYS:N	1:5:B:LYS:CA	1:5:B:LYS:C	1:6:B:GLU:N	17	16.79
(1,866)	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	1:238:B:VAL:N	11	16.77
(1,632)	1:133:B:PRO:C	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	12	16.5
(1,894)	1:320:B:LEU:N	1:320:B:LEU:CA	1:320:B:LEU:C	1:321:B:ARG:N	9	16.48
(1,806)	1:221:B:GLN:C	1:222:B:SER:N	1:222:B:SER:CA	1:222:B:SER:C	17	16.45
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	3	16.38
(1,764)	1:200:B:GLU:C	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	2	16.35
(1,765)	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	1:202:B:ASP:N	19	16.33
(1,557)	1:95:B:ASP:C	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	8	16.31
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	19	16.3
(1,565)	1:99:B:LYS:C	1:100:B:ALA:N	1:100:B:ALA:CA	1:100:B:ALA:C	1	16.24
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	2	16.12
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	4	16.11
(1,905)	1:336:B:THR:C	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	15	16.03
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	9	15.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,785)	1:211:B:ASP:N	1:211:B:ASP:CA	1:211:B:ASP:C	1:212:B:TYR:N	3	15.94
(1,602)	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	1:119:B:GLU:N	7	15.94
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	11	15.82
(1,259)	1:60:B:PHE:N	1:60:B:PHE:CA	1:60:B:PHE:C	1:61:B:LYS:N	2	15.68
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	17	15.67
(1,253)	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	1:58:B:SER:N	16	15.66
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	6	15.65
(1,647)	1:141:B:ASN:N	1:141:B:ASN:CA	1:141:B:ASN:C	1:142:B:ARG:N	13	15.58
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	13	15.58
(1,565)	1:99:B:LYS:C	1:100:B:ALA:N	1:100:B:ALA:CA	1:100:B:ALA:C	18	15.55
(1,601)	1:117:B:ASP:C	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	20	15.5
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	4	15.5
(1,739)	1:188:B:GLU:N	1:188:B:GLU:CA	1:188:B:GLU:C	1:189:B:ALA:N	3	15.37
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	17	15.18
(1,897)	1:331:B:ALA:C	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	10	15.05
(1,253)	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	1:58:B:SER:N	15	15.03
(1,249)	1:55:B:LEU:N	1:55:B:LEU:CA	1:55:B:LEU:C	1:56:B:GLY:N	8	15.02
(1,278)	1:69:B:LEU:C	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	11	15.0
(1,256)	1:58:B:SER:C	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	4	15.0
(1,894)	1:320:B:LEU:N	1:320:B:LEU:CA	1:320:B:LEU:C	1:321:B:ARG:N	2	14.97
(1,800)	1:218:B:LYS:C	1:219:B:VAL:N	1:219:B:VAL:CA	1:219:B:VAL:C	15	14.88
(1,882)	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	1:313:B:ASP:N	19	14.87
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	6	14.8
(1,805)	1:221:B:GLN:N	1:221:B:GLN:CA	1:221:B:GLN:C	1:222:B:SER:N	6	14.77
(1,246)	1:53:B:GLY:C	1:54:B:ILE:N	1:54:B:ILE:CA	1:54:B:ILE:C	17	14.7
(1,905)	1:336:B:THR:C	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	18	14.59
(1,244)	1:52:B:SER:C	1:53:B:GLY:N	1:53:B:GLY:CA	1:53:B:GLY:C	16	14.58
(1,882)	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	1:313:B:ASP:N	13	14.54
(1,899)	1:332:B:GLY:C	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	4	14.5
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	15	14.28
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	5	14.27
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	15	14.24
(1,803)	1:220:B:GLU:N	1:220:B:GLU:CA	1:220:B:GLU:C	1:221:B:GLN:N	9	14.24
(1,798)	1:217:B:LYS:C	1:218:B:LYS:N	1:218:B:LYS:CA	1:218:B:LYS:C	12	14.19
(1,870)	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	1:274:B:GLN:N	14	14.17
(1,634)	1:134:B:THR:C	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	17	14.09
(1,187)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ILE:N	2	14.06
(1,272)	1:66:B:ALA:C	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	17	13.93
(1,145)	1:3:B:ALA:N	1:3:B:ALA:CA	1:3:B:ALA:C	1:4:B:SER:N	14	13.87
(1,758)	1:197:B:LEU:C	1:198:B:ASP:N	1:198:B:ASP:CA	1:198:B:ASP:C	14	13.79
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	4	13.77
(1,642)	1:138:B:TYR:C	1:139:B:TYR:N	1:139:B:TYR:CA	1:139:B:TYR:C	7	13.67
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	4	13.62
(1,732)	1:184:B:GLY:N	1:184:B:GLY:CA	1:184:B:GLY:C	1:185:B:LYS:N	10	13.61
(1,240)	1:50:B:ALA:C	1:51:B:VAL:N	1:51:B:VAL:CA	1:51:B:VAL:C	11	13.6
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	17	13.54
(1,570)	1:102:B:ALA:N	1:102:B:ALA:CA	1:102:B:ALA:C	1:103:B:GLU:N	18	13.52
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	15	13.47
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	8	13.45
(1,265)	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	1:64:B:HIS:N	7	13.44
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	11	13.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	1	13.43
(1,804)	1:220:B:GLU:C	1:221:B:GLN:N	1:221:B:GLN:CA	1:221:B:GLN:C	14	13.32
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	2	13.31
(1,762)	1:199:B:ILE:C	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	12	13.3
(1,146)	1:3:B:ALA:C	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	6	13.28
(1,899)	1:332:B:GLY:C	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	17	13.24
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	3	13.18
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	3	13.12
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	3	13.05
(1,702)	1:169:B:TYR:N	1:169:B:TYR:CA	1:169:B:TYR:C	1:170:B:PHE:N	14	13.04
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	15	12.96
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	10	12.96
(1,763)	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	1:201:B:GLY:N	4	12.91
(1,757)	1:197:B:LEU:N	1:197:B:LEU:CA	1:197:B:LEU:C	1:198:B:ASP:N	14	12.85
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	1	12.83
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	17	12.78
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	10	12.72
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	14	12.66
(1,253)	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	1:58:B:SER:N	3	12.64
(1,256)	1:58:B:SER:C	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	12	12.51
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	9	12.5
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	13	12.48
(1,873)	1:293:B:PRO:C	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	8	12.45
(1,874)	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	1:295:B:ILE:N	9	12.43
(1,147)	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	1:5:B:LYS:N	5	12.41
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	10	12.35
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	12	12.34
(1,763)	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	1:201:B:GLY:N	19	12.33
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	2	12.28
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	15	12.25
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	20	12.19
(1,191)	1:26:B:SER:N	1:26:B:SER:CA	1:26:B:SER:C	1:27:B:GLU:N	11	12.12
(1,809)	1:223:B:LEU:N	1:223:B:LEU:CA	1:223:B:LEU:C	1:224:B:ASN:N	2	12.09
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	14	12.03
(1,896)	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1:328:B:PHE:N	14	12.0
(1,166)	1:13:B:VAL:C	1:14:B:ASN:N	1:14:B:ASN:CA	1:14:B:ASN:C	4	11.99
(1,902)	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	1:335:B:SER:N	14	11.98
(1,895)	1:326:B:ASN:C	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	7	11.97
(1,882)	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	1:313:B:ASP:N	15	11.84
(1,866)	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	1:238:B:VAL:N	12	11.77
(1,866)	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	1:238:B:VAL:N	15	11.73
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	18	11.73
(1,887)	1:314:B:LEU:C	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	13	11.68
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	18	11.67
(1,277)	1:69:B:LEU:N	1:69:B:LEU:CA	1:69:B:LEU:C	1:70:B:ASN:N	11	11.65
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	3	11.59
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	4	11.53
(1,277)	1:69:B:LEU:N	1:69:B:LEU:CA	1:69:B:LEU:C	1:70:B:ASN:N	10	11.52
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	12	11.5
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	1	11.49
(1,581)	1:107:B:MET:C	1:108:B:GLN:N	1:108:B:GLN:CA	1:108:B:GLN:C	7	11.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,253)	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	1:58:B:SER:N	7	11.36
(1,800)	1:218:B:LYS:C	1:219:B:VAL:N	1:219:B:VAL:CA	1:219:B:VAL:C	18	11.26
(1,632)	1:133:B:PRO:C	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	8	11.16
(1,602)	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	1:119:B:GLU:N	20	11.16
(1,251)	1:56:B:GLY:N	1:56:B:GLY:CA	1:56:B:GLY:C	1:57:B:LYS:N	7	11.12
(1,771)	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	1:205:B:THR:N	17	11.01
(1,253)	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	1:58:B:SER:N	8	11.01
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	16	10.99
(1,872)	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	1:275:B:LYS:N	12	10.97
(1,228)	1:44:B:PHE:C	1:45:B:GLY:N	1:45:B:GLY:CA	1:45:B:GLY:C	11	10.97
(1,669)	1:152:B:TYR:N	1:152:B:TYR:CA	1:152:B:TYR:C	1:153:B:ASP:N	8	10.91
(1,635)	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	1:136:B:ALA:N	10	10.88
(1,887)	1:314:B:LEU:C	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	4	10.87
(1,810)	1:223:B:LEU:C	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1	10.86
(1,265)	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	1:64:B:HIS:N	18	10.81
(1,883)	1:312:B:SER:C	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	1	10.65
(1,237)	1:49:B:GLU:N	1:49:B:GLU:CA	1:49:B:GLU:C	1:50:B:ALA:N	12	10.64
(1,249)	1:55:B:LEU:N	1:55:B:LEU:CA	1:55:B:LEU:C	1:56:B:GLY:N	16	10.6
(1,761)	1:199:B:ILE:N	1:199:B:ILE:CA	1:199:B:ILE:C	1:200:B:GLU:N	7	10.59
(1,739)	1:188:B:GLU:N	1:188:B:GLU:CA	1:188:B:GLU:C	1:189:B:ALA:N	11	10.58
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	5	10.49
(1,556)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:ALA:N	9	10.49
(1,636)	1:135:B:ASN:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	19	10.47
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	3	10.45
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	9	10.4
(1,249)	1:55:B:LEU:N	1:55:B:LEU:CA	1:55:B:LEU:C	1:56:B:GLY:N	15	10.29
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	9	10.21
(1,642)	1:138:B:TYR:C	1:139:B:TYR:N	1:139:B:TYR:CA	1:139:B:TYR:C	8	10.15
(1,734)	1:185:B:LYS:N	1:185:B:LYS:CA	1:185:B:LYS:C	1:186:B:PRO:N	13	10.13
(1,256)	1:58:B:SER:C	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	6	10.13
(1,765)	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	1:202:B:ASP:N	17	10.08
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	12	10.08
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	9	10.07
(1,568)	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	1:102:B:ALA:N	11	10.06
(1,771)	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	1:205:B:THR:N	8	10.04
(1,282)	1:71:B:SER:C	1:72:B:ALA:N	1:72:B:ALA:CA	1:72:B:ALA:C	12	10.03
(1,802)	1:219:B:VAL:C	1:220:B:GLU:N	1:220:B:GLU:CA	1:220:B:GLU:C	12	10.0
(1,628)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:LEU:N	7	10.0
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	3	9.88
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	16	9.86
(1,887)	1:314:B:LEU:C	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	17	9.8
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	2	9.79
(1,600)	1:117:B:ASP:N	1:117:B:ASP:CA	1:117:B:ASP:C	1:118:B:TYR:N	11	9.7
(1,718)	1:177:B:GLY:N	1:177:B:GLY:CA	1:177:B:GLY:C	1:178:B:PHE:N	6	9.68
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	20	9.68
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	10	9.66
(1,874)	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	1:295:B:ILE:N	1	9.63
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	2	9.61
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	11	9.6
(1,881)	1:311:B:LEU:C	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	17	9.53
(1,870)	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	1:274:B:GLN:N	2	9.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,764)	1:200:B:GLU:C	1:201:B:GLY:N	1:201:B:GLY:CA	1:201:B:GLY:C	4	9.48
(1,237)	1:49:B:GLU:N	1:49:B:GLU:CA	1:49:B:GLU:C	1:50:B:ALA:N	5	9.48
(1,807)	1:222:B:SER:N	1:222:B:SER:CA	1:222:B:SER:C	1:223:B:LEU:N	1	9.47
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	7	9.43
(1,253)	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	1:58:B:SER:N	17	9.43
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	3	9.41
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	11	9.41
(1,562)	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	1:99:B:LYS:N	10	9.38
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	15	9.37
(1,629)	1:131:B:VAL:C	1:132:B:LEU:N	1:132:B:LEU:CA	1:132:B:LEU:C	4	9.37
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	15	9.31
(1,576)	1:105:B:LEU:N	1:105:B:LEU:CA	1:105:B:LEU:C	1:106:B:LYS:N	4	9.24
(1,901)	1:333:B:ALA:C	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	12	9.2
(1,678)	1:156:B:VAL:C	1:157:B:LYS:N	1:157:B:LYS:CA	1:157:B:LYS:C	11	9.2
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	12	9.17
(1,632)	1:133:B:PRO:C	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	2	9.1
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	9	9.05
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	20	8.99
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	12	8.99
(1,896)	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1:328:B:PHE:N	9	8.9
(1,601)	1:117:B:ASP:C	1:118:B:TYR:N	1:118:B:TYR:CA	1:118:B:TYR:C	10	8.9
(1,734)	1:185:B:LYS:N	1:185:B:LYS:CA	1:185:B:LYS:C	1:186:B:PRO:N	8	8.83
(1,571)	1:102:B:ALA:C	1:103:B:GLU:N	1:103:B:GLU:CA	1:103:B:GLU:C	15	8.78
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	1	8.74
(1,199)	1:30:B:ALA:N	1:30:B:ALA:CA	1:30:B:ALA:C	1:31:B:ASP:N	2	8.69
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	1	8.65
(1,899)	1:332:B:GLY:C	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	16	8.62
(1,635)	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	1:136:B:ALA:N	19	8.53
(1,603)	1:118:B:TYR:C	1:119:B:GLU:N	1:119:B:GLU:CA	1:119:B:GLU:C	3	8.49
(1,255)	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	1:59:B:GLU:N	14	8.48
(1,230)	1:45:B:GLY:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	8	8.47
(1,789)	1:213:B:GLU:N	1:213:B:GLU:CA	1:213:B:GLU:C	1:214:B:SER:N	5	8.41
(1,264)	1:62:B:GLY:C	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	9	8.41
(1,239)	1:50:B:ALA:N	1:50:B:ALA:CA	1:50:B:ALA:C	1:51:B:VAL:N	4	8.41
(1,243)	1:52:B:SER:N	1:52:B:SER:CA	1:52:B:SER:C	1:53:B:GLY:N	4	8.4
(1,734)	1:185:B:LYS:N	1:185:B:LYS:CA	1:185:B:LYS:C	1:186:B:PRO:N	10	8.37
(1,249)	1:55:B:LEU:N	1:55:B:LEU:CA	1:55:B:LEU:C	1:56:B:GLY:N	20	8.37
(1,244)	1:52:B:SER:C	1:53:B:GLY:N	1:53:B:GLY:CA	1:53:B:GLY:C	6	8.35
(1,879)	1:310:B:ASN:C	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	15	8.33
(1,237)	1:49:B:GLU:N	1:49:B:GLU:CA	1:49:B:GLU:C	1:50:B:ALA:N	2	8.32
(1,635)	1:135:B:ASN:N	1:135:B:ASN:CA	1:135:B:ASN:C	1:136:B:ALA:N	5	8.26
(1,560)	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	1:98:B:THR:N	3	8.2
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	5	8.17
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	14	8.17
(1,274)	1:67:B:ASP:C	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	7	8.15
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	2	8.01
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	4	8.0
(1,771)	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	1:205:B:THR:N	20	7.99
(1,869)	1:272:B:ALA:C	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	5	7.96
(1,816)	1:226:B:GLU:C	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	8	7.94
(1,809)	1:223:B:LEU:N	1:223:B:LEU:CA	1:223:B:LEU:C	1:224:B:ASN:N	12	7.91

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,277)	1:69:B:LEU:N	1:69:B:LEU:CA	1:69:B:LEU:C	1:70:B:ASN:N	12	7.87
(1,254)	1:57:B:LYS:C	1:58:B:SER:N	1:58:B:SER:CA	1:58:B:SER:C	17	7.85
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	4	7.82
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	7	7.8
(1,901)	1:333:B:ALA:C	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	2	7.77
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	16	7.73
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	4	7.69
(1,188)	1:24:B:GLU:C	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	15	7.69
(1,805)	1:221:B:GLN:N	1:221:B:GLN:CA	1:221:B:GLN:C	1:222:B:SER:N	11	7.62
(1,785)	1:211:B:ASP:N	1:211:B:ASP:CA	1:211:B:ASP:C	1:212:B:TYR:N	19	7.62
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	13	7.52
(1,256)	1:58:B:SER:C	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	8	7.44
(1,824)	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	1:273:A:ALA:N	7	7.39
(1,562)	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	1:99:B:LYS:N	12	7.37
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	10	7.36
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	2	7.32
(1,529)	1:217:A:LYS:N	1:217:A:LYS:CA	1:217:A:LYS:C	1:218:A:LYS:N	3	7.3
(1,760)	1:198:B:ASP:C	1:199:B:ILE:N	1:199:B:ILE:CA	1:199:B:ILE:C	17	7.29
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	3	7.29
(1,147)	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	1:5:B:LYS:N	10	7.27
(1,823)	1:271:A:GLN:C	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	11	7.25
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	6	7.18
(1,766)	1:201:B:GLY:C	1:202:B:ASP:N	1:202:B:ASP:CA	1:202:B:ASP:C	17	7.16
(1,183)	1:22:B:LYS:N	1:22:B:LYS:CA	1:22:B:LYS:C	1:23:B:LYS:N	1	7.16
(1,275)	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	1:69:B:LEU:N	20	7.14
(1,680)	1:157:B:LYS:C	1:158:B:ASP:N	1:158:B:ASP:CA	1:158:B:ASP:C	1	7.12
(1,679)	1:157:B:LYS:N	1:157:B:LYS:CA	1:157:B:LYS:C	1:158:B:ASP:N	1	7.09
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	9	7.04
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	7	7.04
(1,702)	1:169:B:TYR:N	1:169:B:TYR:CA	1:169:B:TYR:C	1:170:B:PHE:N	3	7.03
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	15	7.02
(1,897)	1:331:B:ALA:C	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	3	6.99
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	2	6.98
(1,870)	1:273:B:ALA:N	1:273:B:ALA:CA	1:273:B:ALA:C	1:274:B:GLN:N	8	6.98
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	19	6.96
(1,551)	1:92:B:PRO:C	1:93:B:GLU:N	1:93:B:GLU:CA	1:93:B:GLU:C	15	6.93
(1,734)	1:185:B:LYS:N	1:185:B:LYS:CA	1:185:B:LYS:C	1:186:B:PRO:N	11	6.91
(1,140)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:ALA:N	3	6.9
(1,727)	1:181:B:TYR:C	1:182:B:ALA:N	1:182:B:ALA:CA	1:182:B:ALA:C	10	6.86
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	19	6.78
(1,187)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ILE:N	19	6.78
(1,894)	1:320:B:LEU:N	1:320:B:LEU:CA	1:320:B:LEU:C	1:321:B:ARG:N	1	6.76
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	11	6.65
(1,150)	1:5:B:LYS:C	1:6:B:GLU:N	1:6:B:GLU:CA	1:6:B:GLU:C	10	6.62
(1,862)	1:337:A:ASP:N	1:337:A:ASP:CA	1:337:A:ASP:C	1:338:A:GLU:N	15	6.6
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	9	6.59
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	14	6.58
(1,771)	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	1:205:B:THR:N	12	6.53
(1,243)	1:52:B:SER:N	1:52:B:SER:CA	1:52:B:SER:C	1:53:B:GLY:N	16	6.45
(1,576)	1:105:B:LEU:N	1:105:B:LEU:CA	1:105:B:LEU:C	1:106:B:LYS:N	18	6.44
(1,550)	1:227:A:LYS:C	1:228:A:THR:N	1:228:A:THR:CA	1:228:A:THR:C	2	6.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,257)	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	1:60:B:PHE:N	11	6.43
(1,257)	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	1:60:B:PHE:N	15	6.41
(1,884)	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	1:314:B:LEU:N	12	6.38
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	1	6.35
(1,699)	1:167:B:PRO:C	1:168:B:SER:N	1:168:B:SER:CA	1:168:B:SER:C	3	6.31
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	8	6.24
(1,567)	1:100:B:ALA:C	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	17	6.16
(1,866)	1:237:B:ASP:N	1:237:B:ASP:CA	1:237:B:ASP:C	1:238:B:VAL:N	18	6.15
(1,836)	1:311:A:LEU:N	1:311:A:LEU:CA	1:311:A:LEU:C	1:312:A:SER:N	11	6.15
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	5	6.08
(1,896)	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1:328:B:PHE:N	4	6.05
(1,646)	1:140:B:ALA:C	1:141:B:ASN:N	1:141:B:ASN:CA	1:141:B:ASN:C	17	6.01
(1,300)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:ALA:N	11	6.01
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	17	5.96
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	9	5.94
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	4	5.93
(1,633)	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1:135:B:ASN:N	4	5.92
(1,471)	1:188:A:GLU:N	1:188:A:GLU:CA	1:188:A:GLU:C	1:189:A:ALA:N	1	5.87
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	6	5.86
(1,874)	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	1:295:B:ILE:N	5	5.84
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	11	5.82
(1,807)	1:222:B:SER:N	1:222:B:SER:CA	1:222:B:SER:C	1:223:B:LEU:N	17	5.77
(1,631)	1:133:B:PRO:N	1:133:B:PRO:CA	1:133:B:PRO:C	1:134:B:THR:N	20	5.75
(1,880)	1:311:B:LEU:N	1:311:B:LEU:CA	1:311:B:LEU:C	1:312:B:SER:N	11	5.7
(1,884)	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	1:314:B:LEU:N	9	5.67
(1,560)	1:97:B:GLU:N	1:97:B:GLU:CA	1:97:B:GLU:C	1:98:B:THR:N	7	5.66
(1,735)	1:186:B:PRO:N	1:186:B:PRO:CA	1:186:B:PRO:C	1:187:B:GLU:N	6	5.63
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	12	5.6
(1,138)	1:70:A:ASN:N	1:70:A:ASN:CA	1:70:A:ASN:C	1:71:A:SER:N	14	5.58
(1,138)	1:70:A:ASN:N	1:70:A:ASN:CA	1:70:A:ASN:C	1:71:A:SER:N	19	5.57
(1,665)	1:150:B:LYS:N	1:150:B:LYS:CA	1:150:B:LYS:C	1:151:B:GLU:N	7	5.53
(1,532)	1:218:A:LYS:C	1:219:A:VAL:N	1:219:A:VAL:CA	1:219:A:VAL:C	13	5.51
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	19	5.5
(1,268)	1:64:B:HIS:C	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	9	5.5
(1,892)	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	1:320:B:LEU:N	8	5.49
(1,817)	1:227:B:LYS:N	1:227:B:LYS:CA	1:227:B:LYS:C	1:228:B:THR:N	7	5.47
(1,706)	1:171:B:ARG:N	1:171:B:ARG:CA	1:171:B:ARG:C	1:172:B:GLY:N	11	5.45
(1,562)	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	1:99:B:LYS:N	5	5.44
(1,285)	1:93:A:GLU:C	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	14	5.39
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	6	5.37
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	2	5.36
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	9	5.36
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	18	5.31
(1,892)	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	1:320:B:LEU:N	6	5.3
(1,700)	1:168:B:SER:N	1:168:B:SER:CA	1:168:B:SER:C	1:169:B:TYR:N	15	5.3
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	4	5.25
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	16	5.22
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	8	5.21
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	2	5.2
(1,665)	1:150:B:LYS:N	1:150:B:LYS:CA	1:150:B:LYS:C	1:151:B:GLU:N	9	5.2
(1,723)	1:179:B:ALA:C	1:180:B:LYS:N	1:180:B:LYS:CA	1:180:B:LYS:C	17	5.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,767)	1:202:B:ASP:N	1:202:B:ASP:CA	1:202:B:ASP:C	1:203:B:ASN:N	3	5.18
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	10	5.17
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	19	5.17
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	14	5.15
(1,631)	1:133:B:PRO:N	1:133:B:PRO:CA	1:133:B:PRO:C	1:134:B:THR:N	6	5.14
(1,541)	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	1:224:A:ASN:N	9	5.13
(1,882)	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	1:313:B:ASP:N	18	5.09
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	15	5.05
(1,285)	1:93:A:GLU:C	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	13	5.03
(1,898)	1:332:B:GLY:N	1:332:B:GLY:CA	1:332:B:GLY:C	1:333:B:ALA:N	5	5.01
(1,771)	1:204:B:ALA:N	1:204:B:ALA:CA	1:204:B:ALA:C	1:205:B:THR:N	1	5.01
(1,632)	1:133:B:PRO:C	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	4	4.99
(1,138)	1:70:A:ASN:N	1:70:A:ASN:CA	1:70:A:ASN:C	1:71:A:SER:N	18	4.99
(1,878)	1:308:B:THR:N	1:308:B:THR:CA	1:308:B:THR:C	1:309:B:PRO:N	13	4.98
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	5	4.97
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	6	4.95
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	14	4.9
(1,823)	1:271:A:GLN:C	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	6	4.89
(1,871)	1:273:B:ALA:C	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	20	4.86
(1,757)	1:197:B:LEU:N	1:197:B:LEU:CA	1:197:B:LEU:C	1:198:B:ASP:N	2	4.85
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	16	4.85
(1,245)	1:53:B:GLY:N	1:53:B:GLY:CA	1:53:B:GLY:C	1:54:B:ILE:N	16	4.82
(1,189)	1:25:B:ILE:N	1:25:B:ILE:CA	1:25:B:ILE:C	1:26:B:SER:N	19	4.78
(1,550)	1:227:A:LYS:C	1:228:A:THR:N	1:228:A:THR:CA	1:228:A:THR:C	16	4.76
(1,632)	1:133:B:PRO:C	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	10	4.75
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	15	4.75
(1,284)	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	1:94:A:ASP:N	14	4.71
(1,631)	1:133:B:PRO:N	1:133:B:PRO:CA	1:133:B:PRO:C	1:134:B:THR:N	8	4.69
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	19	4.68
(1,227)	1:44:B:PHE:N	1:44:B:PHE:CA	1:44:B:PHE:C	1:45:B:GLY:N	11	4.68
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	4	4.61
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	16	4.61
(1,428)	1:165:A:ILE:C	1:166:A:ASP:N	1:166:A:ASP:CA	1:166:A:ASP:C	6	4.61
(1,286)	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	1:95:A:ASP:N	2	4.61
(1,872)	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	1:275:B:LYS:N	20	4.6
(1,735)	1:186:B:PRO:N	1:186:B:PRO:CA	1:186:B:PRO:C	1:187:B:GLU:N	1	4.59
(1,598)	1:116:B:LYS:N	1:116:B:LYS:CA	1:116:B:LYS:C	1:117:B:ASP:N	1	4.59
(1,430)	1:167:A:PRO:N	1:167:A:PRO:CA	1:167:A:PRO:C	1:168:A:SER:N	6	4.55
(1,867)	1:271:B:GLN:C	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	18	4.53
(1,237)	1:49:B:GLU:N	1:49:B:GLU:CA	1:49:B:GLU:C	1:50:B:ALA:N	3	4.52
(1,121)	1:61:A:LYS:C	1:62:A:GLY:N	1:62:A:GLY:CA	1:62:A:GLY:C	3	4.48
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	2	4.43
(1,535)	1:220:A:GLU:N	1:220:A:GLU:CA	1:220:A:GLU:C	1:221:A:GLN:N	19	4.43
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	16	4.39
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	9	4.35
(1,238)	1:49:B:GLU:C	1:50:B:ALA:N	1:50:B:ALA:CA	1:50:B:ALA:C	11	4.32
(1,568)	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	1:102:B:ALA:N	1	4.31
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	20	4.3
(1,147)	1:4:B:SER:N	1:4:B:SER:CA	1:4:B:SER:C	1:5:B:LYS:N	14	4.27
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	9	4.26
(1,365)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	7	4.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,124)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:HIS:N	17	4.26
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	7	4.26
(1,835)	1:310:A:ASN:C	1:311:A:LEU:N	1:311:A:LEU:CA	1:311:A:LEU:C	2	4.25
(1,753)	1:195:B:LYS:N	1:195:B:LYS:CA	1:195:B:LYS:C	1:196:B:VAL:N	5	4.25
(1,111)	1:56:A:GLY:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	5	4.25
(1,275)	1:68:B:ILE:N	1:68:B:ILE:CA	1:68:B:ILE:C	1:69:B:LEU:N	3	4.24
(1,731)	1:183:B:GLN:C	1:184:B:GLY:N	1:184:B:GLY:CA	1:184:B:GLY:C	2	4.23
(1,882)	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	1:313:B:ASP:N	17	4.22
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	16	4.2
(1,904)	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	1:337:B:ASP:N	9	4.19
(1,791)	1:214:B:SER:N	1:214:B:SER:CA	1:214:B:SER:C	1:215:B:ALA:N	5	4.18
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	2	4.17
(1,268)	1:64:B:HIS:C	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	17	4.12
(1,844)	1:315:A:MET:N	1:315:A:MET:CA	1:315:A:MET:C	1:316:A:ASN:N	6	4.08
(1,589)	1:111:B:LYS:C	1:112:B:ALA:N	1:112:B:ALA:CA	1:112:B:ALA:C	1	4.08
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	17	4.05
(1,143)	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	1:3:B:ALA:N	9	4.04
(1,823)	1:271:A:GLN:C	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	15	4.03
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	1	4.03
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	8	3.99
(1,517)	1:211:A:ASP:N	1:211:A:ASP:CA	1:211:A:ASP:C	1:212:A:TYR:N	13	3.98
(1,260)	1:60:B:PHE:C	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	3	3.97
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	1	3.97
(1,842)	1:314:A:LEU:N	1:314:A:LEU:CA	1:314:A:LEU:C	1:315:A:MET:N	10	3.96
(1,761)	1:199:B:ILE:N	1:199:B:ILE:CA	1:199:B:ILE:C	1:200:B:GLU:N	12	3.94
(1,687)	1:161:B:SER:N	1:161:B:SER:CA	1:161:B:SER:C	1:162:B:ALA:N	11	3.94
(1,287)	1:94:A:ASP:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	18	3.93
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	8	3.87
(1,55)	1:28:A:ASP:C	1:29:A:GLY:N	1:29:A:GLY:CA	1:29:A:GLY:C	4	3.86
(1,785)	1:211:B:ASP:N	1:211:B:ASP:CA	1:211:B:ASP:C	1:212:B:TYR:N	11	3.84
(1,281)	1:71:B:SER:N	1:71:B:SER:CA	1:71:B:SER:C	1:72:B:ALA:N	1	3.84
(1,346)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:TYR:N	3	3.83
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	19	3.83
(1,823)	1:271:A:GLN:C	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	8	3.81
(1,140)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:ALA:N	13	3.8
(1,132)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:ILE:N	20	3.79
(1,46)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ILE:N	19	3.79
(1,643)	1:139:B:TYR:N	1:139:B:TYR:CA	1:139:B:TYR:C	1:140:B:ALA:N	13	3.78
(1,769)	1:203:B:ASN:N	1:203:B:ASN:CA	1:203:B:ASN:C	1:204:B:ALA:N	10	3.76
(1,364)	1:133:A:PRO:C	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	17	3.75
(1,287)	1:94:A:ASP:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	3	3.74
(1,845)	1:316:A:ASN:C	1:317:A:ASN:N	1:317:A:ASN:CA	1:317:A:ASN:C	4	3.71
(1,291)	1:96:A:ALA:C	1:97:A:GLU:N	1:97:A:GLU:CA	1:97:A:GLU:C	9	3.71
(1,851)	1:326:A:ASN:C	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	4	3.7
(1,290)	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	1:97:A:GLU:N	1	3.7
(1,287)	1:94:A:ASP:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	17	3.7
(1,892)	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	1:320:B:LEU:N	18	3.69
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	16	3.67
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	11	3.66
(1,576)	1:105:B:LEU:N	1:105:B:LEU:CA	1:105:B:LEU:C	1:106:B:LYS:N	11	3.63
(1,141)	1:71:A:SER:C	1:72:A:ALA:N	1:72:A:ALA:CA	1:72:A:ALA:C	19	3.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,128)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:ALA:N	18	3.62
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	19	3.59
(1,693)	1:164:B:SER:N	1:164:B:SER:CA	1:164:B:SER:C	1:165:B:ILE:N	7	3.57
(1,367)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ALA:N	3	3.57
(1,288)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:ALA:N	10	3.57
(1,367)	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	1:136:A:ALA:N	10	3.55
(1,288)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:ALA:N	12	3.54
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	13	3.49
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	4	3.47
(1,299)	1:100:A:ALA:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	9	3.47
(1,877)	1:307:B:GLY:C	1:308:B:THR:N	1:308:B:THR:CA	1:308:B:THR:C	15	3.46
(1,541)	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	1:224:A:ASN:N	18	3.46
(1,284)	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	1:94:A:ASP:N	18	3.44
(1,695)	1:165:B:ILE:N	1:165:B:ILE:CA	1:165:B:ILE:C	1:166:B:ASP:N	7	3.43
(1,121)	1:61:A:LYS:C	1:62:A:GLY:N	1:62:A:GLY:CA	1:62:A:GLY:C	9	3.4
(1,99)	1:50:A:ALA:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	7	3.39
(1,300)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:ALA:N	10	3.37
(1,497)	1:201:A:GLY:N	1:201:A:GLY:CA	1:201:A:GLY:C	1:202:A:ASP:N	20	3.35
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	16	3.34
(1,546)	1:225:A:LEU:C	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1	3.33
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	7	3.32
(1,263)	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	1:63:B:GLN:N	4	3.32
(1,238)	1:49:B:GLU:C	1:50:B:ALA:N	1:50:B:ALA:CA	1:50:B:ALA:C	3	3.32
(1,237)	1:49:B:GLU:N	1:49:B:GLU:CA	1:49:B:GLU:C	1:50:B:ALA:N	6	3.31
(1,820)	1:236:A:ALA:N	1:236:A:ALA:CA	1:236:A:ALA:C	1:237:A:ASP:N	3	3.3
(1,555)	1:94:B:ASP:C	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	9	3.28
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	12	3.28
(1,501)	1:203:A:ASN:N	1:203:A:ASN:CA	1:203:A:ASN:C	1:204:A:ALA:N	2	3.27
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	17	3.27
(1,433)	1:168:A:SER:C	1:169:A:TYR:N	1:169:A:TYR:CA	1:169:A:TYR:C	18	3.26
(1,265)	1:63:B:GLN:N	1:63:B:GLN:CA	1:63:B:GLN:C	1:64:B:HIS:N	20	3.25
(1,546)	1:225:A:LEU:C	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	5	3.24
(1,543)	1:224:A:ASN:N	1:224:A:ASN:CA	1:224:A:ASN:C	1:225:A:LEU:N	8	3.24
(1,552)	1:93:B:GLU:N	1:93:B:GLU:CA	1:93:B:GLU:C	1:94:B:ASP:N	3	3.23
(1,854)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:ALA:N	13	3.2
(1,294)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:LYS:N	2	3.19
(1,876)	1:295:B:ILE:N	1:295:B:ILE:CA	1:295:B:ILE:C	1:296:B:ARG:N	17	3.18
(1,140)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:ALA:N	19	3.18
(1,538)	1:221:A:GLN:C	1:222:A:SER:N	1:222:A:SER:CA	1:222:A:SER:C	18	3.17
(1,729)	1:182:B:ALA:C	1:183:B:GLN:N	1:183:B:GLN:CA	1:183:B:GLN:C	11	3.14
(1,724)	1:180:B:LYS:N	1:180:B:LYS:CA	1:180:B:LYS:C	1:181:B:TYR:N	17	3.13
(1,119)	1:60:A:PHE:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	3	3.13
(1,856)	1:333:A:ALA:N	1:333:A:ALA:CA	1:333:A:ALA:C	1:334:A:GLN:N	15	3.11
(1,845)	1:316:A:ASN:C	1:317:A:ASN:N	1:317:A:ASN:CA	1:317:A:ASN:C	7	3.11
(1,138)	1:70:A:ASN:N	1:70:A:ASN:CA	1:70:A:ASN:C	1:71:A:SER:N	1	3.11
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	18	3.1
(1,763)	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	1:201:B:GLY:N	18	3.09
(1,284)	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	1:94:A:ASP:N	13	3.09
(1,142)	1:1:B:MET:C	1:2:B:SER:N	1:2:B:SER:CA	1:2:B:SER:C	17	3.09
(1,854)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:ALA:N	8	3.08
(1,876)	1:295:B:ILE:N	1:295:B:ILE:CA	1:295:B:ILE:C	1:296:B:ARG:N	13	3.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,444)	1:174:A:SER:N	1:174:A:SER:CA	1:174:A:SER:C	1:175:A:ARG:N	8	3.06
(1,840)	1:313:A:ASP:N	1:313:A:ASP:CA	1:313:A:ASP:C	1:314:A:LEU:N	6	3.05
(1,828)	1:274:A:GLN:N	1:274:A:GLN:CA	1:274:A:GLN:C	1:275:A:LYS:N	6	3.05
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	16	3.05
(1,550)	1:227:A:LYS:C	1:228:A:THR:N	1:228:A:THR:CA	1:228:A:THR:C	1	3.02
(1,841)	1:313:A:ASP:C	1:314:A:LEU:N	1:314:A:LEU:CA	1:314:A:LEU:C	18	3.0
(1,828)	1:274:A:GLN:N	1:274:A:GLN:CA	1:274:A:GLN:C	1:275:A:LYS:N	15	3.0
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	14	2.99
(1,792)	1:214:B:SER:C	1:215:B:ALA:N	1:215:B:ALA:CA	1:215:B:ALA:C	8	2.96
(1,665)	1:150:B:LYS:N	1:150:B:LYS:CA	1:150:B:LYS:C	1:151:B:GLU:N	4	2.96
(1,895)	1:326:B:ASN:C	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	9	2.94
(1,269)	1:65:B:LEU:N	1:65:B:LEU:CA	1:65:B:LEU:C	1:66:B:ALA:N	9	2.94
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	10	2.93
(1,365)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	9	2.92
(1,809)	1:223:B:LEU:N	1:223:B:LEU:CA	1:223:B:LEU:C	1:224:B:ASN:N	16	2.91
(1,550)	1:227:A:LYS:C	1:228:A:THR:N	1:228:A:THR:CA	1:228:A:THR:C	19	2.91
(1,132)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:ILE:N	2	2.91
(1,98)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:VAL:N	20	2.91
(1,807)	1:222:B:SER:N	1:222:B:SER:CA	1:222:B:SER:C	1:223:B:LEU:N	5	2.9
(1,665)	1:150:B:LYS:N	1:150:B:LYS:CA	1:150:B:LYS:C	1:151:B:GLU:N	2	2.9
(1,835)	1:310:A:ASN:C	1:311:A:LEU:N	1:311:A:LEU:CA	1:311:A:LEU:C	17	2.89
(1,762)	1:199:B:ILE:C	1:200:B:GLU:N	1:200:B:GLU:CA	1:200:B:GLU:C	18	2.89
(1,541)	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	1:224:A:ASN:N	15	2.89
(1,503)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:THR:N	20	2.87
(1,811)	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1:225:B:LEU:N	18	2.85
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	5	2.83
(1,546)	1:225:A:LEU:C	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	2	2.8
(1,288)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:ALA:N	7	2.8
(1,286)	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	1:95:A:ASP:N	17	2.8
(1,233)	1:47:B:GLU:N	1:47:B:GLU:CA	1:47:B:GLU:C	1:48:B:ARG:N	2	2.8
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	20	2.79
(1,295)	1:98:A:THR:C	1:99:A:LYS:N	1:99:A:LYS:CA	1:99:A:LYS:C	19	2.78
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	9	2.78
(1,540)	1:222:A:SER:C	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	3	2.77
(1,822)	1:237:A:ASP:N	1:237:A:ASP:CA	1:237:A:ASP:C	1:238:A:VAL:N	5	2.76
(1,285)	1:93:A:GLU:C	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	4	2.74
(1,277)	1:69:B:LEU:N	1:69:B:LEU:CA	1:69:B:LEU:C	1:70:B:ASN:N	6	2.74
(1,900)	1:333:B:ALA:N	1:333:B:ALA:CA	1:333:B:ALA:C	1:334:B:GLN:N	5	2.72
(1,853)	1:331:A:ALA:C	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	5	2.72
(1,822)	1:237:A:ASP:N	1:237:A:ASP:CA	1:237:A:ASP:C	1:238:A:VAL:N	2	2.72
(1,832)	1:295:A:ILE:N	1:295:A:ILE:CA	1:295:A:ILE:C	1:296:A:ARG:N	19	2.7
(1,632)	1:133:B:PRO:C	1:134:B:THR:N	1:134:B:THR:CA	1:134:B:THR:C	1	2.7
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	1	2.7
(1,557)	1:95:B:ASP:C	1:96:B:ALA:N	1:96:B:ALA:CA	1:96:B:ALA:C	15	2.67
(1,872)	1:274:B:GLN:N	1:274:B:GLN:CA	1:274:B:GLN:C	1:275:B:LYS:N	14	2.64
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	1	2.64
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	9	2.63
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	13	2.63
(1,855)	1:332:A:GLY:C	1:333:A:ALA:N	1:333:A:ALA:CA	1:333:A:ALA:C	8	2.62
(1,823)	1:271:A:GLN:C	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	14	2.61
(1,132)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:ILE:N	15	2.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,494)	1:199:A:ILE:C	1:200:A:GLU:N	1:200:A:GLU:CA	1:200:A:GLU:C	8	2.6
(1,287)	1:94:A:ASP:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	2	2.6
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	7	2.6
(1,823)	1:271:A:GLN:C	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	7	2.58
(1,566)	1:100:B:ALA:N	1:100:B:ALA:CA	1:100:B:ALA:C	1:101:B:LYS:N	12	2.58
(1,132)	1:67:A:ASP:N	1:67:A:ASP:CA	1:67:A:ASP:C	1:68:A:ILE:N	11	2.58
(1,428)	1:165:A:ILE:C	1:166:A:ASP:N	1:166:A:ASP:CA	1:166:A:ASP:C	13	2.57
(1,294)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:LYS:N	13	2.56
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	11	2.55
(1,848)	1:319:A:ALA:N	1:319:A:ALA:CA	1:319:A:ALA:C	1:320:A:LEU:N	18	2.52
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	9	2.51
(1,140)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:ALA:N	14	2.51
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	15	2.49
(1,707)	1:171:B:ARG:C	1:172:B:GLY:N	1:172:B:GLY:CA	1:172:B:GLY:C	4	2.49
(1,285)	1:93:A:GLU:C	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	18	2.48
(1,562)	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	1:99:B:LYS:N	2	2.47
(1,850)	1:320:A:LEU:N	1:320:A:LEU:CA	1:320:A:LEU:C	1:321:A:ARG:N	18	2.44
(1,540)	1:222:A:SER:C	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	18	2.44
(1,894)	1:320:B:LEU:N	1:320:B:LEU:CA	1:320:B:LEU:C	1:321:B:ARG:N	7	2.43
(1,814)	1:225:B:LEU:C	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	6	2.42
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	12	2.4
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	15	2.38
(1,532)	1:218:A:LYS:C	1:219:A:VAL:N	1:219:A:VAL:CA	1:219:A:VAL:C	20	2.37
(1,446)	1:175:A:ARG:N	1:175:A:ARG:CA	1:175:A:ARG:C	1:176:A:LEU:N	1	2.37
(1,562)	1:98:B:THR:N	1:98:B:THR:CA	1:98:B:THR:C	1:99:B:LYS:N	1	2.36
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	8	2.36
(1,121)	1:61:A:LYS:C	1:62:A:GLY:N	1:62:A:GLY:CA	1:62:A:GLY:C	20	2.36
(1,466)	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	1:186:A:PRO:N	5	2.35
(1,412)	1:157:A:LYS:C	1:158:A:ASP:N	1:158:A:ASP:CA	1:158:A:ASP:C	3	2.35
(1,533)	1:219:A:VAL:N	1:219:A:VAL:CA	1:219:A:VAL:C	1:220:A:GLU:N	18	2.34
(1,285)	1:93:A:GLU:C	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	17	2.34
(1,891)	1:318:B:PRO:C	1:319:B:ALA:N	1:319:B:ALA:CA	1:319:B:ALA:C	2	2.32
(1,840)	1:313:A:ASP:N	1:313:A:ASP:CA	1:313:A:ASP:C	1:314:A:LEU:N	8	2.32
(1,822)	1:237:A:ASP:N	1:237:A:ASP:CA	1:237:A:ASP:C	1:238:A:VAL:N	11	2.32
(1,614)	1:124:B:LYS:N	1:124:B:LYS:CA	1:124:B:LYS:C	1:125:B:TYR:N	18	2.29
(1,551)	1:92:B:PRO:C	1:93:B:GLU:N	1:93:B:GLU:CA	1:93:B:GLU:C	3	2.29
(1,544)	1:224:A:ASN:C	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	6	2.28
(1,423)	1:163:A:ILE:N	1:163:A:ILE:CA	1:163:A:ILE:C	1:164:A:SER:N	9	2.28
(1,104)	1:53:A:GLY:N	1:53:A:GLY:CA	1:53:A:GLY:C	1:54:A:ILE:N	8	2.26
(1,868)	1:272:B:ALA:N	1:272:B:ALA:CA	1:272:B:ALA:C	1:273:B:ALA:N	7	2.25
(1,290)	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	1:97:A:GLU:N	13	2.25
(1,820)	1:236:A:ALA:N	1:236:A:ALA:CA	1:236:A:ALA:C	1:237:A:ASP:N	19	2.24
(1,769)	1:203:B:ASN:N	1:203:B:ASN:CA	1:203:B:ASN:C	1:204:B:ALA:N	15	2.24
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	10	2.24
(1,151)	1:6:B:GLU:N	1:6:B:GLU:CA	1:6:B:GLU:C	1:7:B:GLU:N	12	2.24
(1,517)	1:211:A:ASP:N	1:211:A:ASP:CA	1:211:A:ASP:C	1:212:A:TYR:N	11	2.23
(1,124)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:HIS:N	1	2.2
(1,681)	1:158:B:ASP:N	1:158:B:ASP:CA	1:158:B:ASP:C	1:159:B:ALA:N	3	2.19
(1,285)	1:93:A:GLU:C	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	2	2.19
(1,141)	1:71:A:SER:C	1:72:A:ALA:N	1:72:A:ALA:CA	1:72:A:ALA:C	3	2.19
(1,876)	1:295:B:ILE:N	1:295:B:ILE:CA	1:295:B:ILE:C	1:296:B:ARG:N	3	2.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,811)	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1:225:B:LEU:N	19	2.17
(1,365)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	5	2.17
(1,121)	1:61:A:LYS:C	1:62:A:GLY:N	1:62:A:GLY:CA	1:62:A:GLY:C	18	2.17
(1,47)	1:24:A:GLU:C	1:25:A:ILE:N	1:25:A:ILE:CA	1:25:A:ILE:C	4	2.17
(1,494)	1:199:A:ILE:C	1:200:A:GLU:N	1:200:A:GLU:CA	1:200:A:GLU:C	7	2.16
(1,292)	1:97:A:GLU:N	1:97:A:GLU:CA	1:97:A:GLU:C	1:98:A:THR:N	3	2.16
(1,510)	1:207:A:ALA:C	1:208:A:MET:N	1:208:A:MET:CA	1:208:A:MET:C	8	2.15
(1,855)	1:332:A:GLY:C	1:333:A:ALA:N	1:333:A:ALA:CA	1:333:A:ALA:C	17	2.12
(1,850)	1:320:A:LEU:N	1:320:A:LEU:CA	1:320:A:LEU:C	1:321:A:ARG:N	11	2.12
(1,830)	1:294:A:SER:N	1:294:A:SER:CA	1:294:A:SER:C	1:295:A:ILE:N	3	2.12
(1,284)	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	1:94:A:ASP:N	7	2.12
(1,283)	1:92:A:PRO:C	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	3	2.12
(1,882)	1:312:B:SER:N	1:312:B:SER:CA	1:312:B:SER:C	1:313:B:ASP:N	5	2.11
(1,850)	1:320:A:LEU:N	1:320:A:LEU:CA	1:320:A:LEU:C	1:321:A:ARG:N	15	2.11
(1,541)	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	1:224:A:ASN:N	1	2.11
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	18	2.1
(1,288)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:ALA:N	5	2.1
(1,827)	1:273:A:ALA:C	1:274:A:GLN:N	1:274:A:GLN:CA	1:274:A:GLN:C	2	2.09
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	16	2.09
(1,365)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	6	2.08
(1,854)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:ALA:N	9	2.07
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	7	2.06
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	5	2.06
(1,365)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	19	2.05
(1,120)	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	1:62:A:GLY:N	1	2.05
(1,815)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:LYS:N	6	2.04
(1,141)	1:71:A:SER:C	1:72:A:ALA:N	1:72:A:ALA:CA	1:72:A:ALA:C	13	2.04
(1,732)	1:184:B:GLY:N	1:184:B:GLY:CA	1:184:B:GLY:C	1:185:B:LYS:N	1	2.02
(1,306)	1:104:A:ASP:N	1:104:A:ASP:CA	1:104:A:ASP:C	1:105:A:LEU:N	1	2.01
(1,121)	1:61:A:LYS:C	1:62:A:GLY:N	1:62:A:GLY:CA	1:62:A:GLY:C	2	2.01
(1,257)	1:59:B:GLU:N	1:59:B:GLU:CA	1:59:B:GLU:C	1:60:B:PHE:N	12	1.98
(1,397)	1:150:A:LYS:N	1:150:A:LYS:CA	1:150:A:LYS:C	1:151:A:GLU:N	3	1.97
(1,283)	1:92:A:PRO:C	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	7	1.97
(1,138)	1:70:A:ASN:N	1:70:A:ASN:CA	1:70:A:ASN:C	1:71:A:SER:N	10	1.97
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	7	1.95
(1,854)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:ALA:N	7	1.94
(1,851)	1:326:A:ASN:C	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	2	1.94
(1,548)	1:226:A:GLU:C	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	4	1.94
(1,47)	1:24:A:GLU:C	1:25:A:ILE:N	1:25:A:ILE:CA	1:25:A:ILE:C	2	1.94
(1,840)	1:313:A:ASP:N	1:313:A:ASP:CA	1:313:A:ASP:C	1:314:A:LEU:N	2	1.93
(1,568)	1:101:B:LYS:N	1:101:B:LYS:CA	1:101:B:LYS:C	1:102:B:ALA:N	13	1.93
(1,368)	1:135:A:ASN:C	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	10	1.92
(1,896)	1:327:B:LEU:N	1:327:B:LEU:CA	1:327:B:LEU:C	1:328:B:PHE:N	5	1.91
(1,362)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:PRO:N	6	1.91
(1,315)	1:108:A:GLN:C	1:109:A:GLY:N	1:109:A:GLY:CA	1:109:A:GLY:C	18	1.91
(1,286)	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	1:95:A:ASP:N	3	1.91
(1,262)	1:61:B:LYS:C	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	8	1.91
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	18	1.87
(1,48)	1:25:A:ILE:N	1:25:A:ILE:CA	1:25:A:ILE:C	1:26:A:SER:N	10	1.87
(1,906)	1:337:B:ASP:N	1:337:B:ASP:CA	1:337:B:ASP:C	1:338:B:GLU:N	1	1.86
(1,544)	1:224:A:ASN:C	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	14	1.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,826)	1:273:A:ALA:N	1:273:A:ALA:CA	1:273:A:ALA:C	1:274:A:GLN:N	11	1.85
(1,397)	1:150:A:LYS:N	1:150:A:LYS:CA	1:150:A:LYS:C	1:151:A:GLU:N	7	1.85
(1,138)	1:70:A:ASN:N	1:70:A:ASN:CA	1:70:A:ASN:C	1:71:A:SER:N	20	1.84
(1,854)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:ALA:N	20	1.83
(1,886)	1:314:B:LEU:N	1:314:B:LEU:CA	1:314:B:LEU:C	1:315:B:MET:N	3	1.81
(1,829)	1:293:A:PRO:C	1:294:A:SER:N	1:294:A:SER:CA	1:294:A:SER:C	12	1.81
(1,284)	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	1:94:A:ASP:N	6	1.8
(1,118)	1:60:A:PHE:N	1:60:A:PHE:CA	1:60:A:PHE:C	1:61:A:LYS:N	4	1.8
(1,862)	1:337:A:ASP:N	1:337:A:ASP:CA	1:337:A:ASP:C	1:338:A:GLU:N	18	1.79
(1,544)	1:224:A:ASN:C	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	11	1.79
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	10	1.78
(1,524)	1:214:A:SER:C	1:215:A:ALA:N	1:215:A:ALA:CA	1:215:A:ALA:C	5	1.78
(1,150)	1:5:B:LYS:C	1:6:B:GLU:N	1:6:B:GLU:CA	1:6:B:GLU:C	14	1.78
(1,550)	1:227:A:LYS:C	1:228:A:THR:N	1:228:A:THR:CA	1:228:A:THR:C	14	1.77
(1,489)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	9	1.77
(1,844)	1:315:A:MET:N	1:315:A:MET:CA	1:315:A:MET:C	1:316:A:ASN:N	20	1.76
(1,825)	1:272:A:ALA:C	1:273:A:ALA:N	1:273:A:ALA:CA	1:273:A:ALA:C	1	1.76
(1,864)	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	1:237:B:ASP:N	5	1.75
(1,503)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:THR:N	15	1.75
(1,365)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	3	1.75
(1,840)	1:313:A:ASP:N	1:313:A:ASP:CA	1:313:A:ASP:C	1:314:A:LEU:N	14	1.74
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	18	1.74
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	20	1.73
(1,841)	1:313:A:ASP:C	1:314:A:LEU:N	1:314:A:LEU:CA	1:314:A:LEU:C	7	1.73
(1,496)	1:200:A:GLU:C	1:201:A:GLY:N	1:201:A:GLY:CA	1:201:A:GLY:C	14	1.73
(1,811)	1:224:B:ASN:N	1:224:B:ASN:CA	1:224:B:ASN:C	1:225:B:LEU:N	5	1.71
(1,332)	1:117:A:ASP:N	1:117:A:ASP:CA	1:117:A:ASP:C	1:118:A:TYR:N	15	1.71
(1,304)	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	1:104:A:ASP:N	5	1.71
(1,140)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:ALA:N	12	1.7
(1,291)	1:96:A:ALA:C	1:97:A:GLU:N	1:97:A:GLU:CA	1:97:A:GLU:C	1	1.69
(1,273)	1:67:B:ASP:N	1:67:B:ASP:CA	1:67:B:ASP:C	1:68:B:ILE:N	7	1.69
(1,121)	1:61:A:LYS:C	1:62:A:GLY:N	1:62:A:GLY:CA	1:62:A:GLY:C	1	1.69
(1,512)	1:208:A:MET:C	1:209:A:LYS:N	1:209:A:LYS:CA	1:209:A:LYS:C	9	1.68
(1,4)	1:3:A:ALA:N	1:3:A:ALA:CA	1:3:A:ALA:C	1:4:A:SER:N	3	1.68
(1,549)	1:227:A:LYS:N	1:227:A:LYS:CA	1:227:A:LYS:C	1:228:A:THR:N	6	1.67
(1,863)	1:235:B:ASP:C	1:236:B:ALA:N	1:236:B:ALA:CA	1:236:B:ALA:C	15	1.66
(1,300)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:ALA:N	14	1.66
(1,118)	1:60:A:PHE:N	1:60:A:PHE:CA	1:60:A:PHE:C	1:61:A:LYS:N	6	1.66
(1,842)	1:314:A:LEU:N	1:314:A:LEU:CA	1:314:A:LEU:C	1:315:A:MET:N	2	1.65
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	14	1.65
(1,139)	1:70:A:ASN:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	13	1.63
(1,832)	1:295:A:ILE:N	1:295:A:ILE:CA	1:295:A:ILE:C	1:296:A:ARG:N	12	1.62
(1,540)	1:222:A:SER:C	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	16	1.62
(1,840)	1:313:A:ASP:N	1:313:A:ASP:CA	1:313:A:ASP:C	1:314:A:LEU:N	1	1.61
(1,675)	1:155:B:ALA:N	1:155:B:ALA:CA	1:155:B:ALA:C	1:156:B:VAL:N	4	1.61
(1,629)	1:131:B:VAL:C	1:132:B:LEU:N	1:132:B:LEU:CA	1:132:B:LEU:C	1	1.61
(1,822)	1:237:A:ASP:N	1:237:A:ASP:CA	1:237:A:ASP:C	1:238:A:VAL:N	20	1.6
(1,697)	1:166:B:ASP:N	1:166:B:ASP:CA	1:166:B:ASP:C	1:167:B:PRO:N	5	1.6
(1,537)	1:221:A:GLN:N	1:221:A:GLN:CA	1:221:A:GLN:C	1:222:A:SER:N	2	1.6
(1,537)	1:221:A:GLN:N	1:221:A:GLN:CA	1:221:A:GLN:C	1:222:A:SER:N	15	1.6
(1,366)	1:134:A:THR:C	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	13	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:ALA:N	1	1.6
(1,830)	1:294:A:SER:N	1:294:A:SER:CA	1:294:A:SER:C	1:295:A:ILE:N	18	1.58
(1,669)	1:152:B:TYR:N	1:152:B:TYR:CA	1:152:B:TYR:C	1:153:B:ASP:N	14	1.58
(1,472)	1:188:A:GLU:C	1:189:A:ALA:N	1:189:A:ALA:CA	1:189:A:ALA:C	1	1.58
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	8	1.58
(1,874)	1:294:B:SER:N	1:294:B:SER:CA	1:294:B:SER:C	1:295:B:ILE:N	19	1.55
(1,812)	1:224:B:ASN:C	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	2	1.55
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	3	1.54
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	14	1.54
(1,541)	1:223:A:LEU:N	1:223:A:LEU:CA	1:223:A:LEU:C	1:224:A:ASN:N	4	1.54
(1,350)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:GLU:N	11	1.54
(1,263)	1:62:B:GLY:N	1:62:B:GLY:CA	1:62:B:GLY:C	1:63:B:GLN:N	19	1.52
(1,229)	1:45:B:GLY:N	1:45:B:GLY:CA	1:45:B:GLY:C	1:46:B:PHE:N	15	1.52
(1,862)	1:337:A:ASP:N	1:337:A:ASP:CA	1:337:A:ASP:C	1:338:A:GLU:N	7	1.51
(1,467)	1:186:A:PRO:N	1:186:A:PRO:CA	1:186:A:PRO:C	1:187:A:GLU:N	12	1.5
(1,832)	1:295:A:ILE:N	1:295:A:ILE:CA	1:295:A:ILE:C	1:296:A:ARG:N	9	1.48
(1,845)	1:316:A:ASN:C	1:317:A:ASN:N	1:317:A:ASN:CA	1:317:A:ASN:C	6	1.47
(1,835)	1:310:A:ASN:C	1:311:A:LEU:N	1:311:A:LEU:CA	1:311:A:LEU:C	13	1.47
(1,286)	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	1:95:A:ASP:N	13	1.46
(1,844)	1:315:A:MET:N	1:315:A:MET:CA	1:315:A:MET:C	1:316:A:ASN:N	5	1.45
(1,823)	1:271:A:GLN:C	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	13	1.45
(1,629)	1:131:B:VAL:C	1:132:B:LEU:N	1:132:B:LEU:CA	1:132:B:LEU:C	20	1.45
(1,434)	1:169:A:TYR:N	1:169:A:TYR:CA	1:169:A:TYR:C	1:170:A:PHE:N	18	1.45
(1,278)	1:69:B:LEU:C	1:70:B:ASN:N	1:70:B:ASN:CA	1:70:B:ASN:C	3	1.45
(1,844)	1:315:A:MET:N	1:315:A:MET:CA	1:315:A:MET:C	1:316:A:ASN:N	14	1.44
(1,553)	1:93:B:GLU:C	1:94:B:ASP:N	1:94:B:ASP:CA	1:94:B:ASP:C	14	1.44
(1,89)	1:45:A:GLY:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	12	1.44
(1,96)	1:49:A:GLU:N	1:49:A:GLU:CA	1:49:A:GLU:C	1:50:A:ALA:N	19	1.43
(1,800)	1:218:B:LYS:C	1:219:B:VAL:N	1:219:B:VAL:CA	1:219:B:VAL:C	16	1.42
(1,124)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:HIS:N	13	1.42
(1,310)	1:106:A:LYS:N	1:106:A:LYS:CA	1:106:A:LYS:C	1:107:A:MET:N	13	1.41
(1,588)	1:111:B:LYS:N	1:111:B:LYS:CA	1:111:B:LYS:C	1:112:B:ALA:N	1	1.4
(1,550)	1:227:A:LYS:C	1:228:A:THR:N	1:228:A:THR:CA	1:228:A:THR:C	7	1.4
(1,287)	1:94:A:ASP:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	13	1.4
(1,126)	1:64:A:HIS:N	1:64:A:HIS:CA	1:64:A:HIS:C	1:65:A:LEU:N	19	1.39
(1,533)	1:219:A:VAL:N	1:219:A:VAL:CA	1:219:A:VAL:C	1:220:A:GLU:N	10	1.38
(1,46)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ILE:N	5	1.38
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:ALA:N	20	1.38
(1,883)	1:312:B:SER:C	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	17	1.37
(1,848)	1:319:A:ALA:N	1:319:A:ALA:CA	1:319:A:ALA:C	1:320:A:LEU:N	15	1.37
(1,6)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:LYS:N	7	1.37
(1,287)	1:94:A:ASP:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	5	1.36
(1,124)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:HIS:N	5	1.36
(1,855)	1:332:A:GLY:C	1:333:A:ALA:N	1:333:A:ALA:CA	1:333:A:ALA:C	20	1.35
(1,225)	1:43:B:ALA:N	1:43:B:ALA:CA	1:43:B:ALA:C	1:44:B:PHE:N	18	1.35
(1,133)	1:67:A:ASP:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	6	1.34
(1,888)	1:315:B:MET:N	1:315:B:MET:CA	1:315:B:MET:C	1:316:B:ASN:N	20	1.33
(1,850)	1:320:A:LEU:N	1:320:A:LEU:CA	1:320:A:LEU:C	1:321:A:ARG:N	7	1.33
(1,261)	1:61:B:LYS:N	1:61:B:LYS:CA	1:61:B:LYS:C	1:62:B:GLY:N	6	1.33
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	3	1.32
(1,290)	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	1:97:A:GLU:N	6	1.32

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,798)	1:217:B:LYS:C	1:218:B:LYS:N	1:218:B:LYS:CA	1:218:B:LYS:C	5	1.3
(1,636)	1:135:B:ASN:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	4	1.3
(1,361)	1:131:A:VAL:C	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	20	1.3
(1,92)	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	1:48:A:ARG:N	4	1.3
(1,852)	1:327:A:LEU:N	1:327:A:LEU:CA	1:327:A:LEU:C	1:328:A:PHE:N	4	1.29
(1,96)	1:49:A:GLU:N	1:49:A:GLU:CA	1:49:A:GLU:C	1:50:A:ALA:N	8	1.29
(1,842)	1:314:A:LEU:N	1:314:A:LEU:CA	1:314:A:LEU:C	1:315:A:MET:N	17	1.28
(1,734)	1:185:B:LYS:N	1:185:B:LYS:CA	1:185:B:LYS:C	1:186:B:PRO:N	14	1.28
(1,545)	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	1:226:A:GLU:N	18	1.28
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	15	1.26
(1,903)	1:335:B:SER:C	1:336:B:THR:N	1:336:B:THR:CA	1:336:B:THR:C	20	1.25
(1,252)	1:56:B:GLY:C	1:57:B:LYS:N	1:57:B:LYS:CA	1:57:B:LYS:C	15	1.25
(1,855)	1:332:A:GLY:C	1:333:A:ALA:N	1:333:A:ALA:CA	1:333:A:ALA:C	16	1.23
(1,364)	1:133:A:PRO:C	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	19	1.23
(1,47)	1:24:A:GLU:C	1:25:A:ILE:N	1:25:A:ILE:CA	1:25:A:ILE:C	18	1.23
(1,576)	1:105:B:LEU:N	1:105:B:LEU:CA	1:105:B:LEU:C	1:106:B:LYS:N	17	1.22
(1,244)	1:52:B:SER:C	1:53:B:GLY:N	1:53:B:GLY:CA	1:53:B:GLY:C	17	1.22
(1,1)	1:1:A:MET:C	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1	1.22
(1,855)	1:332:A:GLY:C	1:333:A:ALA:N	1:333:A:ALA:CA	1:333:A:ALA:C	14	1.21
(1,818)	1:227:B:LYS:C	1:228:B:THR:N	1:228:B:THR:CA	1:228:B:THR:C	12	1.21
(1,702)	1:169:B:TYR:N	1:169:B:TYR:CA	1:169:B:TYR:C	1:170:B:PHE:N	16	1.21
(1,330)	1:116:A:LYS:N	1:116:A:LYS:CA	1:116:A:LYS:C	1:117:A:ASP:N	20	1.21
(1,113)	1:57:A:LYS:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	2	1.21
(1,698)	1:167:B:PRO:N	1:167:B:PRO:CA	1:167:B:PRO:C	1:168:B:SER:N	11	1.2
(1,121)	1:61:A:LYS:C	1:62:A:GLY:N	1:62:A:GLY:CA	1:62:A:GLY:C	13	1.18
(1,754)	1:195:B:LYS:C	1:196:B:VAL:N	1:196:B:VAL:CA	1:196:B:VAL:C	9	1.16
(1,544)	1:224:A:ASN:C	1:225:A:LEU:N	1:225:A:LEU:CA	1:225:A:LEU:C	3	1.15
(1,824)	1:272:A:ALA:N	1:272:A:ALA:CA	1:272:A:ALA:C	1:273:A:ALA:N	8	1.14
(1,5)	1:3:A:ALA:C	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	8	1.14
(1,835)	1:310:A:ASN:C	1:311:A:LEU:N	1:311:A:LEU:CA	1:311:A:LEU:C	8	1.13
(1,538)	1:221:A:GLN:C	1:222:A:SER:N	1:222:A:SER:CA	1:222:A:SER:C	13	1.12
(1,503)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:THR:N	18	1.12
(1,287)	1:94:A:ASP:C	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	14	1.12
(1,222)	1:41:B:SER:C	1:42:B:GLU:N	1:42:B:GLU:CA	1:42:B:GLU:C	8	1.12
(1,862)	1:337:A:ASP:N	1:337:A:ASP:CA	1:337:A:ASP:C	1:338:A:GLU:N	11	1.1
(1,629)	1:131:B:VAL:C	1:132:B:LEU:N	1:132:B:LEU:CA	1:132:B:LEU:C	17	1.1
(1,884)	1:313:B:ASP:N	1:313:B:ASP:CA	1:313:B:ASP:C	1:314:B:LEU:N	8	1.08
(1,829)	1:293:A:PRO:C	1:294:A:SER:N	1:294:A:SER:CA	1:294:A:SER:C	20	1.07
(1,697)	1:166:B:ASP:N	1:166:B:ASP:CA	1:166:B:ASP:C	1:167:B:PRO:N	14	1.07
(1,862)	1:337:A:ASP:N	1:337:A:ASP:CA	1:337:A:ASP:C	1:338:A:GLU:N	6	1.06
(1,497)	1:201:A:GLY:N	1:201:A:GLY:CA	1:201:A:GLY:C	1:202:A:ASP:N	13	1.05
(1,135)	1:68:A:ILE:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	12	1.05
(1,46)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ILE:N	10	1.05
(1,838)	1:312:A:SER:N	1:312:A:SER:CA	1:312:A:SER:C	1:313:A:ASP:N	8	1.04
(1,501)	1:203:A:ASN:N	1:203:A:ASN:CA	1:203:A:ASN:C	1:204:A:ALA:N	14	1.04
(1,813)	1:225:B:LEU:N	1:225:B:LEU:CA	1:225:B:LEU:C	1:226:B:GLU:N	11	1.03
(1,467)	1:186:A:PRO:N	1:186:A:PRO:CA	1:186:A:PRO:C	1:187:A:GLU:N	7	1.03
(1,244)	1:52:B:SER:C	1:53:B:GLY:N	1:53:B:GLY:CA	1:53:B:GLY:C	11	1.03
(1,901)	1:333:B:ALA:C	1:334:B:GLN:N	1:334:B:GLN:CA	1:334:B:GLN:C	1	1.02
(1,826)	1:273:A:ALA:N	1:273:A:ALA:CA	1:273:A:ALA:C	1:274:A:GLN:N	1	1.01
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	1	1.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,539)	1:222:A:SER:N	1:222:A:SER:CA	1:222:A:SER:C	1:223:A:LEU:N	12	1.01
(1,547)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:LYS:N	13	1.0
(1,124)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:HIS:N	19	1.0