



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 12:42 AM EST

PDB ID : 2N3J
BMRB ID : 25645
Title : Solution Structure of the alpha-crystallin domain from the redox-sensitive chaperone, HSPB1
Authors : Rajagopal, P.; Liu, Y.; Shi, L.; Klevit, R.E.
Deposited on : 2015-06-03

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

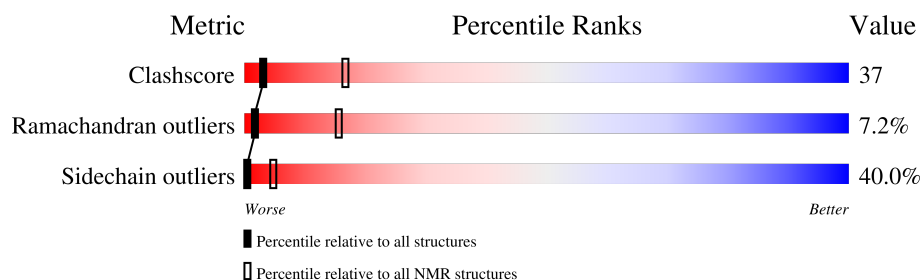
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 20%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	98	
1	B	98	

2 Ensemble composition and analysis

This entry contains 10 models. Model 7 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:94-A:127, A:132-A:170, B:94-B:169 (149)	0.77	7

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3026 atoms, of which 1498 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock protein beta-1.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1513	472	749	135	154	3	
1	B	98	Total	C	H	N	O	S	0
			1513	472	749	135	154	3	

There are 2 discrepancies between the modelled and reference sequences:

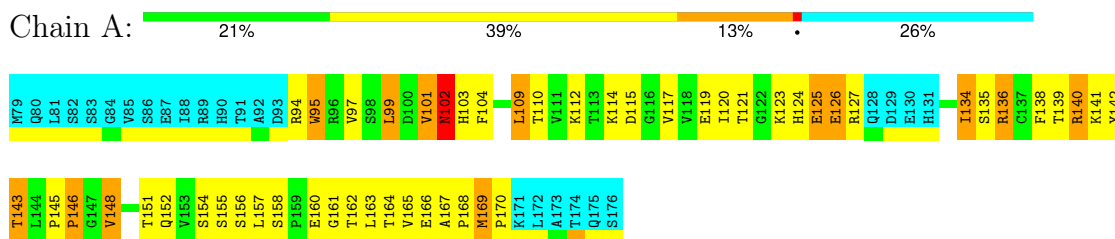
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MET	-	initiating methionine	UNP P04792
B	79	MET	-	initiating methionine	UNP P04792

4 Residue-property plots

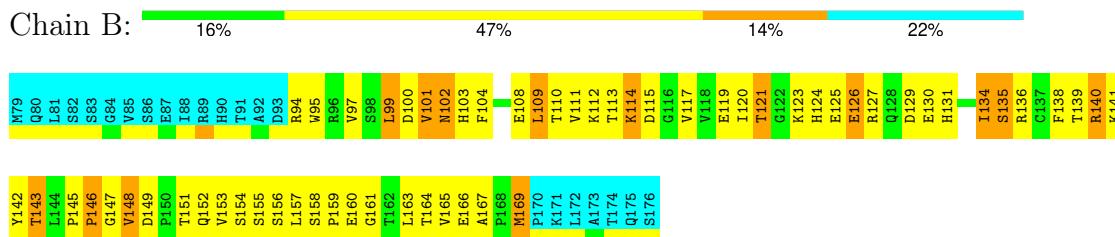
4.1 Average score per residue in the NMR ensemble

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: Heat shock protein beta-1



- Molecule 1: Heat shock protein beta-1

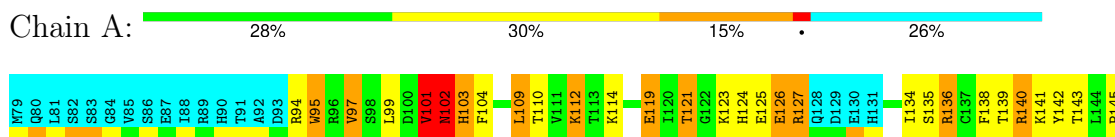


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

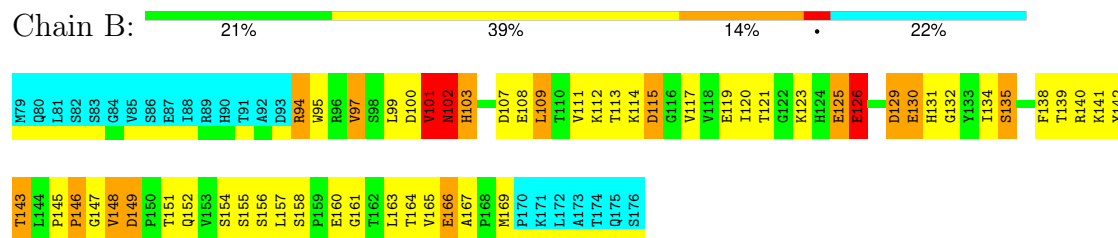
4.2.1 Score per residue for model 1

- Molecule 1: Heat shock protein beta-1



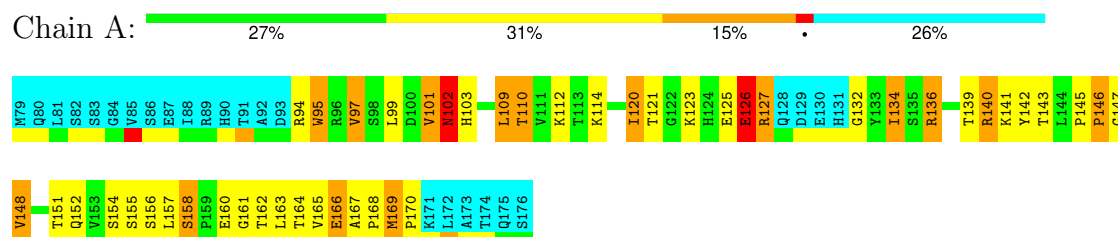


- Molecule 1: Heat shock protein beta-1

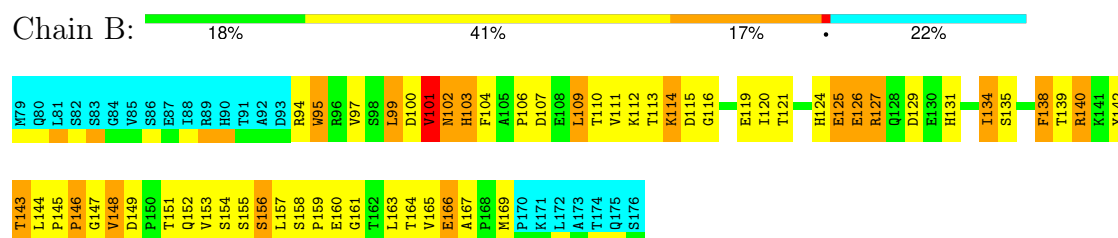


4.2.2 Score per residue for model 2

- Molecule 1: Heat shock protein beta-1

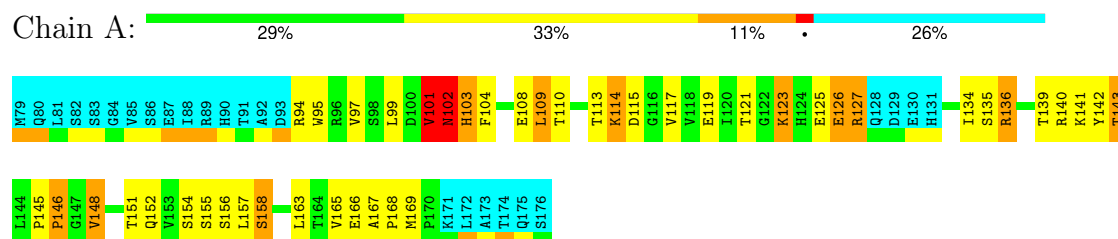


- Molecule 1: Heat shock protein beta-1

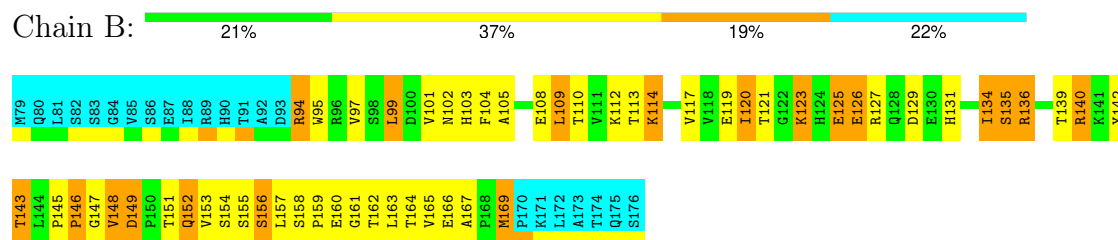


4.2.3 Score per residue for model 3

- Molecule 1: Heat shock protein beta-1

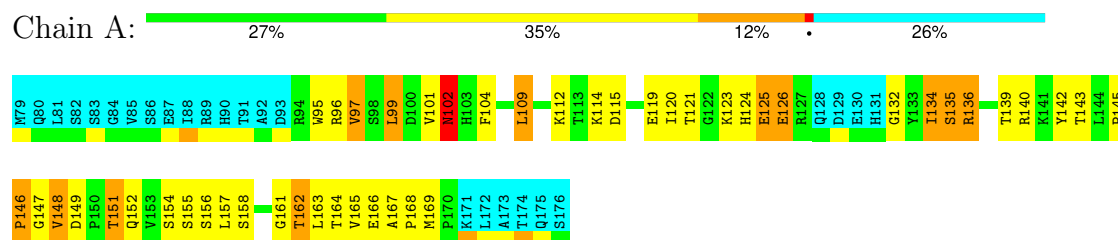


- Molecule 1: Heat shock protein beta-1

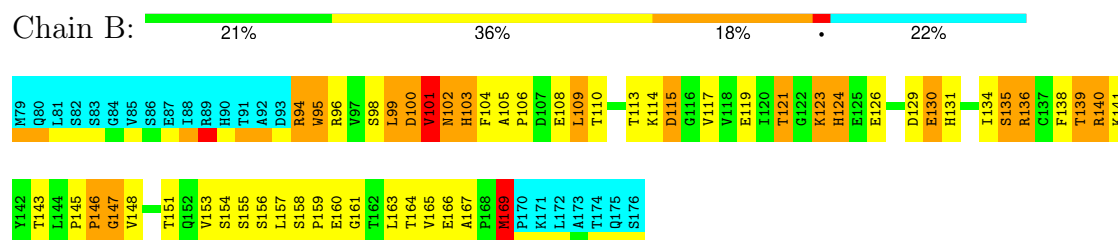


4.2.4 Score per residue for model 4

- Molecule 1: Heat shock protein beta-1

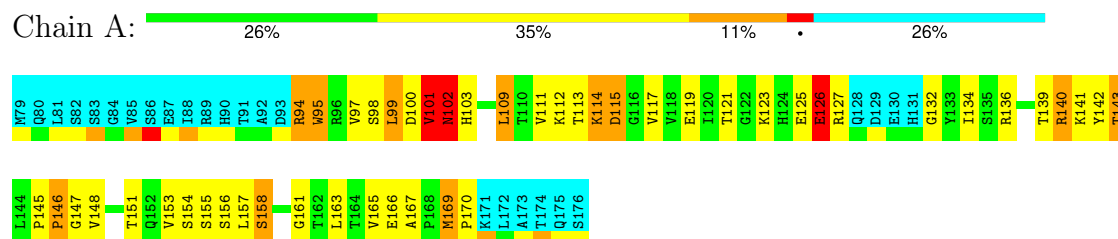


- Molecule 1: Heat shock protein beta-1

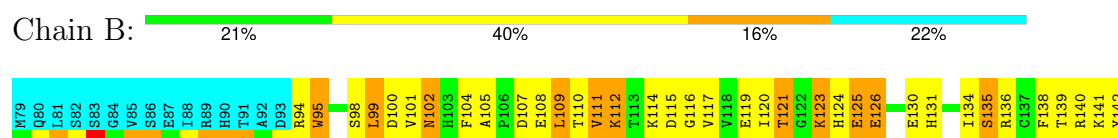


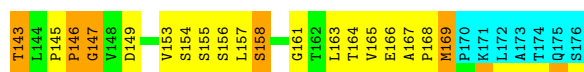
4.2.5 Score per residue for model 5

- Molecule 1: Heat shock protein beta-1



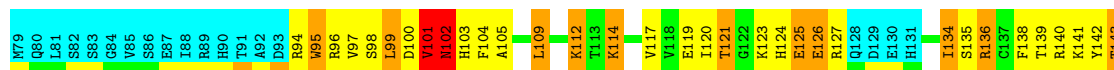
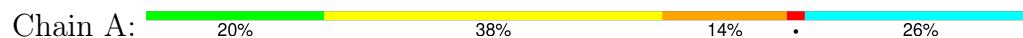
- Molecule 1: Heat shock protein beta-1



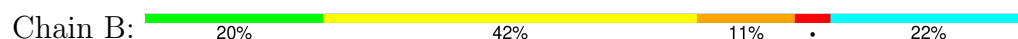


4.2.6 Score per residue for model 6

- Molecule 1: Heat shock protein beta-1

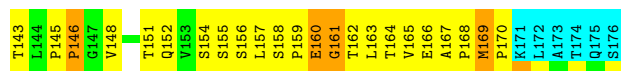
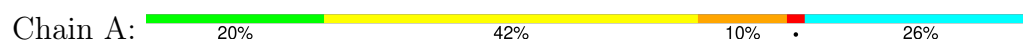


- Molecule 1: Heat shock protein beta-1

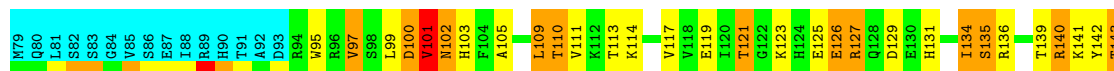
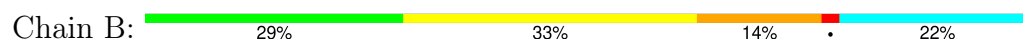


4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Heat shock protein beta-1

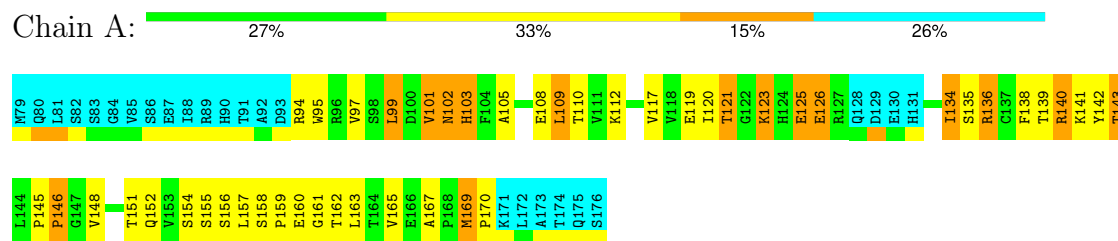


- Molecule 1: Heat shock protein beta-1

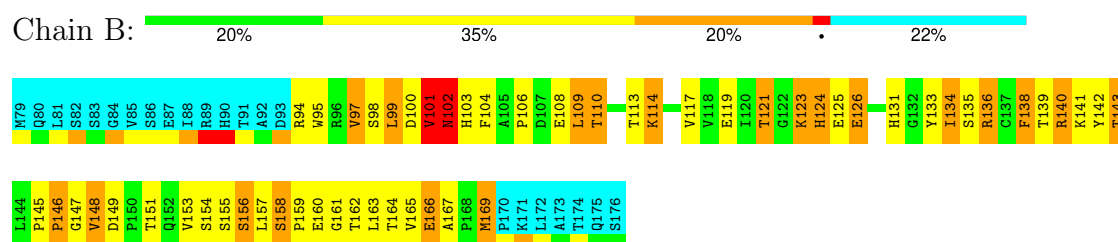


4.2.8 Score per residue for model 8

- Molecule 1: Heat shock protein beta-1

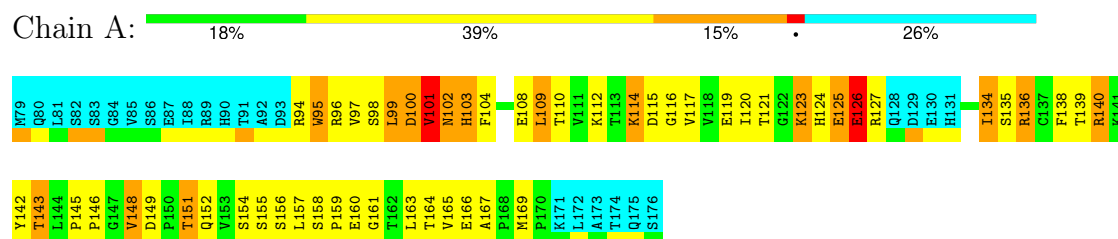


- Molecule 1: Heat shock protein beta-1

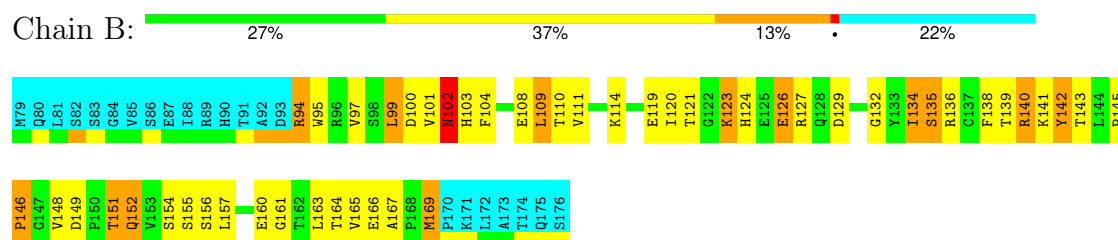


4.2.9 Score per residue for model 9

- Molecule 1: Heat shock protein beta-1

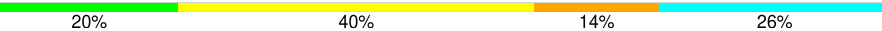


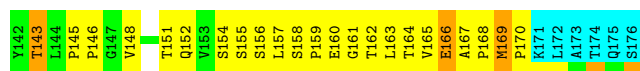
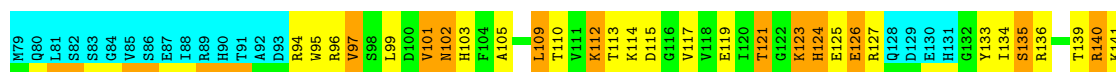
- Molecule 1: Heat shock protein beta-1




4.2.10 Score per residue for model 10

- Molecule 1: Heat shock protein beta-1

Chain A: 



● Molecule 1: Heat shock protein beta-1

Chain B: 



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CS-ROSETTA	structure solution	
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	490
Number of shifts mapped to atoms	490
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	20%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	571	565	565	43±7
1	B	600	583	583	47±6
All	All	11710	11480	11480	869

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:117:VAL:HG22	1:B:143:THR:HG23	0.85	1.47	4	6
1:A:102:ASN:HB3	1:A:109:LEU:HD13	0.79	1.53	1	4
1:B:99:LEU:HD22	1:B:120:ILE:HG12	0.79	1.52	6	3
1:B:102:ASN:HB3	1:B:109:LEU:HD13	0.76	1.57	1	4
1:B:109:LEU:HD22	1:B:157:LEU:HD22	0.74	1.59	8	9
1:A:99:LEU:HD23	1:A:140:ARG:NE	0.74	1.97	7	2
1:B:102:ASN:CB	1:B:109:LEU:HD13	0.73	2.14	5	8
1:A:102:ASN:HB2	1:A:109:LEU:HD13	0.71	1.61	9	2
1:A:109:LEU:HD22	1:A:157:LEU:HD22	0.70	1.61	2	10
1:A:99:LEU:HD22	1:A:120:ILE:HG13	0.69	1.62	2	1
1:B:102:ASN:HB2	1:B:109:LEU:HD13	0.69	1.63	2	3
1:A:127:ARG:CZ	1:A:127:ARG:HB3	0.69	2.16	2	3
1:B:99:LEU:HD22	1:B:120:ILE:HG13	0.68	1.65	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:VAL:HG22	1:A:143:THR:HG23	0.68	1.66	8	4
1:A:140:ARG:NH2	1:A:142:TYR:CD1	0.68	2.62	8	1
1:B:95:TRP:NE1	1:B:97:VAL:HG22	0.67	2.04	1	2
1:A:152:GLN:O	1:A:167:ALA:HB1	0.67	1.89	2	8
1:A:140:ARG:NH2	1:A:142:TYR:CE1	0.67	2.62	8	1
1:B:102:ASN:ND2	1:B:102:ASN:H	0.66	1.88	9	2
1:A:101:VAL:HG11	1:A:138:PHE:CD2	0.65	2.27	7	3
1:A:148:VAL:HA	1:A:169:MET:SD	0.65	2.31	3	2
1:B:102:ASN:OD1	1:B:157:LEU:HD11	0.65	1.91	5	3
1:A:95:TRP:CZ3	1:A:97:VAL:HG21	0.64	2.27	9	4
1:A:119:GLU:CD	1:A:141:LYS:NZ	0.64	2.51	1	2
1:A:127:ARG:CZ	1:A:127:ARG:CB	0.63	2.76	2	2
1:B:109:LEU:CD2	1:B:157:LEU:HD22	0.63	2.23	8	4
1:B:102:ASN:OD1	1:B:109:LEU:HD13	0.63	1.92	6	3
1:A:102:ASN:CB	1:A:109:LEU:HD13	0.63	2.24	1	7
1:A:109:LEU:CD2	1:A:157:LEU:HD22	0.62	2.25	7	5
1:A:102:ASN:ND2	1:A:102:ASN:H	0.62	1.92	1	2
1:A:167:ALA:HB3	1:A:169:MET:HE3	0.61	1.70	3	1
1:B:95:TRP:HB2	1:B:169:MET:SD	0.61	2.35	4	3
1:B:124:HIS:H	1:B:124:HIS:CD2	0.61	2.13	8	1
1:B:114:LYS:O	1:B:116:GLY:N	0.61	2.33	5	3
1:B:102:ASN:OD1	1:B:161:GLY:HA2	0.61	1.95	5	3
1:B:169:MET:SD	1:B:169:MET:N	0.60	2.74	7	2
1:A:99:LEU:HD22	1:A:120:ILE:HG12	0.60	1.73	7	4
1:A:166:GLU:O	1:A:167:ALA:HB2	0.60	1.95	1	7
1:A:102:ASN:OD1	1:A:109:LEU:HD13	0.60	1.96	7	6
1:A:119:GLU:CD	1:A:141:LYS:HZ2	0.60	2.00	7	1
1:A:142:TYR:CE1	1:B:132:GLY:HA3	0.60	2.32	9	2
1:A:99:LEU:HD22	1:A:120:ILE:CG1	0.60	2.27	4	3
1:B:102:ASN:ND2	1:B:102:ASN:N	0.59	2.48	9	2
1:B:140:ARG:NH1	1:B:142:TYR:OH	0.59	2.30	8	1
1:B:102:ASN:ND2	1:B:161:GLY:O	0.59	2.35	9	4
1:B:114:LYS:O	1:B:117:VAL:N	0.59	2.34	5	3
1:B:99:LEU:HD22	1:B:120:ILE:CG1	0.59	2.28	2	4
1:A:95:TRP:NE1	1:A:97:VAL:CG2	0.59	2.65	7	2
1:B:152:GLN:O	1:B:167:ALA:HB1	0.59	1.96	9	3
1:A:95:TRP:NE1	1:A:97:VAL:HG22	0.59	2.13	10	2
1:A:134:ILE:O	1:A:136:ARG:NH2	0.59	2.35	4	1
1:B:130:GLU:N	1:B:130:GLU:CD	0.59	2.56	10	1
1:B:99:LEU:HD23	1:B:140:ARG:NE	0.58	2.12	4	1
1:B:163:LEU:C	1:B:163:LEU:HD13	0.58	2.18	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:158:SER:O	1:A:161:GLY:N	0.58	2.36	4	2
1:B:99:LEU:HD23	1:B:140:ARG:HH11	0.58	1.59	8	1
1:B:99:LEU:HD21	1:B:142:TYR:CE1	0.58	2.33	9	1
1:A:140:ARG:NH2	1:A:142:TYR:OH	0.58	2.34	7	4
1:B:145:PRO:O	1:B:147:GLY:N	0.58	2.37	10	9
1:A:134:ILE:HD12	1:B:140:ARG:NH1	0.58	2.14	2	1
1:A:102:ASN:ND2	1:A:102:ASN:N	0.58	2.50	1	2
1:A:132:GLY:HA3	1:B:142:TYR:CE1	0.58	2.33	2	1
1:A:114:LYS:O	1:A:116:GLY:N	0.58	2.36	9	1
1:B:102:ASN:ND2	1:B:105:ALA:O	0.58	2.34	3	2
1:A:145:PRO:CD	1:A:146:PRO:HD3	0.57	2.29	1	10
1:A:102:ASN:O	1:A:102:ASN:ND2	0.57	2.34	9	3
1:A:99:LEU:HD23	1:A:140:ARG:HE	0.57	1.60	7	1
1:B:102:ASN:OD1	1:B:109:LEU:CD1	0.57	2.52	6	2
1:A:95:TRP:CH2	1:A:148:VAL:HG21	0.57	2.35	2	3
1:A:112:LYS:NZ	1:A:119:GLU:HB2	0.57	2.14	9	1
1:A:165:VAL:O	1:A:165:VAL:HG23	0.57	1.99	7	10
1:A:140:ARG:NE	1:A:142:TYR:OH	0.57	2.35	4	1
1:A:127:ARG:CB	1:A:127:ARG:NH1	0.57	2.68	2	2
1:A:145:PRO:HD2	1:A:146:PRO:CD	0.57	2.30	6	1
1:A:95:TRP:CB	1:A:169:MET:SD	0.57	2.93	5	1
1:A:102:ASN:ND2	1:A:161:GLY:O	0.56	2.37	1	5
1:B:102:ASN:O	1:B:102:ASN:ND2	0.56	2.37	2	3
1:B:145:PRO:HD2	1:B:146:PRO:CD	0.56	2.30	5	7
1:B:108:GLU:OE1	1:B:123:LYS:NZ	0.56	2.37	3	4
1:A:102:ASN:OD1	1:A:161:GLY:HA2	0.56	2.00	8	2
1:B:145:PRO:N	1:B:146:PRO:CD	0.56	2.68	1	9
1:A:140:ARG:NH1	1:A:142:TYR:OH	0.56	2.34	2	2
1:A:125:GLU:O	1:A:126:GLU:C	0.56	2.44	10	8
1:A:158:SER:HB2	1:A:162:THR:HG22	0.56	1.77	4	1
1:B:95:TRP:NE1	1:B:97:VAL:CG2	0.56	2.68	8	2
1:A:102:ASN:OD1	1:A:109:LEU:HD22	0.56	1.99	6	2
1:A:145:PRO:HD2	1:A:146:PRO:HD3	0.56	1.78	9	10
1:A:102:ASN:OD1	1:A:157:LEU:HD11	0.56	1.99	8	2
1:A:163:LEU:C	1:A:163:LEU:HD13	0.56	2.22	2	10
1:A:140:ARG:NH1	1:B:133:TYR:O	0.55	2.29	8	1
1:B:145:PRO:N	1:B:146:PRO:HD2	0.55	2.16	2	8
1:A:134:ILE:HD13	1:A:136:ARG:NH2	0.55	2.16	6	2
1:B:125:GLU:O	1:B:126:GLU:C	0.55	2.45	7	8
1:A:95:TRP:CZ2	1:A:148:VAL:CG2	0.55	2.89	1	2
1:A:99:LEU:CD2	1:A:140:ARG:HB3	0.55	2.31	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:127:ARG:HB2	1:B:127:ARG:NH1	0.55	2.17	7	1
1:A:108:GLU:OE1	1:A:123:LYS:NZ	0.54	2.38	3	1
1:B:126:GLU:HA	1:B:135:SER:OG	0.54	2.02	1	6
1:B:99:LEU:O	1:B:140:ARG:NH2	0.54	2.32	3	2
1:A:112:LYS:NZ	1:A:119:GLU:CB	0.54	2.70	9	2
1:A:114:LYS:O	1:A:117:VAL:HG23	0.54	2.03	5	3
1:B:102:ASN:OD1	1:B:157:LEU:CD1	0.54	2.55	5	1
1:B:95:TRP:CZ3	1:B:97:VAL:HG21	0.54	2.38	6	1
1:B:165:VAL:O	1:B:165:VAL:HG23	0.54	2.03	4	10
1:B:108:GLU:CD	1:B:123:LYS:NZ	0.54	2.61	5	2
1:A:124:HIS:ND1	1:A:125:GLU:N	0.54	2.56	6	1
1:B:145:PRO:CD	1:B:146:PRO:CD	0.54	2.85	5	6
1:A:102:ASN:HD22	1:A:102:ASN:H	0.54	1.46	3	1
1:B:114:LYS:CB	1:B:114:LYS:NZ	0.54	2.71	8	1
1:A:95:TRP:C	1:A:95:TRP:CD1	0.53	2.81	1	1
1:B:149:ASP:O	1:B:153:VAL:HG23	0.53	2.03	7	6
1:A:142:TYR:CZ	1:B:131:HIS:O	0.53	2.61	2	6
1:B:102:ASN:C	1:B:102:ASN:ND2	0.53	2.62	10	1
1:A:100:ASP:C	1:A:101:VAL:HG22	0.53	2.23	9	3
1:B:148:VAL:CG1	1:B:148:VAL:O	0.53	2.56	10	4
1:A:142:TYR:CE1	1:B:131:HIS:O	0.53	2.61	8	2
1:A:102:ASN:OD1	1:A:109:LEU:CD1	0.53	2.56	7	3
1:B:102:ASN:C	1:B:102:ASN:HD22	0.53	2.07	10	2
1:B:145:PRO:CD	1:B:146:PRO:HD3	0.53	2.34	9	4
1:A:95:TRP:HB3	1:A:169:MET:SD	0.53	2.43	10	1
1:B:136:ARG:HD3	1:B:138:PHE:CE1	0.53	2.39	8	1
1:A:102:ASN:O	1:A:105:ALA:N	0.52	2.40	6	2
1:A:141:LYS:NZ	1:B:126:GLU:OE1	0.52	2.42	2	2
1:B:119:GLU:HG2	1:B:141:LYS:HA	0.52	1.82	6	2
1:A:134:ILE:CD1	1:A:136:ARG:NH2	0.52	2.72	6	1
1:B:129:ASP:CG	1:B:130:GLU:N	0.52	2.62	10	4
1:B:96:ARG:NH1	1:B:96:ARG:HB2	0.52	2.19	4	1
1:A:101:VAL:HG11	1:A:138:PHE:CD1	0.52	2.40	1	1
1:B:156:SER:O	1:B:163:LEU:HD22	0.52	2.04	3	4
1:A:127:ARG:NH1	1:A:127:ARG:HB2	0.52	2.19	2	2
1:B:104:PHE:HB2	1:B:124:HIS:CE1	0.52	2.40	2	1
1:B:108:GLU:OE2	1:B:123:LYS:NZ	0.52	2.41	4	4
1:A:112:LYS:NZ	1:A:121:THR:OG1	0.52	2.35	10	4
1:A:101:VAL:O	1:A:103:HIS:N	0.52	2.42	7	5
1:B:94:ARG:NH1	1:B:166:GLU:OE1	0.52	2.42	2	3
1:A:95:TRP:CH2	1:A:148:VAL:CG2	0.52	2.93	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:124:HIS:O	1:B:135:SER:CB	0.52	2.58	4	1
1:B:127:ARG:CB	1:B:127:ARG:CZ	0.52	2.88	7	1
1:B:153:VAL:HA	1:B:167:ALA:HB2	0.51	1.82	10	5
1:A:114:LYS:O	1:A:117:VAL:N	0.51	2.34	5	1
1:A:102:ASN:HD22	1:A:102:ASN:C	0.51	2.08	6	1
1:B:142:TYR:CD1	1:B:142:TYR:N	0.51	2.78	9	5
1:A:102:ASN:CG	1:A:109:LEU:HD13	0.51	2.25	5	5
1:B:140:ARG:HB3	1:B:140:ARG:CZ	0.51	2.34	8	1
1:B:102:ASN:N	1:B:102:ASN:HD22	0.51	2.03	1	2
1:B:102:ASN:CG	1:B:109:LEU:HD13	0.51	2.25	6	3
1:A:158:SER:HB3	1:A:162:THR:OG1	0.51	2.05	2	1
1:A:159:PRO:C	1:A:161:GLY:H	0.51	2.09	9	4
1:B:145:PRO:HD2	1:B:146:PRO:HD3	0.51	1.83	9	6
1:A:127:ARG:N	1:A:135:SER:OG	0.51	2.44	6	1
1:B:101:VAL:C	1:B:103:HIS:H	0.51	2.08	6	3
1:B:143:THR:O	1:B:145:PRO:HD3	0.51	2.05	1	8
1:B:102:ASN:ND2	1:B:102:ASN:C	0.51	2.64	2	1
1:B:153:VAL:HG22	1:B:167:ALA:CB	0.51	2.36	4	5
1:A:167:ALA:HB1	1:A:168:PRO:HD2	0.50	1.83	1	7
1:A:114:LYS:NZ	1:A:119:GLU:OE1	0.50	2.42	5	2
1:B:102:ASN:O	1:B:104:PHE:N	0.50	2.44	3	1
1:A:140:ARG:NH2	1:A:141:LYS:C	0.50	2.65	8	1
1:A:95:TRP:HB2	1:A:169:MET:SD	0.50	2.46	5	1
1:A:126:GLU:OE1	1:B:141:LYS:NZ	0.50	2.43	7	3
1:B:159:PRO:C	1:B:161:GLY:H	0.50	2.09	2	6
1:B:134:ILE:O	1:B:136:ARG:NH2	0.50	2.36	3	1
1:A:142:TYR:OH	1:B:131:HIS:O	0.50	2.26	7	1
1:A:167:ALA:HB3	1:A:169:MET:SD	0.50	2.47	8	1
1:A:140:ARG:HA	1:A:140:ARG:NH1	0.50	2.22	10	1
1:B:100:ASP:C	1:B:101:VAL:HG22	0.50	2.26	1	6
1:B:114:LYS:NZ	1:B:119:GLU:OE2	0.50	2.45	3	6
1:B:168:PRO:C	1:B:169:MET:HG3	0.50	2.28	6	1
1:A:101:VAL:HA	1:A:103:HIS:CE1	0.50	2.42	9	2
1:A:165:VAL:O	1:A:165:VAL:CG2	0.49	2.59	4	9
1:B:101:VAL:O	1:B:103:HIS:N	0.49	2.45	6	2
1:B:149:ASP:O	1:B:153:VAL:CG2	0.49	2.60	7	4
1:A:108:GLU:OE2	1:A:123:LYS:NZ	0.49	2.42	8	2
1:B:127:ARG:NH1	1:B:135:SER:HA	0.49	2.22	9	1
1:A:119:GLU:CD	1:A:141:LYS:HD3	0.49	2.27	10	1
1:A:157:LEU:HD12	1:A:158:SER:N	0.49	2.22	3	1
1:B:140:ARG:NH2	1:B:142:TYR:OH	0.49	2.37	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:114:LYS:NZ	1:B:115:ASP:OD1	0.49	2.45	4	1
1:A:104:PHE:O	1:A:124:HIS:ND1	0.49	2.34	1	2
1:A:101:VAL:HG11	1:A:138:PHE:CE2	0.49	2.42	7	1
1:A:95:TRP:CH2	1:A:97:VAL:HG21	0.49	2.42	1	1
1:A:169:MET:CB	1:A:170:PRO:CD	0.49	2.91	7	1
1:B:102:ASN:O	1:B:105:ALA:N	0.49	2.39	7	3
1:A:153:VAL:HA	1:A:167:ALA:HB2	0.49	1.84	5	1
1:A:101:VAL:HG21	1:A:138:PHE:CD2	0.49	2.43	8	1
1:A:103:HIS:N	1:A:161:GLY:HA3	0.49	2.23	10	2
1:A:102:ASN:ND2	1:A:161:GLY:C	0.49	2.66	1	2
1:B:101:VAL:CG2	1:B:140:ARG:CZ	0.49	2.91	4	1
1:A:101:VAL:CG1	1:A:138:PHE:CD2	0.49	2.96	9	2
1:A:145:PRO:CD	1:A:146:PRO:CD	0.48	2.90	6	1
1:B:94:ARG:NH2	1:B:166:GLU:OE2	0.48	2.40	8	1
1:A:142:TYR:CD1	1:A:142:TYR:N	0.48	2.80	1	3
1:A:95:TRP:CD1	1:A:95:TRP:C	0.48	2.86	9	3
1:A:95:TRP:CG	1:A:96:ARG:N	0.48	2.81	10	1
1:A:102:ASN:N	1:A:102:ASN:HD22	0.48	2.06	5	2
1:A:145:PRO:CB	1:A:146:PRO:HD3	0.48	2.39	1	9
1:B:100:ASP:O	1:B:101:VAL:HG22	0.48	2.08	4	1
1:B:158:SER:O	1:B:161:GLY:N	0.48	2.45	10	3
1:B:119:GLU:C	1:B:120:ILE:HD13	0.48	2.28	6	1
1:A:134:ILE:HD13	1:A:136:ARG:HH21	0.48	1.69	4	1
1:B:107:ASP:OD1	1:B:107:ASP:N	0.48	2.46	6	1
1:A:166:GLU:O	1:A:167:ALA:CB	0.48	2.62	1	3
1:A:136:ARG:NH1	1:B:138:PHE:CZ	0.48	2.82	2	1
1:B:128:GLN:HG2	1:B:129:ASP:N	0.48	2.24	6	1
1:B:104:PHE:O	1:B:136:ARG:NH2	0.48	2.43	10	1
1:B:114:LYS:NZ	1:B:119:GLU:OE1	0.48	2.41	10	1
1:A:101:VAL:C	1:A:103:HIS:H	0.48	2.11	7	3
1:B:115:ASP:O	1:B:115:ASP:CG	0.48	2.50	4	1
1:A:115:ASP:O	1:A:115:ASP:CG	0.47	2.50	5	1
1:A:126:GLU:OE2	1:B:141:LYS:NZ	0.47	2.42	10	4
1:B:163:LEU:C	1:B:163:LEU:CD1	0.47	2.83	1	9
1:B:136:ARG:CZ	1:B:138:PHE:CZ	0.47	2.97	4	1
1:B:124:HIS:ND1	1:B:126:GLU:O	0.47	2.43	9	1
1:B:145:PRO:C	1:B:147:GLY:N	0.47	2.67	7	6
1:B:95:TRP:CB	1:B:169:MET:SD	0.47	3.02	4	2
1:B:148:VAL:O	1:B:148:VAL:CG1	0.47	2.63	7	2
1:B:166:GLU:O	1:B:167:ALA:HB2	0.47	2.10	1	1
1:B:134:ILE:O	1:B:134:ILE:HG23	0.47	2.09	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:ASN:ND2	1:B:102:ASN:O	0.47	2.47	10	2
1:A:153:VAL:HG22	1:A:167:ALA:CB	0.47	2.40	5	1
1:B:168:PRO:O	1:B:169:MET:O	0.47	2.33	6	1
1:B:109:LEU:HD22	1:B:157:LEU:CD2	0.47	2.36	8	1
1:B:101:VAL:N	1:B:103:HIS:CE1	0.47	2.83	1	1
1:B:165:VAL:O	1:B:165:VAL:CG2	0.47	2.63	1	9
1:B:94:ARG:HH12	1:B:166:GLU:CD	0.47	2.14	1	1
1:B:102:ASN:CG	1:B:161:GLY:HA2	0.47	2.30	5	3
1:A:100:ASP:OD1	1:A:140:ARG:NH2	0.47	2.44	6	1
1:B:127:ARG:NH2	1:B:136:ARG:O	0.47	2.47	9	1
1:B:107:ASP:C	1:B:109:LEU:H	0.46	2.14	2	1
1:A:117:VAL:HG13	1:A:143:THR:HG23	0.46	1.86	9	2
1:A:134:ILE:HD11	1:A:136:ARG:HH11	0.46	1.68	8	1
1:B:124:HIS:CD2	1:B:136:ARG:H	0.46	2.27	8	1
1:A:124:HIS:ND1	1:A:127:ARG:HG2	0.46	2.26	9	2
1:B:102:ASN:HD21	1:B:105:ALA:C	0.46	2.12	3	1
1:A:99:LEU:HD22	1:A:120:ILE:HB	0.46	1.86	8	1
1:B:119:GLU:O	1:B:120:ILE:HD12	0.46	2.11	9	2
1:B:109:LEU:HD11	1:B:120:ILE:HG23	0.46	1.88	1	1
1:B:100:ASP:C	1:B:101:VAL:CG2	0.46	2.84	4	1
1:A:117:VAL:HG22	1:A:143:THR:CG2	0.46	2.41	10	1
1:A:140:ARG:CZ	1:A:142:TYR:CZ	0.46	2.99	8	1
1:A:123:LYS:O	1:A:123:LYS:NZ	0.46	2.35	9	2
1:B:124:HIS:CD2	1:B:127:ARG:CZ	0.46	2.99	10	1
1:A:95:TRP:CZ3	1:A:97:VAL:CG2	0.46	2.99	2	3
1:A:109:LEU:HD22	1:A:157:LEU:CD2	0.46	2.35	2	3
1:B:123:LYS:NZ	1:B:123:LYS:O	0.46	2.32	8	2
1:B:145:PRO:CB	1:B:146:PRO:HD3	0.46	2.41	9	1
1:B:95:TRP:CD1	1:B:97:VAL:HG22	0.46	2.46	1	1
1:A:94:ARG:NH1	1:A:166:GLU:OE1	0.45	2.49	9	2
1:B:95:TRP:CD1	1:B:95:TRP:C	0.45	2.90	6	1
1:B:149:ASP:OD1	1:B:152:GLN:N	0.45	2.45	2	1
1:B:108:GLU:CD	1:B:123:LYS:HZ3	0.45	2.15	5	1
1:B:112:LYS:NZ	1:B:121:THR:OG1	0.45	2.40	10	2
1:B:134:ILE:HD11	1:B:136:ARG:NH2	0.45	2.25	7	1
1:A:102:ASN:CB	1:A:109:LEU:CD1	0.45	2.94	10	1
1:B:124:HIS:O	1:B:135:SER:HB3	0.45	2.11	4	2
1:B:112:LYS:NZ	1:B:119:GLU:HB2	0.45	2.25	1	1
1:A:162:THR:O	1:A:162:THR:CG2	0.45	2.65	4	1
1:A:108:GLU:N	1:A:108:GLU:CD	0.45	2.69	7	1
1:A:95:TRP:HE1	1:A:97:VAL:HG22	0.45	1.71	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:ASN:ND2	1:B:161:GLY:CA	0.45	2.79	1	2
1:B:111:VAL:HG13	1:B:120:ILE:CD1	0.45	2.42	2	1
1:B:109:LEU:HA	1:B:121:THR:O	0.45	2.11	8	2
1:B:102:ASN:HB3	1:B:109:LEU:CD1	0.45	2.41	7	1
1:A:169:MET:SD	1:A:169:MET:N	0.45	2.90	1	1
1:A:125:GLU:O	1:A:126:GLU:HB2	0.45	2.12	9	2
1:A:126:GLU:HA	1:A:135:SER:OG	0.45	2.12	4	4
1:B:109:LEU:HG	1:B:110:THR:N	0.45	2.27	6	2
1:A:119:GLU:HA	1:A:140:ARG:O	0.45	2.12	8	1
1:B:124:HIS:NE2	1:B:136:ARG:HG3	0.45	2.27	8	1
1:B:98:SER:HA	1:B:163:LEU:O	0.45	2.11	8	3
1:A:125:GLU:O	1:A:127:ARG:N	0.45	2.50	3	1
1:B:119:GLU:O	1:B:120:ILE:HD13	0.45	2.12	6	1
1:B:157:LEU:HD12	1:B:158:SER:N	0.45	2.27	1	1
1:A:99:LEU:HD23	1:A:140:ARG:HG3	0.45	1.89	2	1
1:B:104:PHE:O	1:B:124:HIS:ND1	0.45	2.34	5	2
1:B:111:VAL:HG13	1:B:120:ILE:HD12	0.44	1.89	5	1
1:B:103:HIS:N	1:B:161:GLY:HA3	0.44	2.28	7	2
1:A:162:THR:HG23	1:A:162:THR:O	0.44	2.12	10	2
1:A:169:MET:HB3	1:A:170:PRO:HD2	0.44	1.90	8	1
1:A:163:LEU:C	1:A:163:LEU:CD1	0.44	2.85	4	7
1:A:114:LYS:NZ	1:A:119:GLU:OE2	0.44	2.49	7	1
1:A:136:ARG:NH1	1:B:138:PHE:CE2	0.44	2.85	9	1
1:B:102:ASN:ND2	1:B:161:GLY:C	0.44	2.70	9	1
1:A:141:LYS:NZ	1:B:126:GLU:OE2	0.44	2.42	3	1
1:A:149:ASP:OD1	1:A:151:THR:N	0.44	2.51	9	2
1:B:99:LEU:CD2	1:B:140:ARG:HB2	0.44	2.42	4	1
1:B:102:ASN:C	1:B:104:PHE:N	0.44	2.69	5	2
1:A:102:ASN:ND2	1:A:105:ALA:O	0.44	2.45	8	3
1:B:147:GLY:O	1:B:149:ASP:N	0.44	2.51	10	1
1:A:141:LYS:HB2	1:A:141:LYS:HZ3	0.44	1.73	6	1
1:B:95:TRP:CE2	1:B:97:VAL:HG22	0.44	2.47	8	1
1:A:114:LYS:HB3	1:A:117:VAL:HB	0.44	1.89	6	4
1:A:143:THR:O	1:A:145:PRO:HD3	0.44	2.12	6	2
1:B:99:LEU:HD23	1:B:140:ARG:NH1	0.44	2.28	8	1
1:A:112:LYS:HZ3	1:A:119:GLU:HB2	0.44	1.69	9	1
1:B:149:ASP:OD1	1:B:151:THR:N	0.44	2.48	9	1
1:A:109:LEU:HG	1:A:110:THR:N	0.43	2.27	2	1
1:A:140:ARG:NH2	1:A:141:LYS:O	0.43	2.46	8	1
1:A:140:ARG:CZ	1:A:140:ARG:HB3	0.43	2.43	2	1
1:B:149:ASP:OD1	1:B:149:ASP:N	0.43	2.49	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:TRP:CZ2	1:A:165:VAL:HG23	0.43	2.49	2	1
1:A:102:ASN:OD1	1:A:161:GLY:CA	0.43	2.67	8	2
1:A:167:ALA:HB3	1:A:169:MET:CE	0.43	2.42	3	1
1:B:104:PHE:CE2	1:B:136:ARG:NH2	0.43	2.86	8	1
1:A:140:ARG:NH2	1:B:131:HIS:ND1	0.43	2.66	4	1
1:B:104:PHE:CD2	1:B:136:ARG:NH2	0.43	2.86	8	1
1:A:96:ARG:CZ	1:A:96:ARG:HB3	0.43	2.44	9	1
1:A:102:ASN:HB3	1:A:109:LEU:CD1	0.43	2.43	10	1
1:A:101:VAL:C	1:A:103:HIS:N	0.43	2.70	6	1
1:A:102:ASN:ND2	1:A:102:ASN:O	0.43	2.51	8	1
1:A:140:ARG:NH2	1:A:141:LYS:N	0.43	2.66	8	1
1:A:140:ARG:CZ	1:A:142:TYR:CE1	0.43	3.01	8	1
1:B:140:ARG:CZ	1:B:140:ARG:CB	0.43	2.97	8	1
1:A:100:ASP:O	1:A:101:VAL:HG22	0.43	2.14	9	1
1:B:102:ASN:OD1	1:B:157:LEU:HD13	0.43	2.13	9	2
1:B:103:HIS:ND1	1:B:103:HIS:N	0.43	2.67	4	1
1:B:134:ILE:HD11	1:B:136:ARG:NH1	0.43	2.29	9	1
1:A:141:LYS:NZ	1:A:141:LYS:HB2	0.43	2.28	1	1
1:A:102:ASN:ND2	1:A:102:ASN:C	0.43	2.73	6	1
1:B:104:PHE:HB3	1:B:136:ARG:CZ	0.43	2.44	10	1
1:A:134:ILE:HA	1:B:139:THR:O	0.42	2.13	4	1
1:A:94:ARG:NH2	1:A:166:GLU:OE2	0.42	2.44	2	1
1:B:117:VAL:HG13	1:B:143:THR:HG23	0.42	1.89	5	1
1:B:119:GLU:HG2	1:B:141:LYS:CB	0.42	2.45	4	1
1:A:95:TRP:O	1:A:166:GLU:HA	0.42	2.13	7	1
1:B:136:ARG:O	1:B:136:ARG:NE	0.42	2.48	10	1
1:A:149:ASP:OD2	1:A:152:GLN:N	0.42	2.45	1	1
1:B:160:GLU:H	1:B:160:GLU:CD	0.42	2.18	1	1
1:B:101:VAL:C	1:B:103:HIS:N	0.42	2.73	6	1
1:A:127:ARG:O	1:A:134:ILE:N	0.42	2.47	9	1
1:A:133:TYR:O	1:B:141:LYS:N	0.42	2.46	10	1
1:A:104:PHE:CE2	1:A:136:ARG:NH2	0.42	2.88	1	1
1:A:169:MET:CB	1:A:170:PRO:HD2	0.42	2.45	8	1
1:B:95:TRP:N	1:B:167:ALA:O	0.42	2.52	2	1
1:B:157:LEU:HD12	1:B:158:SER:H	0.42	1.75	8	1
1:B:142:TYR:N	1:B:142:TYR:CD1	0.42	2.88	3	1
1:A:124:HIS:HB3	1:A:127:ARG:NH2	0.42	2.30	7	1
1:A:140:ARG:HH22	1:A:141:LYS:C	0.42	2.18	8	1
1:B:104:PHE:HB3	1:B:136:ARG:NH1	0.42	2.30	10	1
1:B:127:ARG:NH1	1:B:127:ARG:CB	0.41	2.82	7	1
1:A:140:ARG:NE	1:A:142:TYR:CZ	0.41	2.88	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:95:TRP:CB	1:B:169:MET:HG2	0.41	2.45	8	1
1:A:124:HIS:CD2	1:A:127:ARG:HG3	0.41	2.50	10	1
1:A:101:VAL:N	1:A:103:HIS:CE1	0.41	2.88	3	1
1:B:145:PRO:C	1:B:147:GLY:H	0.41	2.18	3	1
1:B:158:SER:HB2	1:B:162:THR:CG2	0.41	2.45	8	1
1:B:108:GLU:HB3	1:B:123:LYS:O	0.41	2.15	10	1
1:A:99:LEU:HD23	1:A:140:ARG:HD3	0.41	1.93	4	1
1:B:117:VAL:CG1	1:B:141:LYS:HG3	0.41	2.46	7	1
1:A:140:ARG:NH1	1:B:134:ILE:HB	0.41	2.30	10	2
1:A:135:SER:OG	1:A:136:ARG:N	0.41	2.54	3	1
1:B:95:TRP:O	1:B:166:GLU:HA	0.41	2.16	2	1
1:A:119:GLU:HG2	1:A:141:LYS:CB	0.41	2.45	3	2
1:B:102:ASN:O	1:B:102:ASN:CG	0.41	2.58	3	1
1:B:148:VAL:O	1:B:149:ASP:C	0.41	2.59	3	1
1:A:158:SER:C	1:A:160:GLU:N	0.41	2.74	2	1
1:A:114:LYS:O	1:A:115:ASP:C	0.41	2.59	4	1
1:A:104:PHE:CZ	1:A:136:ARG:NH1	0.41	2.89	6	1
1:A:99:LEU:CD2	1:A:140:ARG:CB	0.41	2.98	8	1
1:A:124:HIS:CD2	1:A:127:ARG:CG	0.41	3.03	1	1
1:B:114:LYS:O	1:B:115:ASP:C	0.41	2.59	1	1
1:A:102:ASN:HB3	1:A:161:GLY:O	0.41	2.15	6	1
1:B:100:ASP:CG	1:B:103:HIS:HE2	0.41	2.19	2	1
1:A:132:GLY:HA3	1:B:142:TYR:CZ	0.41	2.50	5	1
1:A:160:GLU:O	1:A:162:THR:N	0.41	2.54	7	1
1:B:119:GLU:CD	1:B:141:LYS:HZ2	0.41	2.16	9	1
1:B:160:GLU:CD	1:B:160:GLU:N	0.41	2.74	9	1
1:A:134:ILE:HD12	1:B:140:ARG:CZ	0.41	2.45	2	1
1:B:104:PHE:CE1	1:B:127:ARG:NH1	0.41	2.89	2	2
1:B:110:THR:N	1:B:121:THR:O	0.41	2.53	7	1
1:A:124:HIS:CG	1:A:127:ARG:HD3	0.41	2.51	10	1
1:B:102:ASN:HD21	1:B:106:PRO:HA	0.41	1.75	10	1
1:B:157:LEU:HD12	1:B:162:THR:O	0.41	2.16	3	1
1:B:157:LEU:HD11	1:B:161:GLY:HA2	0.41	1.91	3	1
1:B:114:LYS:O	1:B:117:VAL:CB	0.41	2.68	7	1
1:B:127:ARG:NH1	1:B:134:ILE:HG23	0.40	2.31	7	1
1:A:119:GLU:HG2	1:A:141:LYS:HA	0.40	1.92	8	1
1:A:100:ASP:C	1:A:101:VAL:CG2	0.40	2.88	9	1
1:B:145:PRO:CD	1:B:146:PRO:HD2	0.40	2.46	5	1
1:A:141:LYS:HB2	1:A:141:LYS:NZ	0.40	2.29	6	1
1:B:100:ASP:OD2	1:B:103:HIS:NE2	0.40	2.45	7	1
1:A:119:GLU:HG2	1:A:141:LYS:HB2	0.40	1.94	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:124:HIS:CD2	1:B:124:HIS:N	0.40	2.82	8	1
1:B:124:HIS:O	1:B:135:SER:OG	0.40	2.35	4	1
1:A:95:TRP:CD1	1:A:95:TRP:O	0.40	2.74	6	1
1:A:149:ASP:OD1	1:A:152:GLN:N	0.40	2.49	9	1
1:B:144:LEU:C	1:B:146:PRO:HD2	0.40	2.37	2	1
1:B:136:ARG:HD2	1:B:138:PHE:CE2	0.40	2.51	5	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/98 (74%)	58±2 (80±3%)	10±2 (13±3%)	5±1 (7±2%)	2	16
1	B	76/98 (78%)	61±2 (81±3%)	9±2 (12±3%)	6±1 (8±2%)	1	15
All	All	1490/1960 (76%)	1197 (80%)	185 (12%)	108 (7%)	2	15

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	126	GLU	10
1	B	146	PRO	10
1	A	101	VAL	9
1	B	101	VAL	9
1	B	126	GLU	8
1	A	102	ASN	7
1	A	146	PRO	7
1	B	102	ASN	5
1	B	160	GLU	5
1	A	147	GLY	4
1	A	160	GLU	4
1	A	94	ARG	3
1	B	106	PRO	3
1	B	115	ASP	3
1	B	94	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	B	147	GLY	3
1	A	170	PRO	2
1	B	169	MET	2
1	B	100	ASP	2
1	B	148	VAL	2
1	A	167	ALA	1
1	B	103	HIS	1
1	A	150	PRO	1
1	B	161	GLY	1
1	A	106	PRO	1
1	A	161	GLY	1
1	A	115	ASP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/88 (75%)	40±2 (61±4%)	26±2 (39±4%)	0	5
1	B	69/88 (78%)	41±3 (59±4%)	28±3 (41±4%)	0	4
All	All	1350/1760 (77%)	810 (60%)	540 (40%)	0	5

All 92 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	102	ASN	10
1	A	109	LEU	10
1	A	121	THR	10
1	A	123	LYS	10
1	A	134	ILE	10
1	A	139	THR	10
1	A	143	THR	10
1	A	148	VAL	10
1	A	151	THR	10
1	A	154	SER	10
1	A	156	SER	10
1	B	99	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	B	109	LEU	10
1	B	121	THR	10
1	B	134	ILE	10
1	B	135	SER	10
1	B	139	THR	10
1	B	140	ARG	10
1	B	154	SER	10
1	B	156	SER	10
1	B	164	THR	10
1	A	99	LEU	9
1	A	136	ARG	9
1	B	102	ASN	9
1	B	123	LYS	9
1	B	143	THR	9
1	B	148	VAL	9
1	B	151	THR	9
1	B	155	SER	9
1	B	169	MET	9
1	A	155	SER	9
1	B	110	THR	9
1	A	101	VAL	8
1	A	169	MET	8
1	A	158	SER	8
1	B	158	SER	8
1	A	95	TRP	7
1	A	97	VAL	7
1	A	110	THR	7
1	A	114	LYS	7
1	B	101	VAL	7
1	B	113	THR	7
1	B	95	TRP	7
1	A	140	ARG	6
1	A	164	THR	6
1	B	97	VAL	6
1	B	129	ASP	6
1	B	166	GLU	6
1	A	112	LYS	5
1	A	135	SER	5
1	B	125	GLU	5
1	B	138	PHE	5
1	B	114	LYS	5
1	A	125	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	103	HIS	4
1	A	127	ARG	4
1	B	111	VAL	4
1	B	126	GLU	4
1	B	130	GLU	4
1	A	166	GLU	4
1	A	113	THR	4
1	B	136	ARG	4
1	B	94	ARG	3
1	B	103	HIS	3
1	B	107	ASP	3
1	A	126	GLU	3
1	B	112	LYS	3
1	B	127	ARG	3
1	A	104	PHE	3
1	A	115	ASP	3
1	B	124	HIS	3
1	A	98	SER	3
1	B	108	GLU	2
1	B	115	ASP	2
1	B	149	ASP	2
1	B	152	GLN	2
1	A	96	ARG	2
1	B	100	ASP	2
1	B	104	PHE	2
1	A	100	ASP	2
1	A	119	GLU	1
1	A	120	ILE	1
1	B	120	ILE	1
1	A	162	THR	1
1	A	111	VAL	1
1	A	149	ASP	1
1	A	152	GLN	1
1	A	138	PHE	1
1	B	142	TYR	1
1	A	94	ARG	1
1	A	124	HIS	1
1	B	128	GLN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 20% for the well-defined parts and 19% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

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

Total number of shifts	490
Number of shifts mapped to atoms	490
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	90	0.41 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	84	0.85 ± 0.25	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	77	-0.46 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 20%, i.e. 409 atoms were assigned a chemical shift out of a possible 1997. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	219/729 (30%)	83/295 (28%)	72/298 (24%)	64/136 (47%)
Sidechain	188/1133 (17%)	118/734 (16%)	68/356 (19%)	2/43 (5%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/135 (1%)	1/68 (1%)	0/60 (0%)	1/7 (14%)
Overall	409/1997 (20%)	202/1097 (18%)	140/714 (20%)	67/186 (36%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 19%, i.e. 490 atoms were assigned a chemical shift out of a possible 2598. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	269/964 (28%)	102/390 (26%)	90/392 (23%)	77/182 (42%)
Sidechain	219/1478 (15%)	130/958 (14%)	86/464 (19%)	3/56 (5%)
Aromatic	2/156 (1%)	1/80 (1%)	0/66 (0%)	1/10 (10%)
Overall	490/2598 (19%)	233/1428 (16%)	176/922 (19%)	81/248 (33%)

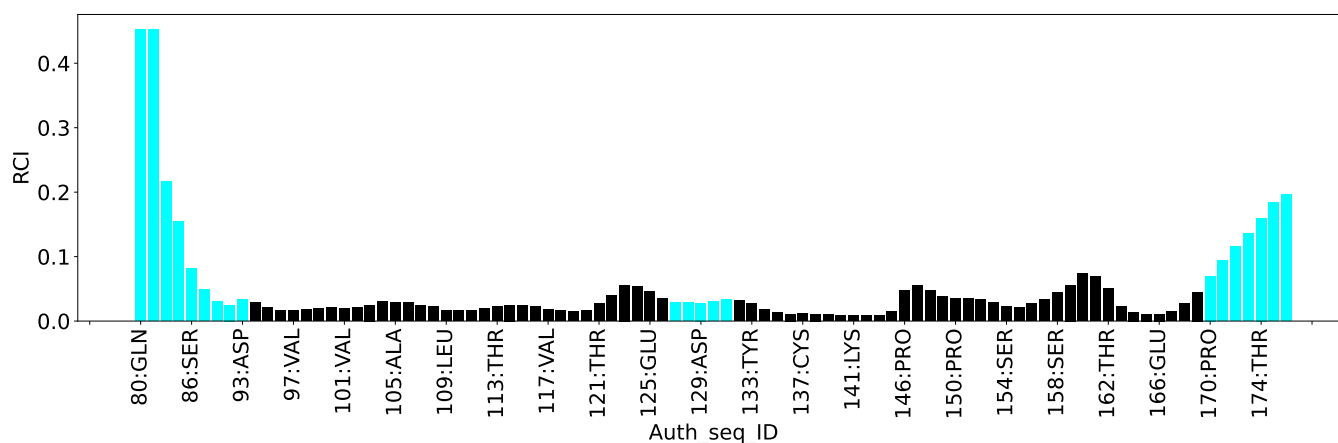
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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	4298
Intra-residue ($ i-j =0$)	899
Sequential ($ i-j =1$)	1094
Medium range ($ i-j >1$ and $ i-j <5$)	533
Long range ($ i-j \geq 5$)	1507
Inter-chain	264
Hydrogen bond restraints	0
Disulfide bond restraints	1
Total dihedral-angle restraints	230
Number of unmapped restraints	0
Number of restraints per residue	23.1
Number of long range restraints per residue ¹	7.7

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	176.7	0.2
0.2-0.5 (Medium)	231.7	0.5
>0.5 (Large)	165.0	7.17

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)	12.8	9.77
10.0-20.0 (Medium)	0.1	10.01
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

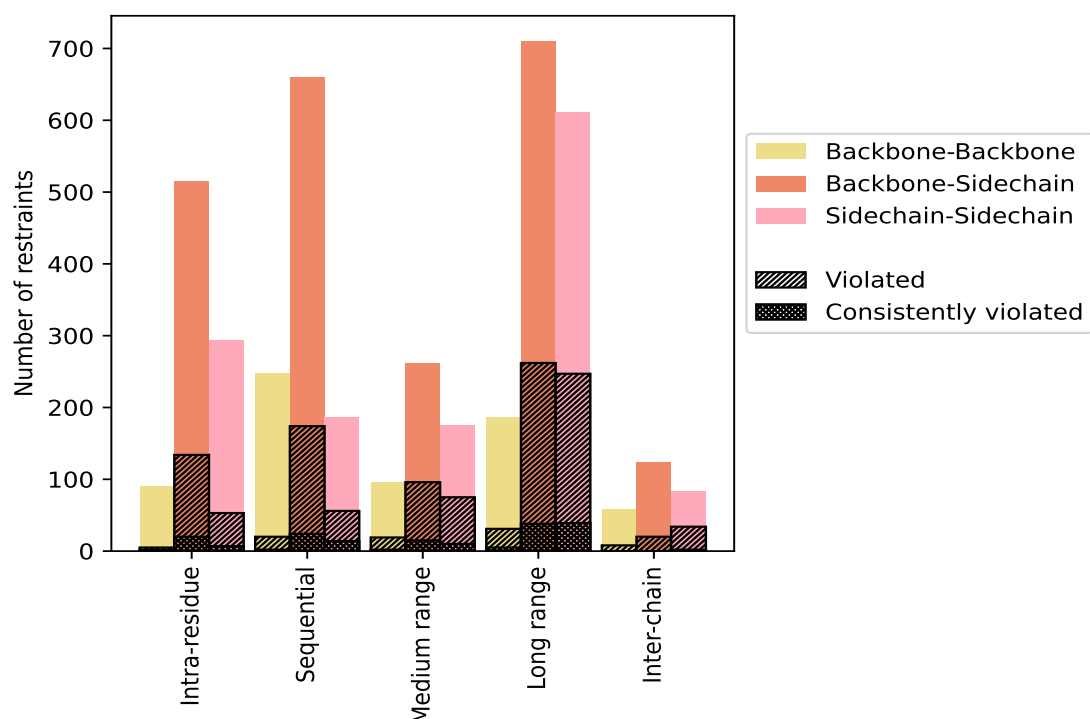
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	899	20.9	192	21.4	4.5	29	3.2	0.7
Backbone-Backbone	90	2.1	5	5.6	0.1	2	2.2	0.0
Backbone-Sidechain	515	12.0	134	26.0	3.1	20	3.9	0.5
Sidechain-Sidechain	294	6.8	53	18.0	1.2	7	2.4	0.2
Sequential ($i-j =1$)	1094	25.5	250	22.9	5.8	40	3.7	0.9
Backbone-Backbone	248	5.8	20	8.1	0.5	2	0.8	0.0
Backbone-Sidechain	660	15.4	174	26.4	4.0	24	3.6	0.6
Sidechain-Sidechain	186	4.3	56	30.1	1.3	14	7.5	0.3
Medium range ($i-j >1$ & $i-j <5$)	533	12.4	190	35.6	4.4	27	5.1	0.6
Backbone-Backbone	96	2.2	19	19.8	0.4	2	2.1	0.0
Backbone-Sidechain	262	6.1	96	36.6	2.2	15	5.7	0.3
Sidechain-Sidechain	175	4.1	75	42.9	1.7	10	5.7	0.2
Long range ($i-j \geq 5$)	1507	35.1	540	35.8	12.6	82	5.4	1.9
Backbone-Backbone	186	4.3	31	16.7	0.7	5	2.7	0.1
Backbone-Sidechain	710	16.5	262	36.9	6.1	38	5.4	0.9
Sidechain-Sidechain	611	14.2	247	40.4	5.7	39	6.4	0.9
Inter-chain	264	6.1	62	23.5	1.4	2	0.8	0.0
Backbone-Backbone	58	1.3	8	13.8	0.2	0	0.0	0.0
Backbone-Sidechain	124	2.9	20	16.1	0.5	0	0.0	0.0
Sidechain-Sidechain	82	1.9	34	41.5	0.8	2	2.4	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	1	0.0	0	0.0	0.0	0	0.0	0.0
Total	4298	100.0	1234	28.7	28.7	180	4.2	4.2
Backbone-Backbone	678	15.8	83	12.2	1.9	11	1.6	0.3
Backbone-Sidechain	2271	52.8	686	30.2	16.0	97	4.3	2.3
Sidechain-Sidechain	1349	31.4	465	34.5	10.8	72	5.3	1.7

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

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



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

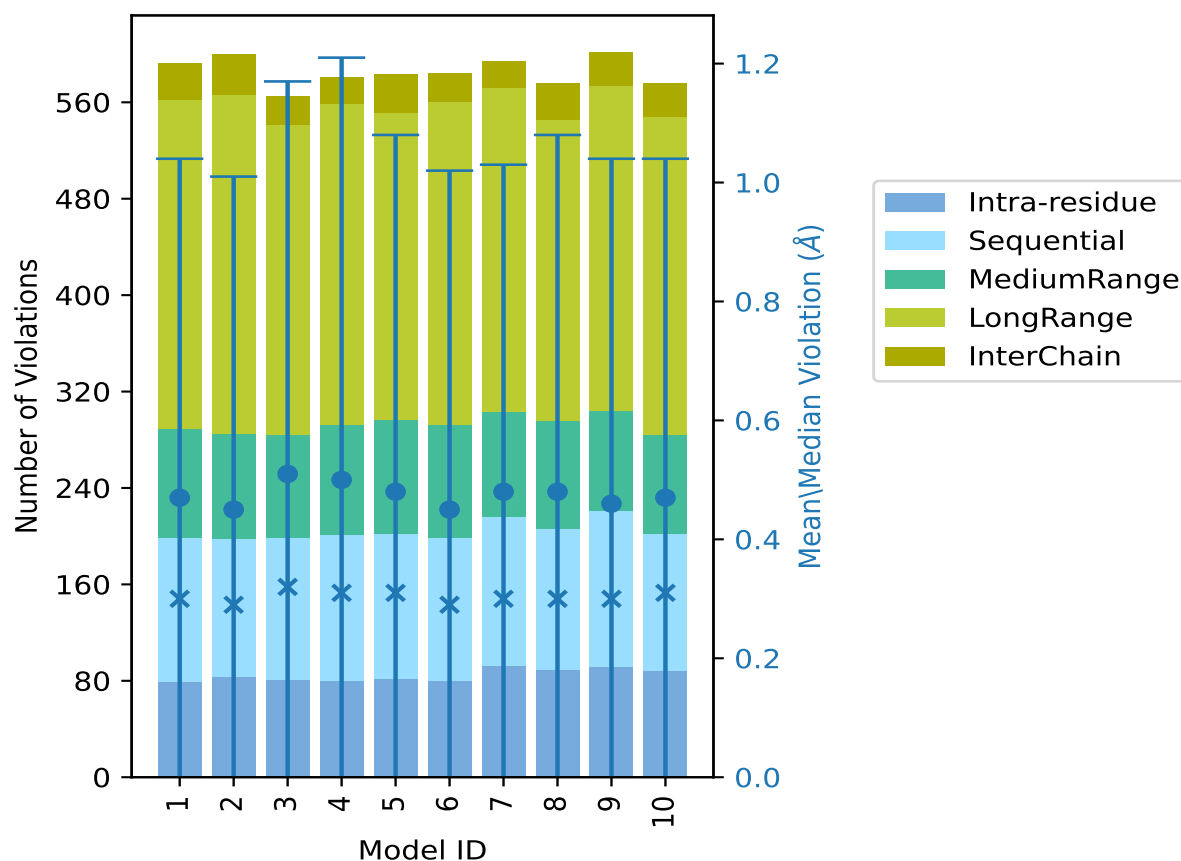
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	79	120	90	273	30	592	0.47	5.27	0.57	0.3
2	83	115	87	281	34	600	0.45	5.46	0.56	0.29
3	81	118	85	257	24	565	0.51	6.11	0.66	0.32
4	80	121	91	267	22	581	0.5	7.16	0.71	0.31
5	82	120	95	254	32	583	0.48	7.17	0.6	0.31
6	80	119	93	268	24	584	0.45	6.06	0.57	0.29
7	93	123	87	269	22	594	0.48	6.94	0.55	0.3
8	89	117	90	250	30	576	0.48	6.54	0.6	0.3
9	92	129	83	270	28	602	0.46	6.42	0.58	0.3
10	88	114	82	264	28	576	0.47	5.28	0.57	0.31

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3063(IR:707, SQ:844, MR:343, LR:967, IC:202) 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	%
41	66	42	111	14	274	1	10.0
31	33	26	62	6	158	2	20.0
30	21	18	69	10	148	3	30.0

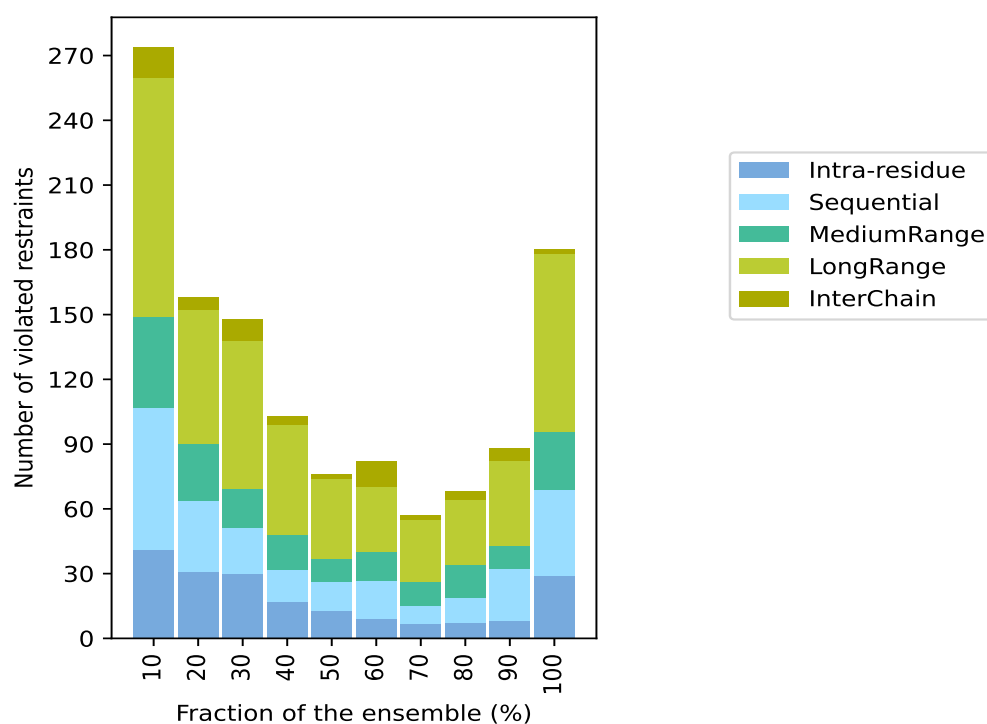
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
17	15	16	51	4	103	4	40.0
13	13	11	37	2	76	5	50.0
9	18	13	30	12	82	6	60.0
7	8	11	29	2	57	7	70.0
7	12	15	30	4	68	8	80.0
8	24	11	39	6	88	9	90.0
29	40	27	82	2	180	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

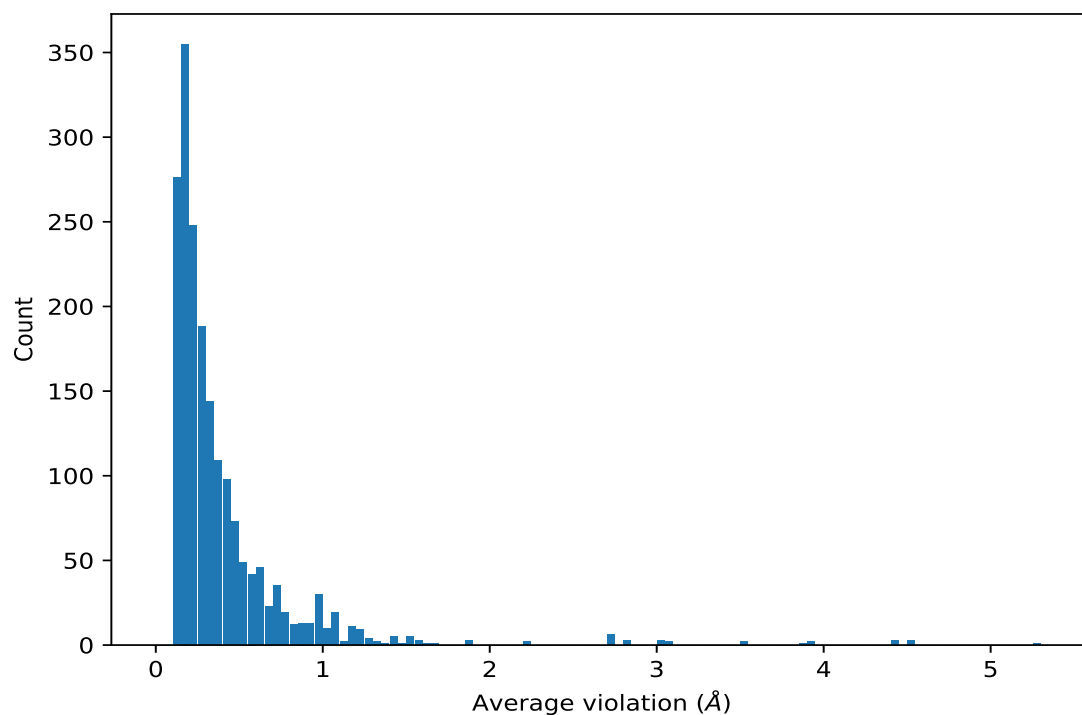


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	10	5.28	1.15	5.49
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG2	10	3.9	1.89	4.2
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG3	10	3.9	1.89	4.2
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	10	3.88	1.42	3.52
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	10	3.04	1.51	3.45
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	10	3.04	1.51	3.45
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	10	3.04	1.51	3.45
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG2	10	2.74	1.96	3.14
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG3	10	2.74	1.96	3.14
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	10	1.61	0.97	1.39
(1,4)	1:89:A:ARG:HB3	1:90:A:HIS:HB3	10	1.57	0.47	1.66
(1,4)	1:89:A:ARG:HB2	1:90:A:HIS:HB3	10	1.57	0.47	1.66
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	10	1.55	0.06	1.56
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	10	1.54	0.16	1.5
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	10	1.51	0.21	1.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	10	1.37	0.37	1.46
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	10	1.29	0.27	1.28
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	10	1.26	0.46	1.31
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	10	1.24	0.29	1.34
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	10	1.24	0.29	1.34
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	10	1.17	0.19	1.18
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	10	1.17	0.19	1.18
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	10	1.17	0.19	1.18
(1,2538)	1:99:B:LEU:HD11	1:112:B:LYS:HG3	10	1.17	0.19	1.18
(1,2538)	1:99:B:LEU:HD12	1:112:B:LYS:HG3	10	1.17	0.19	1.18
(1,2538)	1:99:B:LEU:HD13	1:112:B:LYS:HG3	10	1.17	0.19	1.18
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	10	1.17	0.06	1.15
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	10	1.17	0.06	1.15
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	10	1.17	0.06	1.15
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	10	1.12	0.22	1.19
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	10	1.12	0.22	1.19
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	10	1.09	0.09	1.08
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	10	1.09	0.09	1.08
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	10	1.09	0.09	1.08
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	10	1.06	0.25	1.11
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	10	1.05	0.26	1.1
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	10	1.05	0.26	1.1
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	10	1.05	0.26	1.1
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	10	1.05	0.48	1.27
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	10	1.05	0.44	1.22
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	10	1.04	0.19	1.04
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	10	1.04	0.19	1.04
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	10	1.04	0.19	1.04
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	10	1.01	0.24	1.17
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	10	0.99	0.08	0.98
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	10	0.99	0.08	0.98
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	10	0.99	0.08	0.98
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	10	0.98	0.34	0.86
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	10	0.98	0.34	0.86
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	10	0.98	0.34	0.86
(1,257)	1:99:A:LEU:HD11	1:112:A:LYS:HG3	10	0.98	0.34	0.86
(1,257)	1:99:A:LEU:HD12	1:112:A:LYS:HG3	10	0.98	0.34	0.86
(1,257)	1:99:A:LEU:HD13	1:112:A:LYS:HG3	10	0.98	0.34	0.86
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	10	0.97	0.06	0.96
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	10	0.97	0.06	0.96
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	10	0.97	0.06	0.96
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	10	0.96	0.28	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	10	0.93	0.15	0.92
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	10	0.93	0.32	1.0
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	10	0.91	0.19	0.98
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	10	0.89	0.48	0.82
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG3	10	0.89	0.48	0.82
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	10	0.87	0.18	0.9
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	10	0.87	0.18	0.9
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	10	0.87	0.18	0.9
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	10	0.87	0.23	0.94
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	10	0.87	0.19	0.88
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	10	0.86	0.17	0.86
(1,474)	1:112:A:LYS:HE3	1:114:A:LYS:HB3	10	0.84	0.14	0.86
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	10	0.84	0.14	0.86
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	10	0.84	0.29	0.92
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	10	0.8	0.16	0.86
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	10	0.8	0.23	0.79
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	10	0.8	0.23	0.79
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	10	0.8	0.23	0.79
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	10	0.79	0.21	0.76
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	10	0.79	0.25	0.68
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	10	0.78	0.22	0.84
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	10	0.78	0.13	0.74
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	10	0.77	0.24	0.78
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	10	0.76	0.22	0.7
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	10	0.75	0.27	0.65
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	10	0.75	0.27	0.65
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	10	0.75	0.27	0.65
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	10	0.75	0.27	0.65
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	10	0.75	0.27	0.65
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	10	0.75	0.27	0.65
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	10	0.75	0.24	0.84
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	10	0.74	0.27	0.8
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	10	0.74	0.27	0.8
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	10	0.74	0.27	0.8
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	10	0.74	0.19	0.76
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	10	0.74	0.19	0.76
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	10	0.74	0.19	0.76
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	10	0.72	0.58	0.4
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	10	0.72	0.13	0.7
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	10	0.72	0.13	0.7
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	10	0.72	0.13	0.7
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	10	0.71	0.15	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	10	0.71	0.15	0.76
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	10	0.71	0.15	0.76
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	10	0.71	0.11	0.72
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	10	0.71	0.11	0.72
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	10	0.71	0.11	0.72
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	10	0.69	0.1	0.68
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	10	0.69	0.1	0.68
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	10	0.69	0.1	0.68
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	10	0.69	0.04	0.68
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	10	0.69	0.38	0.55
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	10	0.68	0.1	0.71
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	10	0.67	0.34	0.59
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	10	0.67	0.34	0.59
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	10	0.67	0.34	0.59
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	10	0.67	0.33	0.62
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	10	0.66	0.18	0.7
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	10	0.64	0.26	0.63
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	10	0.64	0.15	0.64
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	10	0.62	0.12	0.66
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	10	0.61	0.13	0.6
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	10	0.61	0.13	0.6
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	10	0.61	0.13	0.6
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	10	0.61	0.16	0.64
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	10	0.61	0.16	0.64
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	10	0.61	0.16	0.64
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	10	0.61	0.32	0.5
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	10	0.6	0.2	0.56
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	10	0.6	0.2	0.56
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	10	0.6	0.2	0.56
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	10	0.6	0.18	0.67
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	10	0.6	0.18	0.67
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	10	0.6	0.18	0.67
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	10	0.6	0.1	0.6
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	10	0.6	0.1	0.6
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	10	0.6	0.1	0.6
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	10	0.6	0.2	0.6
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	10	0.58	0.11	0.6
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB3	10	0.58	0.11	0.6
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	10	0.57	0.24	0.47
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB3	10	0.56	0.08	0.55
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	10	0.56	0.08	0.55
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	10	0.55	0.31	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	10	0.55	0.14	0.58
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	10	0.54	0.23	0.61
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	10	0.54	0.2	0.54
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	10	0.54	0.08	0.53
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	10	0.52	0.17	0.48
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	10	0.52	0.15	0.58
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	10	0.51	0.17	0.46
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	10	0.5	0.21	0.45
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	10	0.5	0.01	0.5
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	10	0.49	0.02	0.48
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	10	0.48	0.2	0.52
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD11	10	0.48	0.12	0.51
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD12	10	0.48	0.12	0.51
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD13	10	0.48	0.12	0.51
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD21	10	0.48	0.12	0.51
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD22	10	0.48	0.12	0.51
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD23	10	0.48	0.12	0.51
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	10	0.48	0.1	0.48
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	10	0.48	0.2	0.54
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	10	0.48	0.13	0.54
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	10	0.48	0.13	0.54
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	10	0.48	0.13	0.54
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	10	0.47	0.15	0.52
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	10	0.47	0.15	0.52
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	10	0.47	0.15	0.52
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	10	0.46	0.06	0.48
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	10	0.46	0.06	0.48
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	10	0.46	0.06	0.48
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	10	0.46	0.15	0.44
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	10	0.45	0.06	0.43
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	10	0.44	0.19	0.5
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	10	0.44	0.05	0.46
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD3	10	0.44	0.17	0.4
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD2	10	0.44	0.17	0.4
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	10	0.44	0.15	0.5
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	10	0.44	0.15	0.5
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	10	0.44	0.15	0.5
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	10	0.43	0.04	0.42
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	10	0.43	0.1	0.42
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD11	10	0.43	0.1	0.42
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD12	10	0.43	0.1	0.42
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD13	10	0.43	0.1	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD21	10	0.43	0.1	0.42
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD22	10	0.43	0.1	0.42
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD23	10	0.43	0.1	0.42
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	10	0.42	0.07	0.41
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	10	0.42	0.07	0.41
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	10	0.42	0.07	0.41
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	10	0.42	0.18	0.46
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	10	0.42	0.05	0.43
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	10	0.42	0.05	0.43
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	10	0.42	0.05	0.43
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	10	0.41	0.07	0.42
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	10	0.41	0.11	0.46
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	10	0.41	0.04	0.4
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	10	0.41	0.04	0.41
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	10	0.41	0.04	0.41
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	10	0.41	0.04	0.41
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	10	0.41	0.11	0.4
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	10	0.41	0.11	0.4
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	10	0.41	0.11	0.4
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	10	0.4	0.06	0.4
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	10	0.4	0.06	0.4
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	10	0.4	0.06	0.4
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	10	0.39	0.02	0.4
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	10	0.39	0.02	0.4
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	10	0.39	0.02	0.4
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	10	0.39	0.1	0.4
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	10	0.38	0.07	0.41
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	10	0.38	0.07	0.41
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	10	0.38	0.07	0.41
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	10	0.38	0.07	0.38
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	10	0.38	0.07	0.38
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	10	0.38	0.07	0.38
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	10	0.38	0.03	0.38
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	10	0.38	0.15	0.36
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	10	0.38	0.12	0.36
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	10	0.38	0.12	0.36
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	10	0.38	0.12	0.36
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	10	0.38	0.13	0.36
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	10	0.36	0.16	0.38
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	10	0.36	0.03	0.36
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	10	0.36	0.2	0.24
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	10	0.36	0.2	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	10	0.36	0.2	0.24
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	10	0.35	0.08	0.35
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	10	0.35	0.1	0.36
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	10	0.35	0.16	0.34
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	10	0.34	0.07	0.36
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	10	0.34	0.13	0.36
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	10	0.34	0.13	0.36
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	10	0.34	0.13	0.36
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	10	0.34	0.06	0.33
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	10	0.33	0.03	0.34
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	10	0.32	0.02	0.34
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	10	0.32	0.02	0.32
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	10	0.32	0.04	0.32
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	10	0.32	0.04	0.32
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	10	0.32	0.04	0.32
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	10	0.32	0.06	0.31
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	10	0.32	0.06	0.31
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	10	0.32	0.06	0.31
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	10	0.32	0.07	0.29
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	10	0.32	0.07	0.29
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	10	0.32	0.07	0.29
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	10	0.3	0.03	0.3
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	10	0.29	0.11	0.29
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	10	0.29	0.11	0.29
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	10	0.29	0.11	0.29
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	10	0.29	0.04	0.3
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	10	0.29	0.04	0.28
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	10	0.29	0.04	0.28
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	10	0.29	0.04	0.28
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	10	0.29	0.07	0.29
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	10	0.29	0.07	0.29
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	10	0.29	0.07	0.29
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	10	0.28	0.09	0.3
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	10	0.28	0.09	0.3
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	10	0.28	0.09	0.3
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	10	0.28	0.1	0.28
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	10	0.27	0.03	0.28
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	10	0.27	0.1	0.24
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	10	0.27	0.1	0.28
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	10	0.26	0.08	0.29
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	10	0.26	0.08	0.29
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	10	0.26	0.08	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	10	0.25	0.1	0.24
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	10	0.25	0.07	0.25
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG2	10	0.25	0.07	0.25
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	10	0.25	0.05	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	10	0.25	0.03	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	10	0.25	0.03	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	10	0.25	0.03	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	10	0.25	0.03	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	10	0.25	0.03	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	10	0.25	0.03	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	10	0.25	0.03	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	10	0.25	0.03	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	10	0.25	0.03	0.24
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	10	0.25	0.12	0.21
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	10	0.24	0.04	0.24
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	10	0.24	0.04	0.24
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	10	0.24	0.04	0.24
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	10	0.24	0.02	0.25
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	10	0.23	0.07	0.2
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	10	0.23	0.07	0.2
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	10	0.23	0.07	0.2
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	10	0.23	0.07	0.2
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	10	0.23	0.07	0.2
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	10	0.23	0.07	0.2
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	10	0.23	0.07	0.2
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	10	0.23	0.07	0.2
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	10	0.23	0.07	0.2
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	10	0.23	0.02	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	10	0.23	0.02	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	10	0.23	0.02	0.24
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	10	0.23	0.05	0.22
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	10	0.23	0.07	0.2
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	10	0.23	0.06	0.23
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	10	0.22	0.06	0.22
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	10	0.22	0.06	0.22
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	10	0.22	0.06	0.22
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	10	0.22	0.04	0.24
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	10	0.22	0.04	0.24
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	10	0.22	0.04	0.24
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	10	0.22	0.02	0.22
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	10	0.22	0.03	0.22
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	10	0.22	0.03	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	10	0.22	0.03	0.22
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	10	0.21	0.02	0.2
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	10	0.21	0.02	0.21
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	10	0.2	0.01	0.2
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	10	0.2	0.01	0.2
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	10	0.2	0.06	0.2
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	10	0.2	0.06	0.2
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	10	0.2	0.06	0.2
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	10	0.2	0.02	0.2
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	10	0.19	0.04	0.2
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	10	0.19	0.02	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	10	0.19	0.02	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	10	0.19	0.02	0.18
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	10	0.18	0.07	0.16
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	10	0.18	0.07	0.16
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	10	0.18	0.07	0.16
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	10	0.18	0.04	0.2
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	10	0.18	0.05	0.18
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG3	10	0.18	0.05	0.18
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	10	0.18	0.05	0.19
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	10	0.18	0.03	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	10	0.18	0.03	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	10	0.18	0.03	0.17
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	10	0.17	0.03	0.16
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	10	0.17	0.03	0.16
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	10	0.17	0.03	0.16
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	10	0.17	0.03	0.16
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	10	0.17	0.03	0.16
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	10	0.17	0.03	0.16
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	10	0.17	0.03	0.16
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	10	0.17	0.03	0.16
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	10	0.17	0.03	0.16
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	10	0.16	0.01	0.16
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	10	0.16	0.01	0.16
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	10	0.15	0.02	0.15
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	10	0.15	0.03	0.15
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	10	0.14	0.02	0.14
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE2	9	3.05	1.55	3.0
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE3	9	3.05	1.55	3.0
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE3	9	2.24	1.38	2.07
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE2	9	2.24	1.38	2.07
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	9	1.69	0.55	1.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2285)	1:89:B:ARG:HB3	1:90:B:HIS:HB3	9	1.42	0.6	1.53
(1,2285)	1:89:B:ARG:HB2	1:90:B:HIS:HB3	9	1.42	0.6	1.53
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	9	1.24	0.16	1.25
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	9	1.07	0.63	0.67
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	9	1.07	0.63	0.67
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	9	1.07	0.63	0.67
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	9	1.05	0.29	0.9
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	9	1.05	0.29	0.9
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	9	1.05	0.29	0.9
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	9	1.05	0.29	0.9
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	9	1.05	0.29	0.9
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	9	1.05	0.29	0.9
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	9	1.0	0.47	0.95
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	9	0.94	0.44	0.85
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	9	0.92	0.33	0.92
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	9	0.91	0.5	0.79
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	9	0.86	0.3	0.86
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	9	0.77	0.22	0.84
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	9	0.73	0.07	0.76
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	9	0.73	0.31	0.76
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	9	0.72	0.23	0.72
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	9	0.72	0.23	0.72
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	9	0.72	0.23	0.72
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	9	0.72	0.23	0.72
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	9	0.72	0.23	0.72
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	9	0.72	0.23	0.72
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	9	0.69	0.41	0.59
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	9	0.69	0.41	0.59
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	9	0.66	0.31	0.6
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	9	0.61	0.29	0.61
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG2	9	0.61	0.29	0.61
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	9	0.59	0.22	0.65
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	9	0.59	0.22	0.65
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	9	0.59	0.22	0.65
(1,2976)	1:123:B:LYS:HD3	1:137:B:CYS:HB2	9	0.59	0.2	0.43
(1,2976)	1:123:B:LYS:HD2	1:137:B:CYS:HB2	9	0.59	0.2	0.43
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	9	0.56	0.08	0.56
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	9	0.55	0.19	0.58
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	9	0.55	0.19	0.58
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	9	0.55	0.19	0.58
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	9	0.54	0.39	0.33
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	9	0.54	0.16	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	9	0.53	0.15	0.56
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	9	0.52	0.25	0.57
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	9	0.52	0.25	0.57
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	9	0.52	0.25	0.57
(1,71)	1:95:A:TRP:HB3	1:168:A:PRO:HB2	9	0.51	0.15	0.43
(1,71)	1:95:A:TRP:HB2	1:168:A:PRO:HB2	9	0.51	0.15	0.43
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	9	0.51	0.17	0.51
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	9	0.51	0.17	0.51
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	9	0.51	0.17	0.51
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	9	0.51	0.07	0.53
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	9	0.48	0.06	0.45
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	9	0.45	0.14	0.47
(1,695)	1:123:A:LYS:HD2	1:137:A:CYS:HB2	9	0.44	0.16	0.42
(1,695)	1:123:A:LYS:HD3	1:137:A:CYS:HB2	9	0.44	0.16	0.42
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	9	0.42	0.17	0.42
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	9	0.4	0.06	0.42
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	9	0.4	0.06	0.42
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	9	0.4	0.06	0.42
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	9	0.4	0.06	0.42
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	9	0.4	0.06	0.42
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	9	0.4	0.06	0.42
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD3	9	0.4	0.17	0.31
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD2	9	0.4	0.17	0.31
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	9	0.39	0.19	0.42
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	9	0.39	0.19	0.42
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	9	0.39	0.19	0.42
(1,2352)	1:95:B:TRP:HB3	1:168:B:PRO:HB2	9	0.39	0.24	0.31
(1,2352)	1:95:B:TRP:HB2	1:168:B:PRO:HB2	9	0.39	0.24	0.31
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	9	0.38	0.13	0.38
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	9	0.38	0.03	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	9	0.38	0.03	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	9	0.38	0.03	0.39
(1,694)	1:123:A:LYS:HD2	1:137:A:CYS:HA	9	0.37	0.11	0.41
(1,694)	1:123:A:LYS:HD3	1:137:A:CYS:HA	9	0.37	0.11	0.41
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	9	0.37	0.08	0.4
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	9	0.37	0.08	0.4
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	9	0.37	0.08	0.4
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	9	0.36	0.12	0.38
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	9	0.35	0.11	0.37
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	9	0.35	0.14	0.37
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	9	0.35	0.2	0.33
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	9	0.35	0.12	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	9	0.35	0.13	0.34
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	9	0.35	0.13	0.34
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	9	0.35	0.13	0.34
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	9	0.34	0.19	0.23
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	9	0.34	0.19	0.23
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	9	0.34	0.19	0.23
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	9	0.34	0.09	0.27
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	9	0.34	0.09	0.27
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	9	0.34	0.09	0.27
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	9	0.33	0.15	0.38
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	9	0.33	0.15	0.32
(1,72)	1:95:A:TRP:HB3	1:168:A:PRO:HB3	9	0.33	0.15	0.25
(1,72)	1:95:A:TRP:HB2	1:168:A:PRO:HB3	9	0.33	0.15	0.25
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	9	0.32	0.1	0.27
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	9	0.32	0.1	0.27
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	9	0.32	0.1	0.27
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	9	0.32	0.09	0.31
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	9	0.32	0.09	0.31
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	9	0.32	0.09	0.31
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	9	0.3	0.19	0.18
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	9	0.3	0.19	0.18
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	9	0.3	0.19	0.18
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD22	9	0.29	0.08	0.24
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD21	9	0.29	0.08	0.24
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE3	9	0.29	0.16	0.22
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE2	9	0.29	0.16	0.22
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	9	0.29	0.06	0.29
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	9	0.29	0.06	0.29
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	9	0.29	0.06	0.29
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	9	0.29	0.09	0.3
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	9	0.29	0.09	0.3
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	9	0.29	0.09	0.3
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	9	0.28	0.11	0.25
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	9	0.27	0.07	0.23
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	9	0.27	0.06	0.26
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	9	0.26	0.07	0.28
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	9	0.25	0.05	0.26
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	9	0.25	0.15	0.15
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	9	0.24	0.07	0.24
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	9	0.24	0.12	0.2
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	9	0.24	0.12	0.2
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	9	0.24	0.12	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	9	0.24	0.1	0.26
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	9	0.22	0.07	0.21
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	9	0.22	0.04	0.23
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	9	0.21	0.07	0.22
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	9	0.21	0.07	0.22
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	9	0.21	0.07	0.22
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	9	0.21	0.07	0.22
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	9	0.21	0.07	0.22
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	9	0.21	0.07	0.22
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	9	0.21	0.02	0.21
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	9	0.21	0.09	0.18
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	9	0.21	0.09	0.18
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	9	0.21	0.09	0.18
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD11	9	0.21	0.03	0.2
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD12	9	0.21	0.03	0.2
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD13	9	0.21	0.03	0.2
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD21	9	0.21	0.03	0.2
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD22	9	0.21	0.03	0.2
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD23	9	0.21	0.03	0.2
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	9	0.2	0.02	0.21
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	9	0.2	0.02	0.21
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	9	0.2	0.02	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	9	0.2	0.02	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	9	0.2	0.02	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	9	0.2	0.02	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	9	0.2	0.02	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	9	0.2	0.02	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	9	0.2	0.02	0.21
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	9	0.19	0.04	0.18
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	9	0.18	0.05	0.18
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	9	0.17	0.02	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	9	0.17	0.04	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	9	0.17	0.04	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	9	0.17	0.04	0.17
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	9	0.16	0.04	0.15
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	9	0.16	0.04	0.13
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	9	0.15	0.05	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	9	0.15	0.05	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	9	0.15	0.05	0.14
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	9	0.14	0.03	0.15
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	9	0.14	0.03	0.15
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	9	0.14	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	9	0.14	0.02	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	9	0.14	0.02	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	9	0.14	0.02	0.14
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	8	4.5	1.66	4.6
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	8	4.5	1.66	4.6
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	8	4.5	1.66	4.6
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	8	4.42	1.88	4.83
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	8	4.42	1.88	4.83
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	8	4.42	1.88	4.83
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE3	8	3.5	1.16	3.49
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE2	8	3.5	1.16	3.49
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG3	8	2.7	0.5	2.6
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG2	8	2.7	0.5	2.6
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	8	1.4	0.52	1.62
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	8	1.4	0.52	1.62
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	8	1.4	0.52	1.62
(1,3)	1:89:A:ARG:HB3	1:90:A:HIS:HB2	8	1.3	0.43	1.36
(1,3)	1:89:A:ARG:HB2	1:90:A:HIS:HB2	8	1.3	0.43	1.36
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	8	1.09	0.37	1.2
(1,2284)	1:89:B:ARG:HB3	1:90:B:HIS:HB2	8	1.02	0.66	0.92
(1,2284)	1:89:B:ARG:HB2	1:90:B:HIS:HB2	8	1.02	0.66	0.92
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	8	0.91	0.5	0.94
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	8	0.7	0.19	0.78
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	8	0.65	0.28	0.74
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	8	0.64	0.3	0.75
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	8	0.61	0.22	0.6
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	8	0.61	0.22	0.6
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	8	0.59	0.22	0.54
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	8	0.59	0.22	0.54
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	8	0.59	0.22	0.54
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	8	0.57	0.27	0.6
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	8	0.57	0.27	0.6
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	8	0.57	0.27	0.6
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	8	0.56	0.25	0.6
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	8	0.56	0.25	0.6
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	8	0.55	0.3	0.48
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	8	0.55	0.3	0.48
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	8	0.55	0.3	0.48
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	8	0.54	0.19	0.56
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	8	0.54	0.24	0.54
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	8	0.52	0.28	0.42
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	8	0.5	0.18	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	8	0.5	0.23	0.5
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	8	0.5	0.15	0.56
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	8	0.48	0.39	0.3
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	8	0.48	0.39	0.3
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	8	0.48	0.39	0.3
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	8	0.47	0.11	0.51
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	8	0.47	0.11	0.51
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	8	0.47	0.11	0.51
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	8	0.41	0.09	0.41
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	8	0.41	0.09	0.41
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	8	0.41	0.09	0.41
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD2	8	0.4	0.12	0.43
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD3	8	0.4	0.12	0.43
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	8	0.39	0.12	0.44
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	8	0.37	0.17	0.44
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	8	0.36	0.11	0.35
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	8	0.36	0.11	0.35
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	8	0.36	0.11	0.35
(1,2975)	1:123:B:LYS:HD2	1:137:B:CYS:HA	8	0.35	0.09	0.31
(1,2975)	1:123:B:LYS:HD3	1:137:B:CYS:HA	8	0.35	0.09	0.31
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	8	0.34	0.07	0.36
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	8	0.33	0.19	0.26
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	8	0.32	0.06	0.32
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	8	0.32	0.06	0.32
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	8	0.32	0.06	0.32
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	8	0.32	0.15	0.28
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	8	0.32	0.15	0.28
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	8	0.32	0.15	0.28
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	8	0.32	0.16	0.24
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	8	0.32	0.16	0.24
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	8	0.32	0.16	0.24
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD22	8	0.32	0.09	0.3
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD21	8	0.32	0.09	0.3
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	8	0.31	0.16	0.31
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	8	0.31	0.1	0.32
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	8	0.31	0.1	0.32
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	8	0.31	0.1	0.32
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	8	0.31	0.1	0.32
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	8	0.31	0.1	0.32
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	8	0.31	0.1	0.32
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	8	0.31	0.16	0.26
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	8	0.31	0.16	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	8	0.31	0.16	0.26
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	8	0.31	0.16	0.26
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	8	0.31	0.16	0.26
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	8	0.31	0.16	0.26
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	8	0.3	0.14	0.3
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	8	0.28	0.11	0.3
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	8	0.27	0.14	0.21
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	8	0.27	0.11	0.24
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	8	0.27	0.11	0.24
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	8	0.27	0.11	0.24
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	8	0.26	0.08	0.3
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	8	0.25	0.07	0.28
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	8	0.24	0.13	0.2
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	8	0.24	0.13	0.2
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	8	0.24	0.13	0.2
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	8	0.24	0.06	0.26
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	8	0.24	0.06	0.26
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	8	0.24	0.06	0.26
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	8	0.23	0.14	0.18
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	8	0.22	0.05	0.22
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	8	0.2	0.07	0.22
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	8	0.2	0.08	0.2
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	8	0.2	0.08	0.2
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	8	0.2	0.08	0.2
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	8	0.19	0.03	0.2
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	8	0.18	0.05	0.19
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	8	0.18	0.05	0.19
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	8	0.18	0.05	0.19
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	8	0.18	0.05	0.19
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	8	0.18	0.05	0.19
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	8	0.18	0.05	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	8	0.18	0.05	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	8	0.18	0.05	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	8	0.18	0.05	0.19
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	8	0.18	0.03	0.18
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	8	0.18	0.03	0.18
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	8	0.18	0.03	0.18
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	8	0.18	0.03	0.18
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	8	0.18	0.03	0.18
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	8	0.18	0.03	0.18
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	8	0.18	0.03	0.18
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	8	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	8	0.18	0.03	0.18
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	8	0.18	0.05	0.18
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	8	0.17	0.06	0.16
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	8	0.17	0.06	0.16
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	8	0.17	0.06	0.16
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	8	0.17	0.04	0.18
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	8	0.17	0.04	0.18
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	8	0.17	0.04	0.18
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	8	0.17	0.05	0.18
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	8	0.17	0.05	0.18
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	8	0.17	0.05	0.18
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	8	0.17	0.05	0.14
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	8	0.16	0.05	0.15
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	8	0.16	0.05	0.15
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	8	0.16	0.05	0.15
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	8	0.16	0.05	0.15
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	8	0.16	0.05	0.15
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	8	0.16	0.05	0.15
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	8	0.16	0.05	0.15
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	8	0.16	0.05	0.15
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	8	0.16	0.05	0.15
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	8	0.16	0.03	0.15
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	8	0.16	0.03	0.15
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	8	0.16	0.03	0.15
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	8	0.16	0.03	0.15
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	8	0.16	0.03	0.15
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	8	0.16	0.03	0.15
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	8	0.16	0.03	0.15
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	8	0.16	0.03	0.15
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	8	0.16	0.03	0.15
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	8	0.15	0.02	0.16
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	8	0.15	0.04	0.16
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	8	0.15	0.02	0.15
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	8	0.13	0.01	0.13
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB1	7	2.8	0.93	2.74
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB2	7	2.8	0.93	2.74
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB3	7	2.8	0.93	2.74
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE3	7	2.74	1.52	2.35
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE2	7	2.74	1.52	2.35
(1,2)	1:88:A:ILE:HG21	1:90:A:HIS:HB3	7	1.86	1.16	1.38
(1,2)	1:88:A:ILE:HG22	1:90:A:HIS:HB3	7	1.86	1.16	1.38
(1,2)	1:88:A:ILE:HG23	1:90:A:HIS:HB3	7	1.86	1.16	1.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2283)	1:88:B:ILE:HG21	1:90:B:HIS:HB3	7	1.53	0.92	1.58
(1,2283)	1:88:B:ILE:HG22	1:90:B:HIS:HB3	7	1.53	0.92	1.58
(1,2283)	1:88:B:ILE:HG23	1:90:B:HIS:HB3	7	1.53	0.92	1.58
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG21	7	1.22	1.02	1.37
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG22	7	1.22	1.02	1.37
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG23	7	1.22	1.02	1.37
(1,2061)	1:134:B:ILE:HA	1:140:A:ARG:HD2	7	0.99	0.28	1.14
(1,2193)	1:134:B:ILE:HA	1:140:A:ARG:HD2	7	0.99	0.28	1.14
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB1	7	0.93	0.11	0.96
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB2	7	0.93	0.11	0.96
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB3	7	0.93	0.11	0.96
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE1	7	0.89	0.23	0.99
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE2	7	0.89	0.23	0.99
(1,3566)	1:168:B:PRO:HD2	1:169:B:MET:HA	7	0.76	0.31	0.84
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE1	7	0.75	0.14	0.81
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE2	7	0.75	0.14	0.81
(1,4267)	1:167:B:ALA:H	1:169:B:MET:H	7	0.73	0.33	0.65
(1,1766)	1:149:A:ASP:H	1:169:A:MET:HG3	7	0.68	0.54	0.54
(1,2282)	1:88:B:ILE:HG21	1:90:B:HIS:HA	7	0.64	0.41	0.51
(1,2282)	1:88:B:ILE:HG22	1:90:B:HIS:HA	7	0.64	0.41	0.51
(1,2282)	1:88:B:ILE:HG23	1:90:B:HIS:HA	7	0.64	0.41	0.51
(1,2322)	1:94:B:ARG:HB3	1:167:B:ALA:HA	7	0.61	0.26	0.67
(1,2969)	1:123:B:LYS:HB2	1:137:B:CYS:HB3	7	0.58	0.21	0.57
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD2	7	0.52	0.16	0.52
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD3	7	0.52	0.16	0.52
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG11	7	0.52	0.32	0.39
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG12	7	0.52	0.32	0.39
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG13	7	0.52	0.32	0.39
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD3	7	0.52	0.37	0.44
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD2	7	0.52	0.37	0.44
(1,1654)	1:134:A:ILE:H	1:127:A:ARG:HB2	7	0.45	0.43	0.3
(1,427)	1:111:A:VAL:HG11	1:112:A:LYS:HE3	7	0.41	0.13	0.31
(1,427)	1:111:A:VAL:HG12	1:112:A:LYS:HE3	7	0.41	0.13	0.31
(1,427)	1:111:A:VAL:HG13	1:112:A:LYS:HE3	7	0.41	0.13	0.31
(1,699)	1:125:A:GLU:HA	1:125:A:GLU:HG2	7	0.4	0.15	0.5
(1,3003)	1:126:B:GLU:HG2	1:135:B:SER:HA	7	0.4	0.24	0.28
(1,2790)	1:114:B:LYS:HA	1:114:B:LYS:HB2	7	0.38	0.13	0.44
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG3	7	0.37	0.21	0.29
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG2	7	0.37	0.21	0.29
(1,2561)	1:102:B:ASN:HB3	1:161:B:GLY:HA3	7	0.34	0.22	0.2
(1,718)	1:126:A:GLU:HG2	1:133:A:TYR:HB3	7	0.34	0.11	0.35
(1,2353)	1:95:B:TRP:HB3	1:168:B:PRO:HB3	7	0.34	0.21	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2353)	1:95:B:TRP:HB2	1:168:B:PRO:HB3	7	0.34	0.21	0.28
(1,4197)	1:162:B:THR:H	1:102:B:ASN:HB3	7	0.34	0.23	0.32
(1,51)	1:95:A:TRP:HA	1:95:A:TRP:HB2	7	0.33	0.07	0.37
(1,1193)	1:158:A:SER:HB3	1:160:A:GLU:HB3	7	0.32	0.14	0.34
(1,1097)	1:154:A:SER:HB3	1:155:A:SER:HA	7	0.3	0.08	0.28
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD21	7	0.28	0.08	0.29
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD22	7	0.28	0.08	0.29
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD23	7	0.28	0.08	0.29
(1,2447)	1:97:B:VAL:HG21	1:118:B:VAL:HB	7	0.27	0.09	0.3
(1,2447)	1:97:B:VAL:HG22	1:118:B:VAL:HB	7	0.27	0.09	0.3
(1,2447)	1:97:B:VAL:HG23	1:118:B:VAL:HB	7	0.27	0.09	0.3
(1,3252)	1:146:B:PRO:HG2	1:147:B:GLY:HA2	7	0.27	0.07	0.28
(1,1621)	1:129:A:ASP:H	1:129:A:ASP:HB2	7	0.26	0.05	0.23
(1,2383)	1:96:B:ARG:HB3	1:166:B:GLU:HB3	7	0.26	0.08	0.25
(1,102)	1:96:A:ARG:HB3	1:166:A:GLU:HB3	7	0.26	0.07	0.28
(1,3295)	1:148:B:VAL:HG11	1:170:B:PRO:HG3	7	0.24	0.03	0.25
(1,3295)	1:148:B:VAL:HG12	1:170:B:PRO:HG3	7	0.24	0.03	0.25
(1,3295)	1:148:B:VAL:HG13	1:170:B:PRO:HG3	7	0.24	0.03	0.25
(1,3436)	1:157:B:LEU:HB2	1:163:B:LEU:HA	7	0.24	0.14	0.22
(1,2783)	1:113:B:THR:HG21	1:150:B:PRO:HB3	7	0.22	0.09	0.22
(1,2783)	1:113:B:THR:HG22	1:150:B:PRO:HB3	7	0.22	0.09	0.22
(1,2783)	1:113:B:THR:HG23	1:150:B:PRO:HB3	7	0.22	0.09	0.22
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG21	7	0.21	0.09	0.19
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG22	7	0.21	0.09	0.19
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG23	7	0.21	0.09	0.19
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG21	7	0.21	0.09	0.19
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG22	7	0.21	0.09	0.19
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG23	7	0.21	0.09	0.19
(1,1168)	1:157:A:LEU:HD11	1:161:A:GLY:HA3	7	0.21	0.05	0.19
(1,1168)	1:157:A:LEU:HD12	1:161:A:GLY:HA3	7	0.21	0.05	0.19
(1,1168)	1:157:A:LEU:HD13	1:161:A:GLY:HA3	7	0.21	0.05	0.19
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG11	7	0.19	0.06	0.19
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG12	7	0.19	0.06	0.19
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG13	7	0.19	0.06	0.19
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG21	7	0.18	0.06	0.15
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG22	7	0.18	0.06	0.15
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG23	7	0.18	0.06	0.15
(1,1149)	1:157:A:LEU:HA	1:163:A:LEU:HB3	7	0.18	0.07	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD21	7	0.16	0.04	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD22	7	0.16	0.04	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD23	7	0.16	0.04	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD11	7	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD12	7	0.16	0.04	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD13	7	0.16	0.04	0.15
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD11	7	0.16	0.03	0.16
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD12	7	0.16	0.03	0.16
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD13	7	0.16	0.03	0.16
(1,1657)	1:134:A:ILE:H	1:133:A:TYR:HB3	7	0.16	0.04	0.14
(1,3936)	1:134:B:ILE:H	1:127:B:ARG:HG2	7	0.16	0.04	0.15
(1,680)	1:123:A:LYS:HA	1:123:A:LYS:HG3	7	0.15	0.02	0.16
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG21	7	0.15	0.04	0.16
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG22	7	0.15	0.04	0.16
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG23	7	0.15	0.04	0.16
(1,23)	1:94:A:ARG:HA	1:94:A:ARG:HB3	7	0.15	0.03	0.13
(1,502)	1:113:A:THR:HG21	1:150:A:PRO:HB3	7	0.14	0.04	0.12
(1,502)	1:113:A:THR:HG22	1:150:A:PRO:HB3	7	0.14	0.04	0.12
(1,502)	1:113:A:THR:HG23	1:150:A:PRO:HB3	7	0.14	0.04	0.12
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD1	7	0.14	0.04	0.13
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD2	7	0.14	0.04	0.13
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD1	7	0.14	0.04	0.13
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD2	7	0.14	0.04	0.13
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD1	7	0.14	0.04	0.13
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD2	7	0.14	0.04	0.13
(1,3288)	1:148:B:VAL:HG11	1:153:B:VAL:HA	7	0.13	0.03	0.12
(1,3288)	1:148:B:VAL:HG12	1:153:B:VAL:HA	7	0.13	0.03	0.12
(1,3288)	1:148:B:VAL:HG13	1:153:B:VAL:HA	7	0.13	0.03	0.12
(1,4034)	1:148:B:VAL:H	1:149:B:ASP:H	7	0.13	0.04	0.11
(1,1)	1:88:A:ILE:HG21	1:90:A:HIS:HA	6	1.22	0.81	0.8
(1,1)	1:88:A:ILE:HG22	1:90:A:HIS:HA	6	1.22	0.81	0.8
(1,1)	1:88:A:ILE:HG23	1:90:A:HIS:HA	6	1.22	0.81	0.8
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD1	6	1.18	0.49	1.25
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD2	6	1.18	0.49	1.25
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD1	6	1.01	0.4	0.92
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD2	6	1.01	0.4	0.92
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG21	6	0.98	0.57	0.84
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG22	6	0.98	0.57	0.84
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG23	6	0.98	0.57	0.84
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE1	6	0.97	0.08	0.98
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE2	6	0.97	0.08	0.98
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE1	6	0.97	0.08	0.98
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE2	6	0.97	0.08	0.98
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE1	6	0.97	0.08	0.98
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE2	6	0.97	0.08	0.98
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE1	6	0.97	0.26	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE2	6	0.97	0.26	0.96
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB1	6	0.95	0.66	0.72
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB2	6	0.95	0.66	0.72
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB3	6	0.95	0.66	0.72
(1,2025)	1:132:B:GLY:HA2	1:140:A:ARG:HA	6	0.84	0.48	0.89
(1,2157)	1:132:B:GLY:HA2	1:140:A:ARG:HA	6	0.84	0.48	0.89
(1,990)	1:148:A:VAL:HA	1:169:A:MET:HB2	6	0.75	0.32	0.85
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE1	6	0.72	0.34	0.83
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE2	6	0.72	0.34	0.83
(1,1012)	1:148:A:VAL:HG11	1:169:A:MET:HB2	6	0.68	0.28	0.78
(1,1012)	1:148:A:VAL:HG12	1:169:A:MET:HB2	6	0.68	0.28	0.78
(1,1012)	1:148:A:VAL:HG13	1:169:A:MET:HB2	6	0.68	0.28	0.78
(1,710)	1:126:A:GLU:HA	1:135:A:SER:HB2	6	0.65	0.28	0.66
(1,1916)	1:162:A:THR:H	1:102:A:ASN:HB3	6	0.63	0.21	0.58
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG21	6	0.63	0.08	0.64
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG22	6	0.63	0.08	0.64
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG23	6	0.63	0.08	0.64
(1,722)	1:126:A:GLU:HG2	1:135:A:SER:HA	6	0.6	0.25	0.48
(1,2907)	1:120:B:ILE:HA	1:120:B:ILE:HG13	6	0.55	0.03	0.54
(1,688)	1:123:A:LYS:HB2	1:137:A:CYS:HB3	6	0.52	0.18	0.5
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB1	6	0.49	0.26	0.6
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB2	6	0.49	0.26	0.6
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB3	6	0.49	0.26	0.6
(1,684)	1:123:A:LYS:HA	1:135:A:SER:HB3	6	0.48	0.3	0.49
(1,2053)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	6	0.47	0.13	0.51
(1,2053)	1:133:A:TYR:HB3	1:141:B:LYS:HD3	6	0.47	0.13	0.51
(1,2185)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	6	0.47	0.13	0.51
(1,2185)	1:133:A:TYR:HB3	1:141:B:LYS:HD3	6	0.47	0.13	0.51
(1,1998)	1:169:A:MET:H	1:169:A:MET:HB2	6	0.46	0.26	0.34
(1,723)	1:126:A:GLU:HG2	1:135:A:SER:HB2	6	0.44	0.16	0.5
(1,3612)	1:95:B:TRP:H	1:95:B:TRP:HB2	6	0.44	0.05	0.43
(1,827)	1:139:A:THR:HA	1:140:A:ARG:HG2	6	0.43	0.26	0.28
(1,99)	1:96:A:ARG:HB3	1:164:A:THR:HB	6	0.43	0.16	0.37
(1,3904)	1:129:B:ASP:H	1:130:B:GLU:HG3	6	0.43	0.16	0.42
(1,3904)	1:129:B:ASP:H	1:130:B:GLU:HG2	6	0.43	0.16	0.42
(1,2081)	1:134:A:ILE:HA	1:140:B:ARG:HD3	6	0.43	0.22	0.38
(1,2213)	1:134:A:ILE:HA	1:140:B:ARG:HD3	6	0.43	0.22	0.38
(1,2687)	1:110:B:THR:HG21	1:112:B:LYS:HE3	6	0.41	0.21	0.4
(1,2687)	1:110:B:THR:HG22	1:112:B:LYS:HE3	6	0.41	0.21	0.4
(1,2687)	1:110:B:THR:HG23	1:112:B:LYS:HE3	6	0.41	0.21	0.4
(1,2687)	1:110:B:THR:HG21	1:112:B:LYS:HE2	6	0.41	0.21	0.4
(1,2687)	1:110:B:THR:HG22	1:112:B:LYS:HE2	6	0.41	0.21	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2687)	1:110:B:THR:HG23	1:112:B:LYS:HE2	6	0.41	0.21	0.4
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB1	6	0.39	0.2	0.47
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB2	6	0.39	0.2	0.47
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB3	6	0.39	0.2	0.47
(1,3460)	1:157:B:LEU:HD21	1:163:B:LEU:HB3	6	0.38	0.11	0.42
(1,3460)	1:157:B:LEU:HD22	1:163:B:LEU:HB3	6	0.38	0.11	0.42
(1,3460)	1:157:B:LEU:HD23	1:163:B:LEU:HB3	6	0.38	0.11	0.42
(1,3491)	1:160:B:GLU:HB2	1:162:B:THR:HB	6	0.38	0.12	0.38
(1,3137)	1:141:B:LYS:HG2	1:142:B:TYR:HB3	6	0.38	0.11	0.37
(1,2037)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	6	0.35	0.11	0.34
(1,2169)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	6	0.35	0.11	0.34
(1,1637)	1:131:A:HIS:H	1:130:A:GLU:HG3	6	0.35	0.2	0.34
(1,1637)	1:131:A:HIS:H	1:130:A:GLU:HG2	6	0.35	0.2	0.34
(1,2996)	1:126:B:GLU:HB2	1:135:B:SER:HB3	6	0.33	0.22	0.24
(1,9)	1:90:A:HIS:HB3	1:91:A:THR:HA	6	0.33	0.18	0.27
(1,3847)	1:123:B:LYS:H	1:109:B:LEU:HB2	6	0.32	0.06	0.32
(1,1210)	1:160:A:GLU:HB2	1:162:A:THR:HB	6	0.3	0.14	0.23
(1,2045)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	6	0.3	0.13	0.26
(1,2045)	1:133:B:TYR:HB3	1:141:A:LYS:HD3	6	0.3	0.13	0.26
(1,2177)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	6	0.3	0.13	0.26
(1,2177)	1:133:B:TYR:HB3	1:141:A:LYS:HD3	6	0.3	0.13	0.26
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG21	6	0.29	0.02	0.3
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG22	6	0.29	0.02	0.3
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG23	6	0.29	0.02	0.3
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD11	6	0.29	0.03	0.3
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD12	6	0.29	0.03	0.3
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD13	6	0.29	0.03	0.3
(1,3748)	1:113:B:THR:H	1:112:B:LYS:HB2	6	0.29	0.08	0.28
(1,3139)	1:141:B:LYS:HG3	1:141:B:LYS:HE2	6	0.29	0.05	0.3
(1,2736)	1:112:B:LYS:HB2	1:112:B:LYS:HE3	6	0.28	0.08	0.29
(1,2736)	1:112:B:LYS:HB2	1:112:B:LYS:HE2	6	0.28	0.08	0.29
(1,2708)	1:111:B:VAL:HG11	1:112:B:LYS:HE3	6	0.28	0.14	0.26
(1,2708)	1:111:B:VAL:HG12	1:112:B:LYS:HE3	6	0.28	0.14	0.26
(1,2708)	1:111:B:VAL:HG13	1:112:B:LYS:HE3	6	0.28	0.14	0.26
(1,2708)	1:111:B:VAL:HG11	1:112:B:LYS:HE2	6	0.28	0.14	0.26
(1,2708)	1:111:B:VAL:HG12	1:112:B:LYS:HE2	6	0.28	0.14	0.26
(1,2708)	1:111:B:VAL:HG13	1:112:B:LYS:HE2	6	0.28	0.14	0.26
(1,4262)	1:167:B:ALA:H	1:166:B:GLU:HB2	6	0.28	0.14	0.26
(1,1197)	1:158:A:SER:HB3	1:159:A:PRO:HD3	6	0.26	0.1	0.24
(1,1634)	1:131:A:HIS:H	1:129:A:ASP:HB3	6	0.24	0.06	0.22
(1,3018)	1:127:B:ARG:HA	1:127:B:ARG:HD3	6	0.24	0.07	0.25
(1,2738)	1:112:B:LYS:HB2	1:120:B:ILE:HA	6	0.23	0.08	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3915)	1:131:B:HIS:H	1:129:B:ASP:HB3	6	0.22	0.09	0.22
(1,4128)	1:155:B:SER:H	1:154:B:SER:HB2	6	0.22	0.08	0.22
(1,2929)	1:120:B:ILE:HG21	1:139:B:THR:HA	6	0.22	0.06	0.22
(1,2929)	1:120:B:ILE:HG22	1:139:B:THR:HA	6	0.22	0.06	0.22
(1,2929)	1:120:B:ILE:HG23	1:139:B:THR:HA	6	0.22	0.06	0.22
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD1	6	0.21	0.07	0.22
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD2	6	0.21	0.07	0.22
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD1	6	0.21	0.07	0.22
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD2	6	0.21	0.07	0.22
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD1	6	0.21	0.07	0.22
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD2	6	0.21	0.07	0.22
(1,2083)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	6	0.2	0.05	0.22
(1,2215)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	6	0.2	0.05	0.22
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG21	6	0.2	0.06	0.19
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG22	6	0.2	0.06	0.19
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG23	6	0.2	0.06	0.19
(1,1173)	1:157:A:LEU:HD11	1:163:A:LEU:HB3	6	0.2	0.04	0.2
(1,1173)	1:157:A:LEU:HD12	1:163:A:LEU:HB3	6	0.2	0.04	0.2
(1,1173)	1:157:A:LEU:HD13	1:163:A:LEU:HB3	6	0.2	0.04	0.2
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD21	6	0.19	0.06	0.2
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD22	6	0.19	0.06	0.2
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD23	6	0.19	0.06	0.2
(1,2928)	1:120:B:ILE:HG21	1:122:B:GLY:HA3	6	0.19	0.05	0.18
(1,2928)	1:120:B:ILE:HG22	1:122:B:GLY:HA3	6	0.19	0.05	0.18
(1,2928)	1:120:B:ILE:HG23	1:122:B:GLY:HA3	6	0.19	0.05	0.18
(1,654)	1:120:A:ILE:HD11	1:140:A:ARG:HD2	6	0.18	0.09	0.15
(1,654)	1:120:A:ILE:HD12	1:140:A:ARG:HD2	6	0.18	0.09	0.15
(1,654)	1:120:A:ILE:HD13	1:140:A:ARG:HD2	6	0.18	0.09	0.15
(1,279)	1:102:A:ASN:HB3	1:161:A:GLY:HA2	6	0.18	0.03	0.18
(1,3358)	1:153:B:VAL:HA	1:168:B:PRO:HD2	6	0.18	0.03	0.18
(1,652)	1:120:A:ILE:HD11	1:140:A:ARG:HB2	6	0.17	0.09	0.14
(1,652)	1:120:A:ILE:HD12	1:140:A:ARG:HB2	6	0.17	0.09	0.14
(1,652)	1:120:A:ILE:HD13	1:140:A:ARG:HB2	6	0.17	0.09	0.14
(1,1647)	1:132:A:GLY:H	1:131:A:HIS:HB3	6	0.17	0.03	0.18
(1,4263)	1:167:B:ALA:H	1:166:B:GLU:HB3	6	0.17	0.06	0.16
(1,664)	1:121:A:THR:HA	1:139:A:THR:HA	6	0.17	0.04	0.16
(1,1391)	1:105:A:ALA:H	1:108:A:GLU:HB3	6	0.16	0.03	0.18
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG21	6	0.15	0.04	0.15
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG22	6	0.15	0.04	0.15
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG23	6	0.15	0.04	0.15
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD11	6	0.14	0.04	0.12
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD12	6	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD13	6	0.14	0.04	0.12
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG21	6	0.13	0.02	0.13
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG22	6	0.13	0.02	0.13
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG23	6	0.13	0.02	0.13
(1,1079)	1:153:A:VAL:HB	1:154:A:SER:HA	6	0.13	0.02	0.12
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG21	6	0.12	0.02	0.12
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG22	6	0.12	0.02	0.12
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG23	6	0.12	0.02	0.12
(1,3928)	1:132:B:GLY:H	1:131:B:HIS:HB3	6	0.12	0.01	0.12
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD1	6	0.11	0.01	0.11
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD2	6	0.11	0.01	0.11
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD1	6	0.11	0.01	0.11
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD2	6	0.11	0.01	0.11
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD1	6	0.11	0.01	0.11
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD2	6	0.11	0.01	0.11
(1,1311)	1:170:A:PRO:HB2	1:170:A:PRO:HG2	6	0.11	0.01	0.11
(1,3592)	1:170:B:PRO:HB2	1:170:B:PRO:HG2	6	0.11	0.0	0.11
(1,1301)	1:169:A:MET:HB3	1:171:A:LYS:HG2	5	1.25	0.28	1.13
(1,1301)	1:169:A:MET:HB3	1:171:A:LYS:HG3	5	1.25	0.28	1.13
(1,2004)	1:171:A:LYS:H	1:169:A:MET:HA	5	1.01	0.29	0.87
(1,3346)	1:152:B:GLN:HB2	1:169:B:MET:HA	5	0.71	0.27	0.77
(1,7)	1:90:A:HIS:HB2	1:91:A:THR:HA	5	0.65	0.26	0.63
(1,1691)	1:140:A:ARG:H	1:120:A:ILE:HB	5	0.64	0.09	0.65
(1,2062)	1:134:B:ILE:HA	1:140:A:ARG:HD3	5	0.63	0.34	0.49
(1,2194)	1:134:B:ILE:HA	1:140:A:ARG:HD3	5	0.63	0.34	0.49
(1,4255)	1:167:B:ALA:H	1:95:B:TRP:HB3	5	0.63	0.22	0.63
(1,3763)	1:114:B:LYS:H	1:115:B:ASP:HB2	5	0.61	0.23	0.64
(1,626)	1:120:A:ILE:HA	1:120:A:ILE:HG13	5	0.56	0.02	0.55
(1,4095)	1:152:B:GLN:HE22	1:170:B:PRO:HD3	5	0.52	0.16	0.5
(1,232)	1:99:A:LEU:HD11	1:120:A:ILE:HG12	5	0.52	0.16	0.59
(1,232)	1:99:A:LEU:HD12	1:120:A:ILE:HG12	5	0.52	0.16	0.59
(1,232)	1:99:A:LEU:HD13	1:120:A:ILE:HG12	5	0.52	0.16	0.59
(1,2314)	1:94:B:ARG:HA	1:169:B:MET:HB2	5	0.51	0.12	0.45
(1,3005)	1:126:B:GLU:HG2	1:135:B:SER:HB3	5	0.5	0.47	0.22
(1,3274)	1:148:B:VAL:HA	1:170:B:PRO:HG2	5	0.46	0.27	0.48
(1,1799)	1:152:A:GLN:HE21	1:152:A:GLN:HB3	5	0.45	0.2	0.43
(1,4280)	1:169:B:MET:H	1:169:B:MET:HB3	5	0.45	0.23	0.45
(1,682)	1:123:A:LYS:HA	1:123:A:LYS:HE3	5	0.42	0.16	0.44
(1,682)	1:123:A:LYS:HA	1:123:A:LYS:HE2	5	0.42	0.16	0.44
(1,449)	1:112:A:LYS:HA	1:112:A:LYS:HE2	5	0.4	0.14	0.47
(1,449)	1:112:A:LYS:HA	1:112:A:LYS:HE3	5	0.4	0.14	0.47
(1,2000)	1:169:A:MET:H	1:169:A:MET:HG3	5	0.4	0.23	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3345)	1:152:B:GLN:HB2	1:168:B:PRO:HD3	5	0.4	0.23	0.38
(1,528)	1:116:A:GLY:HA2	1:148:A:VAL:HB	5	0.36	0.08	0.33
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD1	5	0.33	0.04	0.33
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD2	5	0.33	0.04	0.33
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD1	5	0.33	0.04	0.33
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD2	5	0.33	0.04	0.33
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD1	5	0.33	0.04	0.33
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD2	5	0.33	0.04	0.33
(1,3902)	1:129:B:ASP:H	1:129:B:ASP:HB2	5	0.32	0.06	0.34
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD11	5	0.32	0.12	0.26
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD12	5	0.32	0.12	0.26
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD13	5	0.32	0.12	0.26
(1,4205)	1:162:B:THR:H	1:160:B:GLU:HB2	5	0.31	0.08	0.31
(1,3848)	1:123:B:LYS:H	1:109:B:LEU:HG	5	0.3	0.13	0.24
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE1	5	0.29	0.1	0.28
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE2	5	0.29	0.1	0.28
(1,2993)	1:126:B:GLU:HB3	1:133:B:TYR:HB2	5	0.29	0.18	0.16
(1,2993)	1:126:B:GLU:HB2	1:133:B:TYR:HB2	5	0.29	0.18	0.16
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG21	5	0.27	0.03	0.27
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG22	5	0.27	0.03	0.27
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG23	5	0.27	0.03	0.27
(1,1847)	1:155:A:SER:H	1:154:A:SER:HB2	5	0.27	0.07	0.29
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD11	5	0.27	0.15	0.21
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD12	5	0.27	0.15	0.21
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD13	5	0.27	0.15	0.21
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD11	5	0.25	0.07	0.27
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD12	5	0.25	0.07	0.27
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD13	5	0.25	0.07	0.27
(1,1816)	1:153:A:VAL:H	1:149:A:ASP:HB2	5	0.24	0.11	0.21
(1,1065)	1:152:A:GLN:HB2	1:169:A:MET:HA	5	0.24	0.07	0.24
(1,858)	1:141:A:LYS:HG3	1:141:A:LYS:HE2	5	0.22	0.07	0.2
(1,1626)	1:129:A:ASP:H	1:132:A:GLY:HA3	5	0.22	0.04	0.23
(1,1280)	1:168:A:PRO:HB2	1:170:A:PRO:HD3	5	0.22	0.1	0.24
(1,3249)	1:146:B:PRO:HB3	1:147:B:GLY:HA3	5	0.22	0.18	0.13
(1,3474)	1:158:B:SER:HB3	1:160:B:GLU:HB3	5	0.22	0.12	0.13
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD1	5	0.21	0.12	0.15
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD2	5	0.21	0.12	0.15
(1,1703)	1:142:A:TYR:H	1:141:A:LYS:HG3	5	0.21	0.06	0.22
(1,1703)	1:142:A:TYR:H	1:141:A:LYS:HG2	5	0.21	0.06	0.22
(1,80)	1:96:A:ARG:HA	1:96:A:ARG:HD2	5	0.21	0.06	0.23
(1,80)	1:96:A:ARG:HA	1:96:A:ARG:HD3	5	0.21	0.06	0.23
(1,3910)	1:129:B:ASP:H	1:133:B:TYR:HB2	5	0.21	0.1	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3955)	1:137:B:CYS:H	1:136:B:ARG:HB3	5	0.21	0.07	0.22
(1,4182)	1:161:B:GLY:H	1:102:B:ASN:HB2	5	0.2	0.08	0.2
(1,1598)	1:128:A:GLN:H	1:127:A:ARG:HG2	5	0.2	0.08	0.22
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD21	5	0.2	0.08	0.16
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD22	5	0.2	0.08	0.16
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD23	5	0.2	0.08	0.16
(1,3454)	1:157:B:LEU:HD11	1:163:B:LEU:HB3	5	0.19	0.05	0.17
(1,3454)	1:157:B:LEU:HD12	1:163:B:LEU:HB3	5	0.19	0.05	0.17
(1,3454)	1:157:B:LEU:HD13	1:163:B:LEU:HB3	5	0.19	0.05	0.17
(1,1580)	1:125:A:GLU:H	1:108:A:GLU:HG2	5	0.18	0.07	0.21
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD11	5	0.18	0.05	0.18
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD12	5	0.18	0.05	0.18
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD13	5	0.18	0.05	0.18
(1,2977)	1:123:B:LYS:HD3	1:137:B:CYS:HB3	5	0.18	0.09	0.11
(1,2977)	1:123:B:LYS:HD2	1:137:B:CYS:HB3	5	0.18	0.09	0.11
(1,1525)	1:119:A:GLU:H	1:114:A:LYS:HB3	5	0.17	0.05	0.17
(1,3430)	1:157:B:LEU:HA	1:163:B:LEU:HB3	5	0.17	0.02	0.16
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG21	5	0.17	0.02	0.17
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG22	5	0.17	0.02	0.17
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG23	5	0.17	0.02	0.17
(1,782)	1:131:A:HIS:HB2	1:132:A:GLY:HA2	5	0.16	0.06	0.13
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG21	5	0.16	0.04	0.14
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG22	5	0.16	0.04	0.14
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG23	5	0.16	0.04	0.14
(1,1901)	1:161:A:GLY:H	1:102:A:ASN:HB2	5	0.16	0.02	0.16
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG21	5	0.16	0.05	0.13
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG22	5	0.16	0.05	0.13
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG23	5	0.16	0.05	0.13
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG21	5	0.16	0.05	0.13
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG22	5	0.16	0.05	0.13
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG23	5	0.16	0.05	0.13
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG21	5	0.16	0.05	0.13
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG22	5	0.16	0.05	0.13
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG23	5	0.16	0.05	0.13
(1,605)	1:119:A:GLU:HA	1:120:A:ILE:HG13	5	0.15	0.01	0.16
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD21	5	0.15	0.03	0.16
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD22	5	0.15	0.03	0.16
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD23	5	0.15	0.03	0.16
(1,1282)	1:168:A:PRO:HB3	1:169:A:MET:HA	5	0.15	0.04	0.14
(1,3391)	1:155:B:SER:HA	1:165:B:VAL:HA	5	0.15	0.03	0.15
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG21	5	0.14	0.02	0.15
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG22	5	0.14	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG23	5	0.14	0.02	0.15
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE1	5	0.14	0.04	0.13
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE2	5	0.14	0.04	0.13
(1,857)	1:141:A:LYS:HG2	1:143:A:THR:HA	5	0.14	0.03	0.14
(1,1588)	1:126:A:GLU:H	1:125:A:GLU:HG3	5	0.14	0.02	0.13
(1,2442)	1:97:B:VAL:HG21	1:166:B:GLU:HA	5	0.14	0.03	0.12
(1,2442)	1:97:B:VAL:HG22	1:166:B:GLU:HA	5	0.14	0.03	0.12
(1,2442)	1:97:B:VAL:HG23	1:166:B:GLU:HA	5	0.14	0.03	0.12
(1,1110)	1:155:A:SER:HA	1:165:A:VAL:HA	5	0.14	0.01	0.14
(1,2831)	1:117:B:VAL:HA	1:148:B:VAL:HB	5	0.14	0.03	0.15
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG21	5	0.14	0.03	0.13
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG22	5	0.14	0.03	0.13
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG23	5	0.14	0.03	0.13
(1,3015)	1:127:B:ARG:HA	1:127:B:ARG:HB3	5	0.14	0.04	0.13
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG21	5	0.13	0.02	0.14
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG22	5	0.13	0.02	0.14
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG23	5	0.13	0.02	0.14
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD21	5	0.12	0.02	0.12
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD22	5	0.12	0.02	0.12
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD23	5	0.12	0.02	0.12
(1,734)	1:127:A:ARG:HA	1:127:A:ARG:HB3	5	0.12	0.02	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD11	5	0.12	0.01	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD12	5	0.12	0.01	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD13	5	0.12	0.01	0.11
(1,724)	1:126:A:GLU:HG2	1:135:A:SER:HB3	4	0.95	0.32	1.06
(1,16)	1:93:A:ASP:HA	1:94:A:ARG:HD2	4	0.86	0.4	0.8
(1,4076)	1:152:B:GLN:H	1:170:B:PRO:HD2	4	0.7	0.32	0.79
(1,4076)	1:152:B:GLN:H	1:170:B:PRO:HD3	4	0.7	0.32	0.79
(1,728)	1:126:A:GLU:HG3	1:133:A:TYR:HA	4	0.62	0.21	0.64
(1,2009)	1:171:A:LYS:H	1:171:A:LYS:HB2	4	0.6	0.26	0.6
(1,2009)	1:171:A:LYS:H	1:171:A:LYS:HB3	4	0.6	0.26	0.6
(1,2007)	1:171:A:LYS:H	1:170:A:PRO:HD3	4	0.55	0.21	0.59
(1,3895)	1:128:B:GLN:HE21	1:128:B:GLN:HB2	4	0.55	0.14	0.5
(1,3126)	1:141:B:LYS:HA	1:141:B:LYS:HD3	4	0.52	0.07	0.56
(1,3126)	1:141:B:LYS:HA	1:141:B:LYS:HD2	4	0.52	0.07	0.56
(1,1288)	1:169:A:MET:HA	1:169:A:MET:HG2	4	0.52	0.11	0.52
(1,4024)	1:148:B:VAL:H	1:146:B:PRO:HB3	4	0.5	0.1	0.53
(1,1322)	1:94:A:ARG:H	1:93:A:ASP:HB2	4	0.48	0.11	0.48
(1,2318)	1:94:B:ARG:HB2	1:96:B:ARG:HA	4	0.47	0.33	0.36
(1,3972)	1:140:B:ARG:H	1:120:B:ILE:HB	4	0.47	0.12	0.5
(1,255)	1:99:A:LEU:HD21	1:109:A:LEU:HG	4	0.46	0.13	0.52
(1,255)	1:99:A:LEU:HD22	1:109:A:LEU:HG	4	0.46	0.13	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,255)	1:99:A:LEU:HD23	1:109:A:LEU:HG	4	0.46	0.13	0.52
(1,3116)	1:139:B:THR:HG21	1:141:B:LYS:HE2	4	0.45	0.14	0.49
(1,3116)	1:139:B:THR:HG22	1:141:B:LYS:HE2	4	0.45	0.14	0.49
(1,3116)	1:139:B:THR:HG23	1:141:B:LYS:HE2	4	0.45	0.14	0.49
(1,1114)	1:155:A:SER:HB2	1:163:A:LEU:HA	4	0.45	0.16	0.48
(1,4025)	1:148:B:VAL:H	1:146:B:PRO:HG2	4	0.45	0.12	0.48
(1,2148)	1:143:A:THR:H	1:132:B:GLY:HA2	4	0.44	0.23	0.38
(1,2281)	1:143:A:THR:H	1:132:B:GLY:HA2	4	0.44	0.23	0.38
(1,2980)	1:125:B:GLU:HA	1:125:B:GLU:HG2	4	0.42	0.15	0.5
(1,2299)	1:93:B:ASP:HB2	1:94:B:ARG:HA	4	0.4	0.08	0.37
(1,3569)	1:169:B:MET:HA	1:169:B:MET:HG2	4	0.4	0.23	0.4
(1,455)	1:112:A:LYS:HB2	1:112:A:LYS:HE2	4	0.39	0.07	0.42
(1,455)	1:112:A:LYS:HB2	1:112:A:LYS:HE3	4	0.39	0.07	0.42
(1,405)	1:110:A:THR:HG21	1:112:A:LYS:HD2	4	0.38	0.22	0.34
(1,405)	1:110:A:THR:HG22	1:112:A:LYS:HD2	4	0.38	0.22	0.34
(1,405)	1:110:A:THR:HG23	1:112:A:LYS:HD2	4	0.38	0.22	0.34
(1,405)	1:110:A:THR:HG21	1:112:A:LYS:HD3	4	0.38	0.22	0.34
(1,405)	1:110:A:THR:HG22	1:112:A:LYS:HD3	4	0.38	0.22	0.34
(1,405)	1:110:A:THR:HG23	1:112:A:LYS:HD3	4	0.38	0.22	0.34
(1,2930)	1:120:B:ILE:HG21	1:140:B:ARG:HA	4	0.38	0.14	0.36
(1,2930)	1:120:B:ILE:HG22	1:140:B:ARG:HA	4	0.38	0.14	0.36
(1,2930)	1:120:B:ILE:HG23	1:140:B:ARG:HA	4	0.38	0.14	0.36
(1,1277)	1:168:A:PRO:HA	1:169:A:MET:HG3	4	0.38	0.24	0.38
(1,4084)	1:152:B:GLN:HE21	1:168:B:PRO:HD2	4	0.38	0.13	0.39
(1,434)	1:111:A:VAL:HG11	1:120:A:ILE:HG12	4	0.37	0.08	0.39
(1,434)	1:111:A:VAL:HG12	1:120:A:ILE:HG12	4	0.37	0.08	0.39
(1,434)	1:111:A:VAL:HG13	1:120:A:ILE:HG12	4	0.37	0.08	0.39
(1,1756)	1:148:A:VAL:H	1:170:A:PRO:HG3	4	0.36	0.13	0.36
(1,845)	1:141:A:LYS:HA	1:141:A:LYS:HD3	4	0.36	0.17	0.34
(1,845)	1:141:A:LYS:HA	1:141:A:LYS:HD2	4	0.36	0.17	0.34
(1,1664)	1:135:A:SER:H	1:134:A:ILE:HG13	4	0.36	0.11	0.38
(1,2971)	1:123:B:LYS:HB3	1:137:B:CYS:HB2	4	0.35	0.12	0.34
(1,690)	1:123:A:LYS:HB3	1:137:A:CYS:HB2	4	0.34	0.13	0.38
(1,3604)	1:94:B:ARG:H	1:93:B:ASP:HB3	4	0.32	0.11	0.29
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD21	4	0.31	0.14	0.32
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD22	4	0.31	0.14	0.32
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD23	4	0.31	0.14	0.32
(1,712)	1:126:A:GLU:HB3	1:133:A:TYR:HB2	4	0.29	0.18	0.28
(1,1642)	1:132:A:GLY:H	1:129:A:ASP:HB2	4	0.29	0.16	0.26
(1,166)	1:97:A:VAL:HG21	1:118:A:VAL:HB	4	0.29	0.07	0.3
(1,166)	1:97:A:VAL:HG22	1:118:A:VAL:HB	4	0.29	0.07	0.3
(1,166)	1:97:A:VAL:HG23	1:118:A:VAL:HB	4	0.29	0.07	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,166)	1:97:A:VAL:HG11	1:118:A:VAL:HB	4	0.29	0.07	0.3
(1,166)	1:97:A:VAL:HG12	1:118:A:VAL:HB	4	0.29	0.07	0.3
(1,166)	1:97:A:VAL:HG13	1:118:A:VAL:HB	4	0.29	0.07	0.3
(1,2963)	1:123:B:LYS:HA	1:123:B:LYS:HE3	4	0.28	0.16	0.28
(1,2963)	1:123:B:LYS:HA	1:123:B:LYS:HE2	4	0.28	0.16	0.28
(1,2753)	1:112:B:LYS:HD3	1:120:B:ILE:HA	4	0.27	0.15	0.24
(1,2753)	1:112:B:LYS:HD2	1:120:B:ILE:HA	4	0.27	0.15	0.24
(1,2332)	1:95:B:TRP:HA	1:95:B:TRP:HB2	4	0.27	0.08	0.25
(1,2568)	1:105:B:ALA:HA	1:108:B:GLU:HB3	4	0.27	0.1	0.29
(1,2617)	1:108:B:GLU:HA	1:108:B:GLU:HG2	4	0.26	0.1	0.28
(1,2935)	1:120:B:ILE:HD11	1:140:B:ARG:HD2	4	0.26	0.1	0.26
(1,2935)	1:120:B:ILE:HD12	1:140:B:ARG:HD2	4	0.26	0.1	0.26
(1,2935)	1:120:B:ILE:HD13	1:140:B:ARG:HD2	4	0.26	0.1	0.26
(1,3935)	1:134:B:ILE:H	1:127:B:ARG:HB2	4	0.26	0.08	0.29
(1,3302)	1:148:B:VAL:HG21	1:169:B:MET:HB3	4	0.25	0.06	0.25
(1,3302)	1:148:B:VAL:HG22	1:169:B:MET:HB3	4	0.25	0.06	0.25
(1,3302)	1:148:B:VAL:HG23	1:169:B:MET:HB3	4	0.25	0.06	0.25
(1,457)	1:112:A:LYS:HB2	1:120:A:ILE:HA	4	0.24	0.06	0.22
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD21	4	0.24	0.06	0.22
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD22	4	0.24	0.06	0.22
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD23	4	0.24	0.06	0.22
(1,1314)	1:170:A:PRO:HB3	1:170:A:PRO:HD3	4	0.23	0.03	0.22
(1,1314)	1:170:A:PRO:HB3	1:170:A:PRO:HD2	4	0.23	0.03	0.22
(1,3806)	1:119:B:GLU:H	1:114:B:LYS:HB3	4	0.23	0.1	0.2
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD1	4	0.23	0.1	0.23
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD2	4	0.23	0.1	0.23
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD1	4	0.23	0.1	0.23
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD2	4	0.23	0.1	0.23
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD1	4	0.23	0.1	0.23
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD2	4	0.23	0.1	0.23
(1,3907)	1:129:B:ASP:H	1:132:B:GLY:HA3	4	0.23	0.07	0.21
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG21	4	0.22	0.1	0.2
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG22	4	0.22	0.1	0.2
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG23	4	0.22	0.1	0.2
(1,1743)	1:148:A:VAL:H	1:146:A:PRO:HB3	4	0.22	0.15	0.15
(1,3138)	1:141:B:LYS:HG2	1:143:B:THR:HA	4	0.22	0.04	0.22
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG21	4	0.22	0.1	0.18
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG22	4	0.22	0.1	0.18
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG23	4	0.22	0.1	0.18
(1,1902)	1:161:A:GLY:H	1:102:A:ASN:HB3	4	0.21	0.06	0.2
(1,831)	1:139:A:THR:HB	1:141:A:LYS:HE2	4	0.21	0.06	0.21
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD11	4	0.21	0.05	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD12	4	0.21	0.05	0.23
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD13	4	0.21	0.05	0.23
(1,648)	1:120:A:ILE:HG21	1:139:A:THR:HA	4	0.2	0.08	0.2
(1,648)	1:120:A:ILE:HG22	1:139:A:THR:HA	4	0.2	0.08	0.2
(1,648)	1:120:A:ILE:HG23	1:139:A:THR:HA	4	0.2	0.08	0.2
(1,1796)	1:152:A:GLN:HE21	1:149:A:ASP:HB2	4	0.2	0.04	0.22
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD1	4	0.2	0.06	0.22
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD2	4	0.2	0.06	0.22
(1,337)	1:108:A:GLU:HA	1:108:A:GLU:HG3	4	0.2	0.04	0.18
(1,2560)	1:102:B:ASN:HB3	1:161:B:GLY:HA2	4	0.19	0.03	0.2
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG11	4	0.19	0.06	0.18
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG12	4	0.19	0.06	0.18
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG13	4	0.19	0.06	0.18
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG11	4	0.19	0.06	0.18
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG12	4	0.19	0.06	0.18
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG13	4	0.19	0.06	0.18
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG11	4	0.19	0.06	0.18
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG12	4	0.19	0.06	0.18
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG13	4	0.19	0.06	0.18
(1,2945)	1:121:B:THR:HA	1:139:B:THR:HA	4	0.19	0.03	0.19
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG11	4	0.18	0.07	0.17
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG12	4	0.18	0.07	0.17
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG13	4	0.18	0.07	0.17
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG11	4	0.18	0.07	0.17
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG12	4	0.18	0.07	0.17
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG13	4	0.18	0.07	0.17
(1,2329)	1:94:B:ARG:HD2	1:168:B:PRO:HA	4	0.18	0.08	0.16
(1,1655)	1:134:A:ILE:H	1:127:A:ARG:HG2	4	0.18	0.04	0.18
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG21	4	0.18	0.05	0.16
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG22	4	0.18	0.05	0.16
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG23	4	0.18	0.05	0.16
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG21	4	0.18	0.02	0.17
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG22	4	0.18	0.02	0.17
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG23	4	0.18	0.02	0.17
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD11	4	0.17	0.06	0.16
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD12	4	0.17	0.06	0.16
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD13	4	0.17	0.06	0.16
(1,3143)	1:141:B:LYS:HG3	1:142:B:TYR:HB3	4	0.16	0.03	0.17
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG21	4	0.16	0.03	0.18
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG22	4	0.16	0.03	0.18
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG23	4	0.16	0.03	0.18
(1,4089)	1:152:B:GLN:HE22	1:152:B:GLN:HB2	4	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG21	4	0.16	0.04	0.16
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG22	4	0.16	0.04	0.16
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG23	4	0.16	0.04	0.16
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG21	4	0.16	0.04	0.16
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG22	4	0.16	0.04	0.16
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG23	4	0.16	0.04	0.16
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG21	4	0.16	0.04	0.16
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG22	4	0.16	0.04	0.16
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG23	4	0.16	0.04	0.16
(1,419)	1:111:A:VAL:HA	1:120:A:ILE:HG13	4	0.16	0.03	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG21	4	0.16	0.01	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG22	4	0.16	0.01	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG23	4	0.16	0.01	0.16
(1,562)	1:117:A:VAL:HG11	1:142:A:TYR:HB3	4	0.15	0.04	0.16
(1,562)	1:117:A:VAL:HG12	1:142:A:TYR:HB3	4	0.15	0.04	0.16
(1,562)	1:117:A:VAL:HG13	1:142:A:TYR:HB3	4	0.15	0.04	0.16
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB1	4	0.15	0.06	0.13
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB2	4	0.15	0.06	0.13
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB3	4	0.15	0.06	0.13
(1,2578)	1:105:B:ALA:HB1	1:107:B:ASP:HB3	4	0.15	0.05	0.14
(1,2578)	1:105:B:ALA:HB2	1:107:B:ASP:HB3	4	0.15	0.05	0.14
(1,2578)	1:105:B:ALA:HB3	1:107:B:ASP:HB3	4	0.15	0.05	0.14
(1,2892)	1:119:B:GLU:HA	1:141:B:LYS:HE2	4	0.15	0.03	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD21	4	0.15	0.01	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD22	4	0.15	0.01	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD23	4	0.15	0.01	0.15
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG21	4	0.15	0.03	0.14
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG22	4	0.15	0.03	0.14
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG23	4	0.15	0.03	0.14
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD11	4	0.15	0.01	0.15
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD12	4	0.15	0.01	0.15
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD13	4	0.15	0.01	0.15
(1,1517)	1:118:A:VAL:H	1:142:A:TYR:HB2	4	0.14	0.04	0.14
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD21	4	0.14	0.03	0.14
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD22	4	0.14	0.03	0.14
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD23	4	0.14	0.03	0.14
(1,4183)	1:161:B:GLY:H	1:102:B:ASN:HB3	4	0.14	0.04	0.13
(1,2093)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	4	0.14	0.01	0.14
(1,2093)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	4	0.14	0.01	0.14
(1,2093)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	4	0.14	0.01	0.14
(1,2225)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	4	0.14	0.01	0.14
(1,2225)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	4	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2225)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	4	0.14	0.01	0.14
(1,3360)	1:153:B:VAL:HB	1:154:B:SER:HA	4	0.14	0.01	0.14
(1,3770)	1:114:B:LYS:H	1:119:B:GLU:H	4	0.14	0.02	0.15
(1,3292)	1:148:B:VAL:HG11	1:169:B:MET:HA	4	0.14	0.02	0.14
(1,3292)	1:148:B:VAL:HG12	1:169:B:MET:HA	4	0.14	0.02	0.14
(1,3292)	1:148:B:VAL:HG13	1:169:B:MET:HA	4	0.14	0.02	0.14
(1,3438)	1:157:B:LEU:HB3	1:157:B:LEU:HG	4	0.14	0.01	0.14
(1,1172)	1:157:A:LEU:HD11	1:163:A:LEU:HB2	4	0.13	0.02	0.12
(1,1172)	1:157:A:LEU:HD12	1:163:A:LEU:HB2	4	0.13	0.02	0.12
(1,1172)	1:157:A:LEU:HD13	1:163:A:LEU:HB2	4	0.13	0.02	0.12
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD11	4	0.13	0.02	0.13
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD12	4	0.13	0.02	0.13
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD13	4	0.13	0.02	0.13
(1,1345)	1:97:A:VAL:H	1:165:A:VAL:H	4	0.13	0.01	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD11	4	0.13	0.01	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD12	4	0.13	0.01	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD13	4	0.13	0.01	0.12
(1,2886)	1:119:B:GLU:HA	1:120:B:ILE:HG13	4	0.12	0.02	0.12
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD11	4	0.12	0.02	0.12
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD12	4	0.12	0.02	0.12
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD13	4	0.12	0.02	0.12
(1,1627)	1:129:A:ASP:H	1:132:A:GLY:H	4	0.12	0.01	0.12
(1,3670)	1:105:B:ALA:H	1:106:B:PRO:HD3	4	0.11	0.01	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG21	4	0.11	0.01	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG22	4	0.11	0.01	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG23	4	0.11	0.01	0.12
(1,2290)	1:90:B:HIS:HB3	1:91:B:THR:HA	3	0.93	0.31	0.83
(1,841)	1:140:A:ARG:HG2	1:142:A:TYR:HE1	3	0.82	0.51	0.58
(1,841)	1:140:A:ARG:HG2	1:142:A:TYR:HE2	3	0.82	0.51	0.58
(1,3601)	1:94:B:ARG:H	1:92:B:ALA:HA	3	0.81	0.55	0.45
(1,4285)	1:171:B:LYS:H	1:169:B:MET:HA	3	0.79	0.38	0.65
(1,4293)	1:172:B:LEU:H	1:171:B:LYS:HA	3	0.73	0.26	0.85
(1,4272)	1:169:B:MET:H	1:95:B:TRP:HA	3	0.67	0.16	0.76
(1,4080)	1:152:B:GLN:HE21	1:152:B:GLN:HB3	3	0.65	0.09	0.61
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB1	3	0.6	0.31	0.4
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB2	3	0.6	0.31	0.4
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB3	3	0.6	0.31	0.4
(1,3303)	1:148:B:VAL:HG21	1:170:B:PRO:HG2	3	0.59	0.22	0.46
(1,3303)	1:148:B:VAL:HG22	1:170:B:PRO:HG2	3	0.59	0.22	0.46
(1,3303)	1:148:B:VAL:HG23	1:170:B:PRO:HG2	3	0.59	0.22	0.46
(1,2346)	1:95:B:TRP:HB3	1:95:B:TRP:HE3	3	0.56	0.03	0.57
(1,65)	1:95:A:TRP:HB3	1:95:A:TRP:HE3	3	0.56	0.01	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4048)	1:149:B:ASP:H	1:170:B:PRO:HG3	3	0.53	0.2	0.62
(1,3603)	1:94:B:ARG:H	1:93:B:ASP:HB2	3	0.53	0.09	0.54
(1,2513)	1:99:B:LEU:HD11	1:120:B:ILE:HG12	3	0.49	0.09	0.43
(1,2513)	1:99:B:LEU:HD12	1:120:B:ILE:HG12	3	0.49	0.09	0.43
(1,2513)	1:99:B:LEU:HD13	1:120:B:ILE:HG12	3	0.49	0.09	0.43
(1,1623)	1:129:A:ASP:H	1:130:A:GLU:HG3	3	0.48	0.08	0.44
(1,3557)	1:168:B:PRO:HA	1:169:B:MET:HG2	3	0.47	0.4	0.23
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG21	3	0.47	0.26	0.42
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG22	3	0.47	0.26	0.42
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG23	3	0.47	0.26	0.42
(1,1331)	1:95:A:TRP:H	1:95:A:TRP:HB2	3	0.46	0.04	0.47
(1,406)	1:110:A:THR:HG21	1:112:A:LYS:HE3	3	0.45	0.13	0.39
(1,406)	1:110:A:THR:HG22	1:112:A:LYS:HE3	3	0.45	0.13	0.39
(1,406)	1:110:A:THR:HG23	1:112:A:LYS:HE3	3	0.45	0.13	0.39
(1,715)	1:126:A:GLU:HB2	1:135:A:SER:HB3	3	0.44	0.21	0.32
(1,3613)	1:95:B:TRP:H	1:95:B:TRP:HE3	3	0.43	0.08	0.45
(1,18)	1:93:A:ASP:HB2	1:94:A:ARG:HA	3	0.42	0.12	0.5
(1,3096)	1:136:B:ARG:HG3	1:138:B:PHE:HA	3	0.42	0.19	0.32
(1,1640)	1:132:A:GLY:H	1:128:A:GLN:HG2	3	0.41	0.07	0.44
(1,1332)	1:95:A:TRP:H	1:95:A:TRP:HE3	3	0.4	0.03	0.41
(1,2715)	1:111:B:VAL:HG11	1:120:B:ILE:HG12	3	0.38	0.12	0.3
(1,2715)	1:111:B:VAL:HG12	1:120:B:ILE:HG12	3	0.38	0.12	0.3
(1,2715)	1:111:B:VAL:HG13	1:120:B:ILE:HG12	3	0.38	0.12	0.3
(1,2619)	1:108:B:GLU:HA	1:123:B:LYS:HD2	3	0.37	0.22	0.27
(1,2625)	1:108:B:GLU:HG2	1:123:B:LYS:HD2	3	0.37	0.15	0.27
(1,704)	1:125:A:GLU:HA	1:135:A:SER:HB3	3	0.37	0.35	0.13
(1,1974)	1:167:A:ALA:H	1:95:A:TRP:HB3	3	0.37	0.04	0.36
(1,33)	1:94:A:ARG:HA	1:169:A:MET:HB2	3	0.35	0.18	0.37
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB1	3	0.35	0.21	0.3
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB2	3	0.35	0.21	0.3
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB3	3	0.35	0.21	0.3
(1,3092)	1:136:B:ARG:HA	1:136:B:ARG:HG2	3	0.35	0.06	0.38
(1,1924)	1:162:A:THR:H	1:160:A:GLU:HB2	3	0.35	0.11	0.4
(1,612)	1:119:A:GLU:HA	1:141:A:LYS:HE3	3	0.33	0.1	0.33
(1,2075)	1:134:B:ILE:HD11	1:140:A:ARG:HG2	3	0.33	0.08	0.28
(1,2075)	1:134:B:ILE:HD12	1:140:A:ARG:HG2	3	0.33	0.08	0.28
(1,2075)	1:134:B:ILE:HD13	1:140:A:ARG:HG2	3	0.33	0.08	0.28
(1,2207)	1:134:B:ILE:HD11	1:140:A:ARG:HG2	3	0.33	0.08	0.28
(1,2207)	1:134:B:ILE:HD12	1:140:A:ARG:HG2	3	0.33	0.08	0.28
(1,2207)	1:134:B:ILE:HD13	1:140:A:ARG:HG2	3	0.33	0.08	0.28
(1,826)	1:139:A:THR:HA	1:140:A:ARG:HB2	3	0.33	0.04	0.35
(1,847)	1:141:A:LYS:HA	1:141:A:LYS:HE3	3	0.33	0.03	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,344)	1:108:A:GLU:HG2	1:123:A:LYS:HD3	3	0.33	0.11	0.25
(1,344)	1:108:A:GLU:HG2	1:123:A:LYS:HD2	3	0.33	0.11	0.25
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG21	3	0.32	0.05	0.29
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG22	3	0.32	0.05	0.29
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG23	3	0.32	0.05	0.29
(1,3304)	1:149:B:ASP:HA	1:149:B:ASP:HB3	3	0.32	0.1	0.35
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD21	3	0.32	0.07	0.29
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD22	3	0.32	0.07	0.29
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD23	3	0.32	0.07	0.29
(1,1321)	1:94:A:ARG:H	1:93:A:ASP:HA	3	0.31	0.06	0.34
(1,1514)	1:118:A:VAL:H	1:119:A:GLU:HG3	3	0.31	0.16	0.21
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG21	3	0.3	0.11	0.23
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG22	3	0.3	0.11	0.23
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG23	3	0.3	0.11	0.23
(1,1085)	1:153:A:VAL:HG21	1:155:A:SER:HB3	3	0.3	0.11	0.31
(1,1085)	1:153:A:VAL:HG22	1:155:A:SER:HB3	3	0.3	0.11	0.31
(1,1085)	1:153:A:VAL:HG23	1:155:A:SER:HB3	3	0.3	0.11	0.31
(1,1085)	1:153:A:VAL:HG11	1:155:A:SER:HB3	3	0.3	0.11	0.31
(1,1085)	1:153:A:VAL:HG12	1:155:A:SER:HB3	3	0.3	0.11	0.31
(1,1085)	1:153:A:VAL:HG13	1:155:A:SER:HB3	3	0.3	0.11	0.31
(1,4037)	1:148:B:VAL:H	1:170:B:PRO:HG3	3	0.3	0.14	0.39
(1,2626)	1:108:B:GLU:HG2	1:123:B:LYS:HE2	3	0.29	0.07	0.3
(1,2626)	1:108:B:GLU:HG2	1:123:B:LYS:HE3	3	0.29	0.07	0.3
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG21	3	0.29	0.12	0.36
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG22	3	0.29	0.12	0.36
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG23	3	0.29	0.12	0.36
(1,336)	1:108:A:GLU:HA	1:108:A:GLU:HG2	3	0.29	0.05	0.28
(1,3060)	1:131:B:HIS:HA	1:131:B:HIS:HE1	3	0.29	0.08	0.33
(1,1179)	1:157:A:LEU:HD21	1:163:A:LEU:HB3	3	0.28	0.03	0.26
(1,1179)	1:157:A:LEU:HD22	1:163:A:LEU:HB3	3	0.28	0.03	0.26
(1,1179)	1:157:A:LEU:HD23	1:163:A:LEU:HB3	3	0.28	0.03	0.26
(1,2686)	1:110:B:THR:HG21	1:112:B:LYS:HD3	3	0.28	0.04	0.26
(1,2686)	1:110:B:THR:HG22	1:112:B:LYS:HD3	3	0.28	0.04	0.26
(1,2686)	1:110:B:THR:HG23	1:112:B:LYS:HD3	3	0.28	0.04	0.26
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD21	3	0.28	0.08	0.23
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD22	3	0.28	0.08	0.23
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD23	3	0.28	0.08	0.23
(1,808)	1:135:A:SER:HA	1:135:A:SER:HB2	3	0.27	0.01	0.27
(1,3607)	1:94:B:ARG:H	1:168:B:PRO:HA	3	0.27	0.12	0.19
(1,2759)	1:112:B:LYS:HE3	1:121:B:THR:HB	3	0.27	0.17	0.19
(1,2759)	1:112:B:LYS:HE2	1:121:B:THR:HB	3	0.27	0.17	0.19
(1,917)	1:144:A:LEU:HB3	1:147:A:GLY:HA2	3	0.27	0.11	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2018)	1:97:B:VAL:HG21	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2018)	1:97:B:VAL:HG22	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2018)	1:97:B:VAL:HG23	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2018)	1:97:B:VAL:HG11	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2018)	1:97:B:VAL:HG12	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2018)	1:97:B:VAL:HG13	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2150)	1:97:B:VAL:HG21	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2150)	1:97:B:VAL:HG22	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2150)	1:97:B:VAL:HG23	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2150)	1:97:B:VAL:HG11	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2150)	1:97:B:VAL:HG12	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2150)	1:97:B:VAL:HG13	1:131:A:HIS:HB3	3	0.27	0.05	0.26
(1,2629)	1:108:B:GLU:HG3	1:123:B:LYS:HE3	3	0.27	0.11	0.34
(1,2629)	1:108:B:GLU:HG3	1:123:B:LYS:HE2	3	0.27	0.11	0.34
(1,478)	1:112:A:LYS:HE2	1:121:A:THR:HB	3	0.26	0.07	0.26
(1,478)	1:112:A:LYS:HE3	1:121:A:THR:HB	3	0.26	0.07	0.26
(1,3395)	1:155:B:SER:HB2	1:163:B:LEU:HA	3	0.26	0.11	0.27
(1,4281)	1:169:B:MET:H	1:169:B:MET:HG3	3	0.25	0.05	0.25
(1,2957)	1:122:B:GLY:HA3	1:137:B:CYS:HA	3	0.25	0.14	0.18
(1,4191)	1:161:B:GLY:H	1:160:B:GLU:HG3	3	0.25	0.08	0.23
(1,4191)	1:161:B:GLY:H	1:160:B:GLU:HG2	3	0.25	0.08	0.23
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD11	3	0.25	0.12	0.18
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD12	3	0.25	0.12	0.18
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD13	3	0.25	0.12	0.18
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD11	3	0.25	0.12	0.18
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD12	3	0.25	0.12	0.18
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD13	3	0.25	0.12	0.18
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD11	3	0.25	0.12	0.18
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD12	3	0.25	0.12	0.18
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD13	3	0.25	0.12	0.18
(1,3027)	1:128:B:GLN:HA	1:128:B:GLN:HG3	3	0.24	0.16	0.17
(1,348)	1:108:A:GLU:HG3	1:123:A:LYS:HE3	3	0.24	0.12	0.19
(1,348)	1:108:A:GLU:HG3	1:123:A:LYS:HE2	3	0.24	0.12	0.19
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD21	3	0.24	0.0	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD22	3	0.24	0.0	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD23	3	0.24	0.0	0.24
(1,746)	1:128:A:GLN:HA	1:128:A:GLN:HG3	3	0.24	0.05	0.2
(1,2020)	1:97:A:VAL:HG11	1:131:B:HIS:HB3	3	0.24	0.04	0.26
(1,2020)	1:97:A:VAL:HG12	1:131:B:HIS:HB3	3	0.24	0.04	0.26
(1,2020)	1:97:A:VAL:HG13	1:131:B:HIS:HB3	3	0.24	0.04	0.26
(1,2152)	1:97:A:VAL:HG11	1:131:B:HIS:HB3	3	0.24	0.04	0.26
(1,2152)	1:97:A:VAL:HG12	1:131:B:HIS:HB3	3	0.24	0.04	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2152)	1:97:A:VAL:HG13	1:131:B:HIS:HB3	3	0.24	0.04	0.26
(1,2891)	1:119:B:GLU:HA	1:141:B:LYS:HD3	3	0.23	0.05	0.2
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD21	3	0.22	0.01	0.23
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD22	3	0.22	0.01	0.23
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD23	3	0.22	0.01	0.23
(1,3595)	1:170:B:PRO:HB3	1:170:B:PRO:HD3	3	0.22	0.03	0.22
(1,3595)	1:170:B:PRO:HB3	1:170:B:PRO:HD2	3	0.22	0.03	0.22
(1,1318)	1:171:A:LYS:HA	1:171:A:LYS:HD3	3	0.22	0.06	0.23
(1,1318)	1:171:A:LYS:HA	1:171:A:LYS:HD2	3	0.22	0.06	0.23
(1,2894)	1:119:B:GLU:HB3	1:121:B:THR:HB	3	0.22	0.01	0.21
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG21	3	0.22	0.06	0.19
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG22	3	0.22	0.06	0.19
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG23	3	0.22	0.06	0.19
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG21	3	0.22	0.06	0.19
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG22	3	0.22	0.06	0.19
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG23	3	0.22	0.06	0.19
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG21	3	0.22	0.06	0.19
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG22	3	0.22	0.06	0.19
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG23	3	0.22	0.06	0.19
(1,862)	1:141:A:LYS:HG3	1:142:A:TYR:HB3	3	0.21	0.04	0.24
(1,749)	1:128:A:GLN:HA	1:133:A:TYR:HE1	3	0.21	0.03	0.2
(1,749)	1:128:A:GLN:HA	1:133:A:TYR:HE2	3	0.21	0.03	0.2
(1,3654)	1:102:B:ASN:HD21	1:161:B:GLY:HA2	3	0.21	0.06	0.21
(1,3795)	1:118:B:VAL:H	1:119:B:GLU:HG3	3	0.21	0.01	0.21
(1,1014)	1:148:A:VAL:HG11	1:170:A:PRO:HG3	3	0.2	0.02	0.2
(1,1014)	1:148:A:VAL:HG12	1:170:A:PRO:HG3	3	0.2	0.02	0.2
(1,1014)	1:148:A:VAL:HG13	1:170:A:PRO:HG3	3	0.2	0.02	0.2
(1,773)	1:130:A:GLU:HA	1:130:A:GLU:HG3	3	0.2	0.03	0.2
(1,1327)	1:94:A:ARG:H	1:169:A:MET:HG2	3	0.2	0.06	0.22
(1,3664)	1:102:B:ASN:HD22	1:161:B:GLY:HA3	3	0.2	0.03	0.21
(1,1276)	1:168:A:PRO:HA	1:169:A:MET:HG2	3	0.19	0.07	0.18
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD11	3	0.19	0.05	0.18
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD12	3	0.19	0.05	0.18
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD13	3	0.19	0.05	0.18
(1,700)	1:125:A:GLU:HA	1:125:A:GLU:HG3	3	0.19	0.03	0.2
(1,1383)	1:102:A:ASN:HD22	1:161:A:GLY:HA3	3	0.19	0.04	0.19
(1,2716)	1:111:B:VAL:HG21	1:120:B:ILE:HG13	3	0.19	0.05	0.17
(1,2716)	1:111:B:VAL:HG22	1:120:B:ILE:HG13	3	0.19	0.05	0.17
(1,2716)	1:111:B:VAL:HG23	1:120:B:ILE:HG13	3	0.19	0.05	0.17
(1,2716)	1:111:B:VAL:HG11	1:120:B:ILE:HG13	3	0.19	0.05	0.17
(1,2716)	1:111:B:VAL:HG12	1:120:B:ILE:HG13	3	0.19	0.05	0.17
(1,2716)	1:111:B:VAL:HG13	1:120:B:ILE:HG13	3	0.19	0.05	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3663)	1:102:B:ASN:HD22	1:161:B:GLY:HA2	3	0.19	0.02	0.18
(1,558)	1:117:A:VAL:HG11	1:141:A:LYS:HE2	3	0.19	0.02	0.18
(1,558)	1:117:A:VAL:HG12	1:141:A:LYS:HE2	3	0.19	0.02	0.18
(1,558)	1:117:A:VAL:HG13	1:141:A:LYS:HE2	3	0.19	0.02	0.18
(1,737)	1:127:A:ARG:HA	1:127:A:ARG:HD3	3	0.18	0.05	0.21
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD11	3	0.18	0.03	0.19
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD12	3	0.18	0.03	0.19
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD13	3	0.18	0.03	0.19
(1,2310)	1:94:B:ARG:HA	1:168:B:PRO:HA	3	0.18	0.04	0.18
(1,4196)	1:162:B:THR:H	1:102:B:ASN:HB2	3	0.18	0.04	0.18
(1,1545)	1:120:A:ILE:H	1:140:A:ARG:HG3	3	0.18	0.04	0.2
(1,2330)	1:94:B:ARG:HD3	1:168:B:PRO:HA	3	0.18	0.09	0.12
(1,2518)	1:99:B:LEU:HD21	1:101:B:VAL:HB	3	0.18	0.01	0.17
(1,2518)	1:99:B:LEU:HD22	1:101:B:VAL:HB	3	0.18	0.01	0.17
(1,2518)	1:99:B:LEU:HD23	1:101:B:VAL:HB	3	0.18	0.01	0.17
(1,2918)	1:120:B:ILE:HB	1:142:B:TYR:HE1	3	0.18	0.04	0.15
(1,2918)	1:120:B:ILE:HB	1:142:B:TYR:HE2	3	0.18	0.04	0.15
(1,1489)	1:114:A:LYS:H	1:119:A:GLU:H	3	0.17	0.02	0.17
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG21	3	0.17	0.06	0.13
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG22	3	0.17	0.06	0.13
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG23	3	0.17	0.06	0.13
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG21	3	0.17	0.06	0.13
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG22	3	0.17	0.06	0.13
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG23	3	0.17	0.06	0.13
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG21	3	0.17	0.06	0.13
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG22	3	0.17	0.06	0.13
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG23	3	0.17	0.06	0.13
(1,849)	1:141:A:LYS:HB2	1:141:A:LYS:HE2	3	0.17	0.03	0.18
(1,3133)	1:141:B:LYS:HG2	1:141:B:LYS:HE2	3	0.17	0.03	0.17
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG11	3	0.16	0.04	0.15
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG12	3	0.16	0.04	0.15
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG13	3	0.16	0.04	0.15
(1,2361)	1:96:B:ARG:HA	1:96:B:ARG:HD3	3	0.16	0.01	0.15
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD11	3	0.16	0.02	0.15
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD12	3	0.16	0.02	0.15
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD13	3	0.16	0.02	0.15
(1,1373)	1:102:A:ASN:HD21	1:161:A:GLY:HA2	3	0.16	0.02	0.15
(1,1581)	1:125:A:GLU:H	1:108:A:GLU:HG3	3	0.16	0.05	0.14
(1,1611)	1:128:A:GLN:HE22	1:128:A:GLN:H	3	0.16	0.04	0.15
(1,2028)	1:132:B:GLY:HA2	1:142:A:TYR:HB3	3	0.16	0.0	0.16
(1,2160)	1:132:B:GLY:HA2	1:142:A:TYR:HB3	3	0.16	0.0	0.16
(1,331)	1:107:A:ASP:HA	1:108:A:GLU:HG2	3	0.15	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,649)	1:120:A:ILE:HG21	1:140:A:ARG:HA	3	0.15	0.07	0.11
(1,649)	1:120:A:ILE:HG22	1:140:A:ARG:HA	3	0.15	0.07	0.11
(1,649)	1:120:A:ILE:HG23	1:140:A:ARG:HA	3	0.15	0.07	0.11
(1,766)	1:129:A:ASP:HA	1:130:A:GLU:HB2	3	0.15	0.03	0.14
(1,766)	1:129:A:ASP:HA	1:130:A:GLU:HB3	3	0.15	0.03	0.14
(1,1925)	1:162:A:THR:H	1:160:A:GLU:HG3	3	0.15	0.03	0.14
(1,1925)	1:162:A:THR:H	1:160:A:GLU:HG2	3	0.15	0.03	0.14
(1,101)	1:96:A:ARG:HB3	1:166:A:GLU:HA	3	0.15	0.03	0.16
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD11	3	0.15	0.04	0.14
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD12	3	0.15	0.04	0.14
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD13	3	0.15	0.04	0.14
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB1	3	0.15	0.03	0.16
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB2	3	0.15	0.03	0.16
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB3	3	0.15	0.03	0.16
(1,1389)	1:105:A:ALA:H	1:106:A:PRO:HD3	3	0.14	0.02	0.15
(1,3037)	1:128:B:GLN:HB3	1:133:B:TYR:HD1	3	0.14	0.03	0.13
(1,3037)	1:128:B:GLN:HB3	1:133:B:TYR:HD2	3	0.14	0.03	0.13
(1,3869)	1:126:B:GLU:H	1:125:B:GLU:HG3	3	0.14	0.02	0.14
(1,779)	1:131:A:HIS:HA	1:131:A:HIS:HE1	3	0.14	0.02	0.15
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD11	3	0.14	0.05	0.11
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD12	3	0.14	0.05	0.11
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD13	3	0.14	0.05	0.11
(1,1576)	1:124:A:HIS:H	1:136:A:ARG:HA	3	0.14	0.04	0.11
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG21	3	0.14	0.03	0.12
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG22	3	0.14	0.03	0.12
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG23	3	0.14	0.03	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG21	3	0.14	0.03	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG22	3	0.14	0.03	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG23	3	0.14	0.03	0.12
(1,992)	1:148:A:VAL:HA	1:170:A:PRO:HB3	3	0.14	0.03	0.14
(1,3455)	1:157:B:LEU:HD11	1:163:B:LEU:HG	3	0.13	0.03	0.12
(1,3455)	1:157:B:LEU:HD12	1:163:B:LEU:HG	3	0.13	0.03	0.12
(1,3455)	1:157:B:LEU:HD13	1:163:B:LEU:HG	3	0.13	0.03	0.12
(1,4278)	1:169:B:MET:H	1:169:B:MET:HA	3	0.13	0.02	0.14
(1,3453)	1:157:B:LEU:HD11	1:163:B:LEU:HB2	3	0.13	0.02	0.14
(1,3453)	1:157:B:LEU:HD12	1:163:B:LEU:HB2	3	0.13	0.02	0.14
(1,3453)	1:157:B:LEU:HD13	1:163:B:LEU:HB2	3	0.13	0.02	0.14
(1,236)	1:99:A:LEU:HD11	1:164:A:THR:HA	3	0.13	0.01	0.13
(1,236)	1:99:A:LEU:HD12	1:164:A:THR:HA	3	0.13	0.01	0.13
(1,236)	1:99:A:LEU:HD13	1:164:A:THR:HA	3	0.13	0.01	0.13
(1,571)	1:118:A:VAL:HB	1:142:A:TYR:HD1	3	0.13	0.01	0.13
(1,571)	1:118:A:VAL:HB	1:142:A:TYR:HD2	3	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2304)	1:94:B:ARG:HA	1:94:B:ARG:HB3	3	0.13	0.02	0.13
(1,161)	1:97:A:VAL:HG21	1:166:A:GLU:HA	3	0.12	0.01	0.12
(1,161)	1:97:A:VAL:HG22	1:166:A:GLU:HA	3	0.12	0.01	0.12
(1,161)	1:97:A:VAL:HG23	1:166:A:GLU:HA	3	0.12	0.01	0.12
(1,1668)	1:135:A:SER:H	1:135:A:SER:HB3	3	0.12	0.03	0.11
(1,1870)	1:157:A:LEU:H	1:157:A:LEU:HB3	3	0.12	0.01	0.12
(1,2798)	1:115:B:ASP:HB3	1:150:B:PRO:HG2	3	0.12	0.0	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG21	3	0.12	0.0	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG22	3	0.12	0.0	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG23	3	0.12	0.0	0.12
(1,4043)	1:149:B:ASP:H	1:152:B:GLN:HB2	3	0.12	0.01	0.13
(1,759)	1:128:A:GLN:HG2	1:133:A:TYR:HA	3	0.12	0.01	0.11
(1,1849)	1:155:A:SER:H	1:156:A:SER:HA	3	0.12	0.01	0.12
(1,143)	1:97:A:VAL:HG11	1:142:A:TYR:HE1	3	0.11	0.02	0.1
(1,143)	1:97:A:VAL:HG11	1:142:A:TYR:HE2	3	0.11	0.02	0.1
(1,143)	1:97:A:VAL:HG12	1:142:A:TYR:HE1	3	0.11	0.02	0.1
(1,143)	1:97:A:VAL:HG12	1:142:A:TYR:HE2	3	0.11	0.02	0.1
(1,143)	1:97:A:VAL:HG13	1:142:A:TYR:HE1	3	0.11	0.02	0.1
(1,143)	1:97:A:VAL:HG13	1:142:A:TYR:HE2	3	0.11	0.02	0.1
(1,2885)	1:119:B:GLU:HA	1:120:B:ILE:HG12	3	0.11	0.01	0.11
(1,719)	1:126:A:GLU:HG2	1:133:A:TYR:HD1	3	0.11	0.01	0.11
(1,719)	1:126:A:GLU:HG2	1:133:A:TYR:HD2	3	0.11	0.01	0.11
(1,2302)	1:93:B:ASP:HB3	1:94:B:ARG:HG2	2	1.48	0.17	1.48
(1,1614)	1:128:A:GLN:HE21	1:128:A:GLN:HB2	2	0.9	0.23	0.9
(1,2012)	1:172:A:LEU:H	1:171:A:LYS:HA	2	0.9	0.07	0.9
(1,3271)	1:148:B:VAL:HA	1:169:B:MET:HB2	2	0.87	0.11	0.87
(1,3293)	1:148:B:VAL:HG11	1:169:B:MET:HB2	2	0.7	0.14	0.7
(1,3293)	1:148:B:VAL:HG12	1:169:B:MET:HB2	2	0.7	0.14	0.7
(1,3293)	1:148:B:VAL:HG13	1:169:B:MET:HB2	2	0.7	0.14	0.7
(1,1482)	1:114:A:LYS:H	1:115:A:ASP:HB2	2	0.62	0.19	0.62
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG21	2	0.58	0.41	0.58
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG22	2	0.58	0.41	0.58
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG23	2	0.58	0.41	0.58
(1,2545)	1:100:B:ASP:HB2	1:162:B:THR:HB	2	0.56	0.13	0.56
(1,4065)	1:152:B:GLN:H	1:149:B:ASP:HB3	2	0.55	0.24	0.55
(1,4086)	1:152:B:GLN:HE21	1:170:B:PRO:HD3	2	0.53	0.35	0.53
(1,2991)	1:126:B:GLU:HA	1:135:B:SER:HB2	2	0.52	0.29	0.52
(1,770)	1:129:A:ASP:HB3	1:130:A:GLU:HA	2	0.52	0.04	0.52
(1,345)	1:108:A:GLU:HG2	1:123:A:LYS:HE2	2	0.46	0.01	0.46
(1,1608)	1:128:A:GLN:HE22	1:128:A:GLN:HB2	2	0.46	0.27	0.46
(1,834)	1:139:A:THR:HG21	1:140:A:ARG:HG3	2	0.46	0.01	0.46
(1,834)	1:139:A:THR:HG22	1:140:A:ARG:HG3	2	0.46	0.01	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,834)	1:139:A:THR:HG23	1:140:A:ARG:HG3	2	0.46	0.01	0.46
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG21	2	0.46	0.18	0.46
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG22	2	0.46	0.18	0.46
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG23	2	0.46	0.18	0.46
(1,2068)	1:134:B:ILE:HG21	1:140:A:ARG:HD3	2	0.43	0.09	0.43
(1,2068)	1:134:B:ILE:HG22	1:140:A:ARG:HD3	2	0.43	0.09	0.43
(1,2068)	1:134:B:ILE:HG23	1:140:A:ARG:HD3	2	0.43	0.09	0.43
(1,2200)	1:134:B:ILE:HG21	1:140:A:ARG:HD3	2	0.43	0.09	0.43
(1,2200)	1:134:B:ILE:HG22	1:140:A:ARG:HD3	2	0.43	0.09	0.43
(1,2200)	1:134:B:ILE:HG23	1:140:A:ARG:HD3	2	0.43	0.09	0.43
(1,1920)	1:162:A:THR:H	1:158:A:SER:HB2	2	0.42	0.24	0.42
(1,2008)	1:171:A:LYS:H	1:171:A:LYS:HA	2	0.42	0.01	0.42
(1,2313)	1:94:B:ARG:HA	1:168:B:PRO:HD3	2	0.41	0.14	0.41
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD21	2	0.4	0.02	0.4
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD22	2	0.4	0.02	0.4
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD23	2	0.4	0.02	0.4
(1,2013)	1:172:A:LEU:H	1:172:A:LEU:HB2	2	0.39	0.22	0.39
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG21	2	0.38	0.05	0.38
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG22	2	0.38	0.05	0.38
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG23	2	0.38	0.05	0.38
(1,1656)	1:134:A:ILE:H	1:127:A:ARG:HG3	2	0.36	0.24	0.36
(1,4036)	1:148:B:VAL:H	1:170:B:PRO:HB2	2	0.35	0.19	0.35
(1,247)	1:99:A:LEU:HD21	1:140:A:ARG:HG3	2	0.34	0.1	0.34
(1,247)	1:99:A:LEU:HD22	1:140:A:ARG:HG3	2	0.34	0.1	0.34
(1,247)	1:99:A:LEU:HD23	1:140:A:ARG:HG3	2	0.34	0.1	0.34
(1,3492)	1:160:B:GLU:HG2	1:162:B:THR:HB	2	0.34	0.02	0.34
(1,4290)	1:171:B:LYS:H	1:171:B:LYS:HB3	2	0.34	0.01	0.34
(1,4290)	1:171:B:LYS:H	1:171:B:LYS:HB2	2	0.34	0.01	0.34
(1,472)	1:112:A:LYS:HD2	1:120:A:ILE:HA	2	0.33	0.12	0.33
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD21	2	0.33	0.01	0.33
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD22	2	0.33	0.01	0.33
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD23	2	0.33	0.01	0.33
(1,3889)	1:128:B:GLN:HE22	1:128:B:GLN:HB2	2	0.33	0.18	0.33
(1,1767)	1:149:A:ASP:H	1:170:A:PRO:HG3	2	0.32	0.13	0.32
(1,2529)	1:99:B:LEU:HD21	1:140:B:ARG:HD2	2	0.32	0.06	0.32
(1,2529)	1:99:B:LEU:HD22	1:140:B:ARG:HD2	2	0.32	0.06	0.32
(1,2529)	1:99:B:LEU:HD23	1:140:B:ARG:HD2	2	0.32	0.06	0.32
(1,1323)	1:94:A:ARG:H	1:93:A:ASP:HB3	2	0.3	0.01	0.3
(1,1326)	1:94:A:ARG:H	1:168:A:PRO:HA	2	0.3	0.08	0.3
(1,1805)	1:152:A:GLN:HE21	1:170:A:PRO:HD3	2	0.29	0.05	0.29
(1,3602)	1:94:B:ARG:H	1:93:B:ASP:HA	2	0.29	0.03	0.29
(1,338)	1:108:A:GLU:HA	1:123:A:LYS:HD2	2	0.29	0.06	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3862)	1:125:B:GLU:H	1:108:B:GLU:HG3	2	0.29	0.02	0.29
(1,1915)	1:162:A:THR:H	1:102:A:ASN:HB2	2	0.28	0.02	0.28
(1,19)	1:93:A:ASP:HB2	1:94:A:ARG:HG2	2	0.28	0.02	0.28
(1,3014)	1:126:B:GLU:HG3	1:135:B:SER:HB3	2	0.28	0.1	0.28
(1,264)	1:100:A:ASP:HB2	1:162:A:THR:HB	2	0.26	0.12	0.26
(1,635)	1:120:A:ILE:HB	1:140:A:ARG:HD2	2	0.26	0.06	0.26
(1,1650)	1:132:A:GLY:H	1:133:A:TYR:HD1	2	0.26	0.03	0.26
(1,1650)	1:132:A:GLY:H	1:133:A:TYR:HD2	2	0.26	0.03	0.26
(1,3120)	1:140:B:ARG:HB2	1:140:B:ARG:HD2	2	0.26	0.07	0.26
(1,2060)	1:134:B:ILE:HA	1:140:A:ARG:HG3	2	0.26	0.02	0.26
(1,2192)	1:134:B:ILE:HA	1:140:A:ARG:HG3	2	0.26	0.02	0.26
(1,3599)	1:171:B:LYS:HA	1:171:B:LYS:HD2	2	0.25	0.04	0.25
(1,3599)	1:171:B:LYS:HA	1:171:B:LYS:HD3	2	0.25	0.04	0.25
(1,703)	1:125:A:GLU:HA	1:135:A:SER:HB2	2	0.24	0.08	0.24
(1,2754)	1:112:B:LYS:HE2	1:114:B:LYS:HB2	2	0.24	0.11	0.24
(1,2754)	1:112:B:LYS:HE3	1:114:B:LYS:HB2	2	0.24	0.11	0.24
(1,3865)	1:125:B:GLU:H	1:126:B:GLU:H	2	0.24	0.0	0.24
(1,2965)	1:123:B:LYS:HA	1:135:B:SER:HB3	2	0.24	0.02	0.24
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG21	2	0.24	0.0	0.24
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG22	2	0.24	0.0	0.24
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG23	2	0.24	0.0	0.24
(1,3908)	1:129:B:ASP:H	1:132:B:GLY:H	2	0.24	0.02	0.24
(1,69)	1:95:A:TRP:HB3	1:166:A:GLU:HB2	2	0.23	0.11	0.23
(1,1584)	1:125:A:GLU:H	1:126:A:GLU:H	2	0.23	0.04	0.23
(1,3366)	1:153:B:VAL:HG11	1:155:B:SER:HB3	2	0.23	0.0	0.23
(1,3366)	1:153:B:VAL:HG12	1:155:B:SER:HB3	2	0.23	0.0	0.23
(1,3366)	1:153:B:VAL:HG13	1:155:B:SER:HB3	2	0.23	0.0	0.23
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG11	2	0.22	0.04	0.22
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG12	2	0.22	0.04	0.22
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG13	2	0.22	0.04	0.22
(1,4052)	1:151:B:THR:H	1:149:B:ASP:HB3	2	0.22	0.01	0.22
(1,1191)	1:158:A:SER:HB2	1:160:A:GLU:HG2	2	0.22	0.06	0.22
(1,1910)	1:161:A:GLY:H	1:160:A:GLU:HG3	2	0.22	0.04	0.22
(1,3861)	1:125:B:GLU:H	1:108:B:GLU:HG2	2	0.22	0.01	0.22
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD21	2	0.21	0.05	0.21
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD22	2	0.21	0.05	0.21
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD23	2	0.21	0.05	0.21
(1,2592)	1:106:B:PRO:HA	1:109:B:LEU:HB2	2	0.2	0.06	0.2
(1,2981)	1:125:B:GLU:HA	1:125:B:GLU:HG3	2	0.2	0.0	0.2
(1,3672)	1:105:B:ALA:H	1:108:B:GLU:HB3	2	0.2	0.06	0.2
(1,2613)	1:107:B:ASP:HA	1:108:B:GLU:HG3	2	0.2	0.07	0.2
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD11	2	0.2	0.02	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD12	2	0.2	0.02	0.2
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD13	2	0.2	0.02	0.2
(1,756)	1:128:A:GLN:HB3	1:133:A:TYR:HD1	2	0.2	0.04	0.2
(1,756)	1:128:A:GLN:HB3	1:133:A:TYR:HD2	2	0.2	0.04	0.2
(1,3868)	1:126:B:GLU:H	1:125:B:GLU:HG2	2	0.19	0.01	0.19
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD21	2	0.18	0.04	0.18
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD22	2	0.18	0.04	0.18
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD23	2	0.18	0.04	0.18
(1,717)	1:126:A:GLU:HG2	1:127:A:ARG:HG3	2	0.18	0.04	0.18
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG21	2	0.18	0.04	0.18
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG22	2	0.18	0.04	0.18
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG23	2	0.18	0.04	0.18
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG21	2	0.18	0.04	0.18
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG22	2	0.18	0.04	0.18
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG23	2	0.18	0.04	0.18
(1,296)	1:105:A:ALA:HB1	1:107:A:ASP:HB2	2	0.18	0.0	0.18
(1,296)	1:105:A:ALA:HB2	1:107:A:ASP:HB2	2	0.18	0.0	0.18
(1,296)	1:105:A:ALA:HB3	1:107:A:ASP:HB2	2	0.18	0.0	0.18
(1,1104)	1:155:A:SER:HA	1:156:A:SER:HB3	2	0.18	0.01	0.18
(1,3759)	1:114:B:LYS:H	1:112:B:LYS:HD3	2	0.18	0.04	0.18
(1,1733)	1:147:A:GLY:H	1:146:A:PRO:HG2	2	0.18	0.03	0.18
(1,2540)	1:100:B:ASP:HA	1:100:B:ASP:HB3	2	0.18	0.03	0.18
(1,3000)	1:126:B:GLU:HG2	1:133:B:TYR:HD1	2	0.18	0.0	0.18
(1,3000)	1:126:B:GLU:HG2	1:133:B:TYR:HD2	2	0.18	0.0	0.18
(1,4115)	1:154:B:SER:H	1:155:B:SER:HB2	2	0.18	0.03	0.18
(1,4194)	1:161:B:GLY:H	1:162:B:THR:HB	2	0.18	0.0	0.18
(1,602)	1:119:A:GLU:HA	1:119:A:GLU:HG3	2	0.17	0.0	0.17
(1,1643)	1:132:A:GLY:H	1:130:A:GLU:HB2	2	0.17	0.06	0.17
(1,1643)	1:132:A:GLY:H	1:130:A:GLU:HB3	2	0.17	0.06	0.17
(1,2749)	1:112:B:LYS:HG2	1:121:B:THR:HB	2	0.17	0.06	0.17
(1,610)	1:119:A:GLU:HA	1:141:A:LYS:HD3	2	0.17	0.02	0.17
(1,1844)	1:154:A:SER:H	1:168:A:PRO:HD2	2	0.17	0.05	0.17
(1,2559)	1:102:B:ASN:HB2	1:161:B:GLY:HA3	2	0.17	0.04	0.17
(1,4125)	1:154:B:SER:H	1:168:B:PRO:HD2	2	0.17	0.01	0.17
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD11	2	0.16	0.02	0.16
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD12	2	0.16	0.02	0.16
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD13	2	0.16	0.02	0.16
(1,3093)	1:136:B:ARG:HA	1:136:B:ARG:HD2	2	0.16	0.04	0.16
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD11	2	0.16	0.02	0.16
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD12	2	0.16	0.02	0.16
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD13	2	0.16	0.02	0.16
(1,3481)	1:159:B:PRO:HA	1:159:B:PRO:HG3	2	0.16	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,248)	1:99:A:LEU:HD21	1:140:A:ARG:HD2	2	0.16	0.05	0.16
(1,248)	1:99:A:LEU:HD22	1:140:A:ARG:HD2	2	0.16	0.05	0.16
(1,248)	1:99:A:LEU:HD23	1:140:A:ARG:HD2	2	0.16	0.05	0.16
(1,298)	1:105:A:ALA:HB1	1:108:A:GLU:HB2	2	0.16	0.01	0.16
(1,298)	1:105:A:ALA:HB2	1:108:A:GLU:HB2	2	0.16	0.01	0.16
(1,298)	1:105:A:ALA:HB3	1:108:A:GLU:HB2	2	0.16	0.01	0.16
(1,1606)	1:128:A:GLN:H	1:133:A:TYR:HD1	2	0.15	0.01	0.15
(1,1606)	1:128:A:GLN:H	1:133:A:TYR:HD2	2	0.15	0.01	0.15
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB1	2	0.15	0.03	0.15
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB2	2	0.15	0.03	0.15
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB3	2	0.15	0.03	0.15
(1,1958)	1:165:A:VAL:H	1:166:A:GLU:HB3	2	0.15	0.04	0.15
(1,3903)	1:129:B:ASP:H	1:129:B:ASP:HB3	2	0.15	0.03	0.15
(1,29)	1:94:A:ARG:HA	1:168:A:PRO:HA	2	0.15	0.03	0.15
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD21	2	0.15	0.02	0.15
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD22	2	0.15	0.02	0.15
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD23	2	0.15	0.02	0.15
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG21	2	0.14	0.03	0.14
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG22	2	0.14	0.03	0.14
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG23	2	0.14	0.03	0.14
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG21	2	0.14	0.03	0.14
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG22	2	0.14	0.03	0.14
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG23	2	0.14	0.03	0.14
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG21	2	0.14	0.03	0.14
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG22	2	0.14	0.03	0.14
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG23	2	0.14	0.03	0.14
(1,764)	1:129:A:ASP:HA	1:129:A:ASP:HB3	2	0.14	0.02	0.14
(1,1382)	1:102:A:ASN:HD22	1:161:A:GLY:HA2	2	0.14	0.02	0.14
(1,2883)	1:119:B:GLU:HA	1:119:B:GLU:HG3	2	0.14	0.0	0.14
(1,3479)	1:159:B:PRO:HA	1:159:B:PRO:HB3	2	0.14	0.01	0.14
(1,3608)	1:94:B:ARG:H	1:169:B:MET:HG2	2	0.14	0.01	0.14
(1,60)	1:95:A:TRP:HB2	1:95:A:TRP:HE3	2	0.14	0.02	0.14
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG11	2	0.14	0.01	0.14
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG12	2	0.14	0.01	0.14
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG13	2	0.14	0.01	0.14
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG11	2	0.14	0.01	0.14
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG12	2	0.14	0.01	0.14
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG13	2	0.14	0.01	0.14
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG11	2	0.14	0.01	0.14
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG12	2	0.14	0.01	0.14
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG13	2	0.14	0.01	0.14
(1,1174)	1:157:A:LEU:HD11	1:163:A:LEU:HG	2	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1174)	1:157:A:LEU:HD12	1:163:A:LEU:HG	2	0.14	0.01	0.14
(1,1174)	1:157:A:LEU:HD13	1:163:A:LEU:HG	2	0.14	0.01	0.14
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG21	2	0.14	0.01	0.14
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG22	2	0.14	0.01	0.14
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG23	2	0.14	0.01	0.14
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG21	2	0.14	0.01	0.14
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG22	2	0.14	0.01	0.14
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG23	2	0.14	0.01	0.14
(1,2357)	1:95:B:TRP:HE3	1:166:B:GLU:HA	2	0.14	0.01	0.14
(1,3498)	1:161:B:GLY:HA3	1:163:B:LEU:HA	2	0.14	0.02	0.14
(1,812)	1:136:A:ARG:HA	1:136:A:ARG:HD2	2	0.13	0.0	0.13
(1,852)	1:141:A:LYS:HG2	1:141:A:LYS:HE2	2	0.13	0.0	0.13
(1,1428)	1:109:A:LEU:H	1:109:A:LEU:HB3	2	0.13	0.01	0.13
(1,1546)	1:120:A:ILE:H	1:142:A:TYR:H	2	0.13	0.02	0.13
(1,1600)	1:128:A:GLN:H	1:127:A:ARG:HD2	2	0.13	0.02	0.13
(1,1622)	1:129:A:ASP:H	1:129:A:ASP:HB3	2	0.13	0.02	0.13
(1,1806)	1:152:A:GLN:HE22	1:149:A:ASP:HB2	2	0.13	0.03	0.13
(1,3266)	1:148:B:VAL:HA	1:149:B:ASP:HB3	2	0.13	0.02	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD11	2	0.13	0.0	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD12	2	0.13	0.0	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD13	2	0.13	0.0	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD21	2	0.13	0.0	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD22	2	0.13	0.0	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD23	2	0.13	0.0	0.13
(1,4239)	1:165:B:VAL:H	1:166:B:GLU:HB3	2	0.13	0.01	0.13
(1,604)	1:119:A:GLU:HA	1:120:A:ILE:HG12	2	0.12	0.02	0.12
(1,608)	1:119:A:GLU:HA	1:141:A:LYS:HA	2	0.12	0.01	0.12
(1,1762)	1:149:A:ASP:H	1:152:A:GLN:HB2	2	0.12	0.02	0.12
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD11	2	0.12	0.01	0.12
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD12	2	0.12	0.01	0.12
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD13	2	0.12	0.01	0.12
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD21	2	0.12	0.01	0.12
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD22	2	0.12	0.01	0.12
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD23	2	0.12	0.01	0.12
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG21	2	0.12	0.02	0.12
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG22	2	0.12	0.02	0.12
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG23	2	0.12	0.02	0.12
(1,2866)	1:118:B:VAL:HG11	1:142:B:TYR:HD1	2	0.12	0.01	0.12
(1,2866)	1:118:B:VAL:HG11	1:142:B:TYR:HD2	2	0.12	0.01	0.12
(1,2866)	1:118:B:VAL:HG12	1:142:B:TYR:HD1	2	0.12	0.01	0.12
(1,2866)	1:118:B:VAL:HG12	1:142:B:TYR:HD2	2	0.12	0.01	0.12
(1,2866)	1:118:B:VAL:HG13	1:142:B:TYR:HD1	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2866)	1:118:B:VAL:HG13	1:142:B:TYR:HD2	2	0.12	0.01	0.12
(1,2900)	1:119:B:GLU:HG2	1:141:B:LYS:HE3	2	0.12	0.02	0.12
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG21	2	0.12	0.01	0.12
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG22	2	0.12	0.01	0.12
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG23	2	0.12	0.01	0.12
(1,3879)	1:128:B:GLN:H	1:127:B:ARG:HG2	2	0.12	0.02	0.12
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD11	2	0.12	0.01	0.12
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD12	2	0.12	0.01	0.12
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD13	2	0.12	0.01	0.12
(1,853)	1:141:A:LYS:HG2	1:141:A:LYS:HE3	2	0.12	0.02	0.12
(1,1834)	1:154:A:SER:H	1:155:A:SER:HB2	2	0.12	0.02	0.12
(1,2704)	1:111:B:VAL:HB	1:112:B:LYS:HA	2	0.12	0.02	0.12
(1,3278)	1:148:B:VAL:HB	1:150:B:PRO:HA	2	0.12	0.02	0.12
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD11	2	0.12	0.01	0.12
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD12	2	0.12	0.01	0.12
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD13	2	0.12	0.01	0.12
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD21	2	0.12	0.01	0.12
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD22	2	0.12	0.01	0.12
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD23	2	0.12	0.01	0.12
(1,2382)	1:96:B:ARG:HB3	1:166:B:GLU:HA	2	0.12	0.01	0.12
(1,2933)	1:120:B:ILE:HD11	1:140:B:ARG:HB2	2	0.12	0.01	0.12
(1,2933)	1:120:B:ILE:HD12	1:140:B:ARG:HB2	2	0.12	0.01	0.12
(1,2933)	1:120:B:ILE:HD13	1:140:B:ARG:HB2	2	0.12	0.01	0.12
(1,1217)	1:161:A:GLY:HA3	1:163:A:LEU:HA	2	0.12	0.02	0.12
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG11	2	0.12	0.02	0.12
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG12	2	0.12	0.02	0.12
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG13	2	0.12	0.02	0.12
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG21	2	0.12	0.0	0.12
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG22	2	0.12	0.0	0.12
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG23	2	0.12	0.0	0.12
(1,2023)	1:131:A:HIS:HB2	1:142:B:TYR:HD1	2	0.12	0.0	0.12
(1,2023)	1:131:A:HIS:HB2	1:142:B:TYR:HD2	2	0.12	0.0	0.12
(1,2155)	1:131:A:HIS:HB2	1:142:B:TYR:HD1	2	0.12	0.0	0.12
(1,2155)	1:131:A:HIS:HB2	1:142:B:TYR:HD2	2	0.12	0.0	0.12
(1,2291)	1:91:B:THR:HA	1:91:B:THR:HB	2	0.12	0.0	0.12
(1,3723)	1:110:B:THR:H	1:122:B:GLY:H	2	0.12	0.0	0.12
(1,517)	1:115:A:ASP:HB3	1:150:A:PRO:HG2	2	0.11	0.01	0.11
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG21	2	0.11	0.01	0.11
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG22	2	0.11	0.01	0.11
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG23	2	0.11	0.01	0.11
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD21	2	0.11	0.01	0.11
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD22	2	0.11	0.01	0.11

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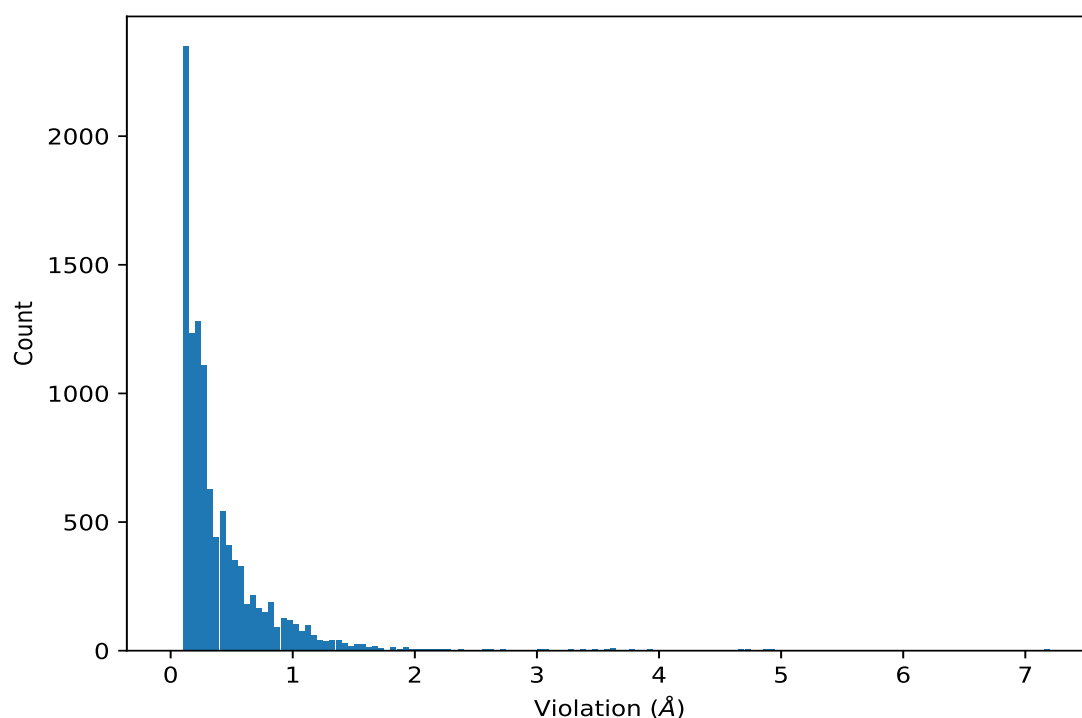
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD23	2	0.11	0.01	0.11
(1,1804)	1:152:A:GLN:HE21	1:169:A:MET:HA	2	0.11	0.01	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD21	2	0.11	0.0	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD22	2	0.11	0.0	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD23	2	0.11	0.0	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD21	2	0.11	0.0	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD22	2	0.11	0.0	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD23	2	0.11	0.0	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD21	2	0.11	0.0	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD22	2	0.11	0.0	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD23	2	0.11	0.0	0.11
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD11	2	0.11	0.0	0.11
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD12	2	0.11	0.0	0.11
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD13	2	0.11	0.0	0.11
(1,1616)	1:128:A:GLN:HE21	1:128:A:GLN:HG2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	5	7.17
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	5	7.17
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	5	7.17
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	4	7.16
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	4	7.16
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	4	7.16
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG3	7	6.94
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	5	6.54
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	8	6.54
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	9	6.42
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	3	6.11
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	3	6.11
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	3	6.11
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	6	6.06
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	6	6.06
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	6	6.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	3	6.0
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	4	5.86
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	6	5.81
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE2	4	5.7
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG3	3	5.63
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	3	5.52
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	2	5.46
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	8	5.41
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	8	5.41
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	8	5.41
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	2	5.36
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	2	5.36
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	2	5.36
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE2	10	5.28
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG2	1	5.27
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG3	4	5.23
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE2	10	5.1
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG2	6	5.1
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG2	10	5.07
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	7	5.01
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	9	4.91
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	9	4.91
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	9	4.91
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	9	4.91
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	10	4.89
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	4	4.86
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	9	4.86
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	9	4.86
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	9	4.86
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE3	5	4.74
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	3	4.7
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	3	4.7
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	3	4.7
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE3	1	4.68
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB1	5	4.65
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB2	5	4.65
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB3	5	4.65
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	4	4.64
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	4	4.64
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	4	4.64
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	1	4.56
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	1	4.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	1	4.56
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE2	4	4.52
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE2	2	4.44
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE2	4	4.36
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	1	4.3
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	1	4.3
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	1	4.3
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG2	3	4.25
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	8	4.19
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	8	4.19
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	8	4.19
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG2	2	4.14
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG2	8	4.13
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE2	1	4.0
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG3	8	3.99
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG2	2	3.93
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	10	3.92
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	10	3.92
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	10	3.92
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	9	3.8
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	9	3.8
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	9	3.8
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG3	3	3.79
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE3	6	3.73
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE2	4	3.72
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	8	3.71
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	2	3.66
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	2	3.66
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	2	3.66
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	8	3.64
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	8	3.64
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	8	3.64
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE2	7	3.64
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	4	3.63
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	4	3.63
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	4	3.63
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE3	6	3.62
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	2	3.59
(1,2)	1:88:A:ILE:HG21	1:90:A:HIS:HB3	5	3.57
(1,2)	1:88:A:ILE:HG22	1:90:A:HIS:HB3	5	3.57
(1,2)	1:88:A:ILE:HG23	1:90:A:HIS:HB3	5	3.57
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	10	3.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:88:A:ILE:HG21	1:90:A:HIS:HB3	3	3.45
(1,2)	1:88:A:ILE:HG22	1:90:A:HIS:HB3	3	3.45
(1,2)	1:88:A:ILE:HG23	1:90:A:HIS:HB3	3	3.45
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	1	3.44
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	6	3.42
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG2	6	3.4
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	1	3.38
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB1	9	3.36
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB2	9	3.36
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB3	9	3.36
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	7	3.27
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	7	3.27
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	7	3.27
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE2	3	3.25
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE2	2	3.24
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	1	3.14
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	1	3.14
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	1	3.14
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG2	10	3.09
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB1	4	3.07
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB2	4	3.07
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB3	4	3.07
(1,2283)	1:88:B:ILE:HG21	1:90:B:HIS:HB3	7	3.04
(1,2283)	1:88:B:ILE:HG22	1:90:B:HIS:HB3	7	3.04
(1,2283)	1:88:B:ILE:HG23	1:90:B:HIS:HB3	7	3.04
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE2	8	3.0
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG2	1	2.87
(1,1)	1:88:A:ILE:HG21	1:90:A:HIS:HA	5	2.84
(1,1)	1:88:A:ILE:HG22	1:90:A:HIS:HA	5	2.84
(1,1)	1:88:A:ILE:HG23	1:90:A:HIS:HA	5	2.84
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB1	6	2.74
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB2	6	2.74
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB3	6	2.74
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG3	9	2.71
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG21	3	2.7
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG22	3	2.7
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG23	3	2.7
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG3	7	2.64
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	4	2.64
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	8	2.64
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG2	9	2.63
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE3	5	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE2	8	2.58
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG3	1	2.57
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG21	5	2.56
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG22	5	2.56
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG23	5	2.56
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	5	2.47
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG3	4	2.45
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	7	2.41
(1,2283)	1:88:B:ILE:HG21	1:90:B:HIS:HB3	10	2.36
(1,2283)	1:88:B:ILE:HG22	1:90:B:HIS:HB3	10	2.36
(1,2283)	1:88:B:ILE:HG23	1:90:B:HIS:HB3	10	2.36
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE2	7	2.35
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE2	7	2.31
(1,2285)	1:89:B:ARG:HB2	1:90:B:HIS:HB3	6	2.3
(1,2011)	1:172:A:LEU:H	1:145:A:PRO:HA	1	2.28
(1,2284)	1:89:B:ARG:HB3	1:90:B:HIS:HB2	8	2.25
(1,4)	1:89:A:ARG:HB2	1:90:A:HIS:HB3	8	2.25
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	6	2.23
(1,2)	1:88:A:ILE:HG21	1:90:A:HIS:HB3	7	2.23
(1,2)	1:88:A:ILE:HG22	1:90:A:HIS:HB3	7	2.23
(1,2)	1:88:A:ILE:HG23	1:90:A:HIS:HB3	7	2.23
(1,4)	1:89:A:ARG:HB2	1:90:A:HIS:HB3	7	2.2
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE3	7	2.18
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE2	9	2.17
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG3	2	2.17
(1,3582)	1:169:B:MET:HB3	1:171:B:LYS:HG2	8	2.15
(1,2285)	1:89:B:ARG:HB2	1:90:B:HIS:HB3	2	2.14
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG21	3	2.14
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG22	3	2.14
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG23	3	2.14
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	9	2.13
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE2	9	2.11
(1,3)	1:89:A:ARG:HB3	1:90:A:HIS:HB2	10	2.08
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE3	1	2.07
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	10	2.07
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	10	2.07
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	10	2.07
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE2	9	2.05
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB1	8	2.01
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB2	8	2.01
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB3	8	2.01
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD1	4	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD2	4	2.01
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	10	1.99
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	4	1.98
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	4	1.98
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	4	1.98
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	4	1.95
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	4	1.95
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	4	1.95
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB1	1	1.94
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB2	1	1.94
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB3	1	1.94
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	1	1.94
(1,2283)	1:88:B:ILE:HG21	1:90:B:HIS:HB3	5	1.93
(1,2283)	1:88:B:ILE:HG22	1:90:B:HIS:HB3	5	1.93
(1,2283)	1:88:B:ILE:HG23	1:90:B:HIS:HB3	5	1.93
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB1	1	1.91
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB2	1	1.91
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB3	1	1.91
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	5	1.87
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	5	1.87
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	5	1.87
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	5	1.85
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	5	1.85
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	5	1.85
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	8	1.84
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	7	1.84
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	7	1.84
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	7	1.84
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	8	1.84
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	1	1.83
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB1	10	1.83
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB2	10	1.83
(1,1987)	1:169:A:MET:H	1:92:A:ALA:HB3	10	1.83
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	8	1.83
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	1	1.8
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	3	1.8
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	7	1.8
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	7	1.8
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	7	1.8
(1,2285)	1:89:B:ARG:HB3	1:90:B:HIS:HB3	3	1.79
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	8	1.78
(1,3583)	1:169:B:MET:HB2	1:171:B:LYS:HE2	9	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	6	1.74
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	6	1.74
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	6	1.74
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	10	1.74
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB1	7	1.73
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB2	7	1.73
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB3	7	1.73
(1,4)	1:89:A:ARG:HB2	1:90:A:HIS:HB3	4	1.73
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	9	1.71
(1,4)	1:89:A:ARG:HB3	1:90:A:HIS:HB3	10	1.71
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	10	1.7
(1,4)	1:89:A:ARG:HB2	1:90:A:HIS:HB3	6	1.7
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	2	1.69
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	2	1.69
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	2	1.69
(1,1)	1:88:A:ILE:HG21	1:90:A:HIS:HA	3	1.69
(1,1)	1:88:A:ILE:HG22	1:90:A:HIS:HA	3	1.69
(1,1)	1:88:A:ILE:HG23	1:90:A:HIS:HA	3	1.69
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	3	1.68
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	4	1.68
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	2	1.68
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	2	1.67
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	10	1.67
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	7	1.66
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG3	3	1.66
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	1	1.66
(1,2302)	1:93:B:ASP:HB3	1:94:B:ARG:HG2	7	1.65
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	3	1.65
(1,1301)	1:169:A:MET:HB3	1:171:A:LYS:HG3	6	1.65
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	5	1.64
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	7	1.64
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	4	1.63
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	4	1.63
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	6	1.63
(1,4)	1:89:A:ARG:HB3	1:90:A:HIS:HB3	1	1.62
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	3	1.61
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	3	1.61
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	4	1.61
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	3	1.61
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	3	1.6
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	7	1.6
(1,3601)	1:94:B:ARG:H	1:92:B:ALA:HA	7	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	4	1.59
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	4	1.59
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	4	1.59
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	4	1.59
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	4	1.59
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	4	1.59
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	3	1.59
(1,4292)	1:172:B:LEU:H	1:145:B:PRO:HA	5	1.58
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	9	1.58
(1,2283)	1:88:B:ILE:HG21	1:90:B:HIS:HB3	1	1.58
(1,2283)	1:88:B:ILE:HG22	1:90:B:HIS:HB3	1	1.58
(1,2283)	1:88:B:ILE:HG23	1:90:B:HIS:HB3	1	1.58
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	8	1.58
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	10	1.58
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	7	1.57
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	5	1.57
(1,4)	1:89:A:ARG:HB3	1:90:A:HIS:HB3	3	1.57
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	5	1.56
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	10	1.55
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	10	1.55
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	10	1.55
(1,2285)	1:89:B:ARG:HB2	1:90:B:HIS:HB3	4	1.55
(1,2284)	1:89:B:ARG:HB2	1:90:B:HIS:HB2	2	1.55
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	5	1.55
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	1	1.55
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	2	1.55
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	2	1.54
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	6	1.54
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	4	1.54
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	4	1.54
(1,3)	1:89:A:ARG:HB2	1:90:A:HIS:HB2	8	1.54
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD1	9	1.53
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD2	9	1.53
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	4	1.53
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	7	1.53
(1,2285)	1:89:B:ARG:HB3	1:90:B:HIS:HB3	8	1.53
(1,2157)	1:132:B:GLY:HA2	1:140:A:ARG:HA	8	1.53
(1,2025)	1:132:B:GLY:HA2	1:140:A:ARG:HA	8	1.53
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	4	1.52
(1,1320)	1:94:A:ARG:H	1:92:A:ALA:HA	1	1.52
(1,841)	1:140:A:ARG:HG2	1:142:A:TYR:HE1	3	1.52
(1,841)	1:140:A:ARG:HG2	1:142:A:TYR:HE2	3	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	7	1.52
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	2	1.52
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD1	7	1.51
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD2	7	1.51
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	4	1.5
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	10	1.5
(1,1301)	1:169:A:MET:HB3	1:171:A:LYS:HG3	4	1.5
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	4	1.5
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	6	1.5
(1,3)	1:89:A:ARG:HB2	1:90:A:HIS:HB2	4	1.5
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	6	1.49
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	1	1.49
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	10	1.49
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	9	1.49
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	9	1.48
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG3	4	1.48
(1,2004)	1:171:A:LYS:H	1:169:A:MET:HA	10	1.48
(1,1654)	1:134:A:ILE:H	1:127:A:ARG:HB2	1	1.48
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	1	1.48
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	2	1.47
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	2	1.47
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	5	1.47
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	5	1.47
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	5	1.47
(1,2284)	1:89:B:ARG:HB3	1:90:B:HIS:HB2	3	1.46
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	3	1.46
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	2	1.46
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	9	1.45
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	8	1.45
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	8	1.45
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	8	1.45
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	2	1.45
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	2	1.45
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	2	1.45
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	2	1.45
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	2	1.45
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	2	1.45
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	6	1.45
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	5	1.45
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG2	10	1.44
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	8	1.44
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	7	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	7	1.44
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	1	1.44
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	1	1.44
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	1	1.44
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	8	1.44
(1,286)	1:105:A:ALA:HA	1:108:A:GLU:HB2	9	1.44
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	3	1.44
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	3	1.44
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	3	1.44
(1,16)	1:93:A:ASP:HA	1:94:A:ARG:HD2	5	1.43
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	9	1.42
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	9	1.42
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	9	1.42
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	3	1.41
(1,1766)	1:149:A:ASP:H	1:169:A:MET:HG3	10	1.41
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	7	1.41
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB1	5	1.4
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB2	5	1.4
(1,4284)	1:171:B:LYS:H	1:92:B:ALA:HB3	5	1.4
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	5	1.4
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	9	1.4
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	9	1.4
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	5	1.4
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	9	1.39
(1,3005)	1:126:B:GLU:HG2	1:135:B:SER:HB3	4	1.38
(1,2285)	1:89:B:ARG:HB2	1:90:B:HIS:HB3	9	1.38
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	1	1.38
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	1	1.38
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	1	1.38
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	1	1.38
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	1	1.38
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	1	1.38
(1,2)	1:88:A:ILE:HG21	1:90:A:HIS:HB3	6	1.38
(1,2)	1:88:A:ILE:HG22	1:90:A:HIS:HB3	6	1.38
(1,2)	1:88:A:ILE:HG23	1:90:A:HIS:HB3	6	1.38
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG21	6	1.37
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG22	6	1.37
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG23	6	1.37
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG21	10	1.37
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG22	10	1.37
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG23	10	1.37
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD2	3	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	1	1.37
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	1	1.37
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	1	1.37
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE1	8	1.37
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE2	8	1.37
(1,1766)	1:149:A:ASP:H	1:169:A:MET:HG3	5	1.36
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	10	1.36
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	7	1.36
(1,3)	1:89:A:ARG:HB3	1:90:A:HIS:HB2	1	1.36
(1,3)	1:89:A:ARG:HB2	1:90:A:HIS:HB2	7	1.36
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	6	1.35
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	6	1.35
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	9	1.35
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	9	1.35
(1,2290)	1:90:B:HIS:HB3	1:91:B:THR:HA	7	1.35
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	9	1.35
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	1	1.34
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	1	1.34
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	1	1.34
(1,2327)	1:94:B:ARG:HG3	1:168:B:PRO:HA	7	1.34
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	8	1.34
(1,110)	1:96:A:ARG:HG3	1:166:A:GLU:HB3	10	1.34
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	6	1.33
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	3	1.33
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	9	1.33
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	6	1.33
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	2	1.32
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	2	1.32
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	9	1.32
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	9	1.32
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	9	1.32
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	6	1.32
(1,2538)	1:99:B:LEU:HD11	1:112:B:LYS:HG3	6	1.32
(1,2538)	1:99:B:LEU:HD12	1:112:B:LYS:HG3	6	1.32
(1,2538)	1:99:B:LEU:HD13	1:112:B:LYS:HG3	6	1.32
(1,4285)	1:171:B:LYS:H	1:169:B:MET:HA	5	1.31
(1,2302)	1:93:B:ASP:HB3	1:94:B:ARG:HG2	3	1.31
(1,2282)	1:88:B:ILE:HG21	1:90:B:HIS:HA	7	1.31
(1,2282)	1:88:B:ILE:HG22	1:90:B:HIS:HA	7	1.31
(1,2282)	1:88:B:ILE:HG23	1:90:B:HIS:HA	7	1.31
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE2	3	1.31
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	8	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	8	1.31
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	8	1.31
(1,2193)	1:134:B:ILE:HA	1:140:A:ARG:HD2	2	1.3
(1,2061)	1:134:B:ILE:HA	1:140:A:ARG:HD2	2	1.3
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	3	1.3
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	3	1.3
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	3	1.3
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	1	1.3
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	1	1.3
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	1	1.3
(1,257)	1:99:A:LEU:HD11	1:112:A:LYS:HG3	7	1.3
(1,257)	1:99:A:LEU:HD12	1:112:A:LYS:HG3	7	1.3
(1,257)	1:99:A:LEU:HD13	1:112:A:LYS:HG3	7	1.3
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	1	1.29
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	1	1.29
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	1	1.29
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	5	1.29
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	5	1.29
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	5	1.29
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	1	1.28
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	2	1.28
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	7	1.28
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	5	1.27
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	9	1.27
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	5	1.27
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	9	1.27
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD1	1	1.27
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD2	1	1.27
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	8	1.26
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	3	1.26
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD1	3	1.26
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD2	3	1.26
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	1	1.26
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	4	1.26
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	9	1.25
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	3	1.25
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	8	1.25
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	10	1.25
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	10	1.25
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	10	1.25
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	10	1.25
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	10	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	10	1.25
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD1	7	1.25
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD2	7	1.25
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	2	1.25
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	4	1.25
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	4	1.25
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	7	1.24
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	5	1.24
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	10	1.24
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	10	1.24
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	10	1.24
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	10	1.24
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	10	1.24
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	10	1.24
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	10	1.24
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	1	1.24
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	1	1.24
(1,724)	1:126:A:GLU:HG2	1:135:A:SER:HB3	7	1.24
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	9	1.23
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	9	1.23
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	9	1.23
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	6	1.23
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	9	1.23
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	2	1.23
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE1	10	1.23
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE2	10	1.23
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	6	1.23
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	7	1.22
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	7	1.22
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	7	1.22
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	2	1.22
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	2	1.22
(1,4267)	1:167:B:ALA:H	1:169:B:MET:H	2	1.21
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	6	1.21
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	10	1.21
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	10	1.21
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	10	1.21
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	6	1.21
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	4	1.21
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	4	1.21
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	4	1.21
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	6	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	6	1.21
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	6	1.21
(1,4)	1:89:A:ARG:HB3	1:90:A:HIS:HB3	9	1.21
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	2	1.2
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	3	1.2
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	5	1.2
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	2	1.2
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	2	1.2
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	2	1.2
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	2	1.2
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	2	1.2
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	9	1.2
(1,2193)	1:134:B:ILE:HA	1:140:A:ARG:HD2	7	1.2
(1,2061)	1:134:B:ILE:HA	1:140:A:ARG:HD2	7	1.2
(1,2004)	1:171:A:LYS:H	1:169:A:MET:HA	9	1.2
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	8	1.2
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	8	1.2
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	2	1.2
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE1	1	1.2
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE2	1	1.2
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	6	1.19
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	7	1.19
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	8	1.19
(1,2157)	1:132:B:GLY:HA2	1:140:A:ARG:HA	2	1.19
(1,2025)	1:132:B:GLY:HA2	1:140:A:ARG:HA	2	1.19
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	6	1.19
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	6	1.19
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	6	1.19
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	5	1.19
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	2	1.19
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	2	1.19
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	8	1.19
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	8	1.19
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	8	1.19
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	9	1.18
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	2	1.18
(1,724)	1:126:A:GLU:HG2	1:135:A:SER:HB3	9	1.18
(1,3)	1:89:A:ARG:HB2	1:90:A:HIS:HB2	6	1.18
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	1	1.17
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	1	1.17
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	1	1.17
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	5	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	5	1.17
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	5	1.17
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	5	1.17
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	5	1.17
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	5	1.17
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	1	1.17
(1,2282)	1:88:B:ILE:HG21	1:90:B:HIS:HA	2	1.17
(1,2282)	1:88:B:ILE:HG22	1:90:B:HIS:HA	2	1.17
(1,2282)	1:88:B:ILE:HG23	1:90:B:HIS:HA	2	1.17
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	3	1.17
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	3	1.17
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	3	1.17
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	6	1.16
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	6	1.16
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	6	1.16
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	2	1.16
(1,2391)	1:96:B:ARG:HG3	1:166:B:GLU:HB3	6	1.16
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	6	1.16
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	7	1.16
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	7	1.16
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	7	1.16
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	7	1.16
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	9	1.16
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	10	1.15
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	10	1.15
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	4	1.15
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	4	1.15
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	4	1.15
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	3	1.15
(1,2193)	1:134:B:ILE:HA	1:140:A:ARG:HD2	9	1.15
(1,2061)	1:134:B:ILE:HA	1:140:A:ARG:HD2	9	1.15
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	2	1.15
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	2	1.15
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	2	1.15
(1,2193)	1:134:B:ILE:HA	1:140:A:ARG:HD2	1	1.14
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	7	1.14
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	7	1.14
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	7	1.14
(1,2061)	1:134:B:ILE:HA	1:140:A:ARG:HD2	1	1.14
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	7	1.14
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	7	1.14
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	7	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1614)	1:128:A:GLN:HE21	1:128:A:GLN:HB2	7	1.14
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	9	1.14
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	3	1.14
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE3	6	1.13
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	8	1.13
(1,3566)	1:168:B:PRO:HD2	1:169:B:MET:HA	6	1.13
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	9	1.13
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	9	1.13
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	9	1.13
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	3	1.13
(1,2300)	1:93:B:ASP:HB2	1:94:B:ARG:HG2	7	1.13
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB1	3	1.13
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB2	3	1.13
(1,2003)	1:171:A:LYS:H	1:92:A:ALA:HB3	3	1.13
(1,1301)	1:169:A:MET:HB3	1:171:A:LYS:HG2	9	1.13
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	5	1.13
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	3	1.13
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	4	1.12
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	6	1.12
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	8	1.12
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	7	1.12
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	7	1.12
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	7	1.12
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	7	1.12
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	4	1.12
(1,2194)	1:134:B:ILE:HA	1:140:A:ARG:HD3	3	1.12
(1,2157)	1:132:B:GLY:HA2	1:140:A:ARG:HA	4	1.12
(1,2062)	1:134:B:ILE:HA	1:140:A:ARG:HD3	3	1.12
(1,2025)	1:132:B:GLY:HA2	1:140:A:ARG:HA	4	1.12
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	8	1.12
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	8	1.12
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	8	1.12
(1,710)	1:126:A:GLU:HA	1:135:A:SER:HB2	2	1.12
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	9	1.12
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	9	1.12
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	9	1.12
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD1	10	1.11
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD2	10	1.11
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	9	1.11
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	9	1.11
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	9	1.11
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	10	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	10	1.11
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	3	1.11
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	9	1.11
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	3	1.11
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	3	1.11
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	3	1.11
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	5	1.11
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	5	1.11
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	5	1.11
(1,990)	1:148:A:VAL:HA	1:169:A:MET:HB2	3	1.11
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE1	3	1.11
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE2	3	1.11
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE1	3	1.11
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE2	3	1.11
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE1	3	1.11
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE2	3	1.11
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	9	1.1
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	2	1.1
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	2	1.1
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	2	1.1
(1,2284)	1:89:B:ARG:HB2	1:90:B:HIS:HB2	6	1.1
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	9	1.1
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	6	1.1
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	6	1.1
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	6	1.1
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE1	1	1.1
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE2	1	1.1
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	8	1.1
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	9	1.1
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	2	1.1
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	2	1.1
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	2	1.1
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG11	10	1.1
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG12	10	1.1
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG13	10	1.1
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	5	1.1
(1,2)	1:88:A:ILE:HG21	1:90:A:HIS:HB3	2	1.1
(1,2)	1:88:A:ILE:HG22	1:90:A:HIS:HB3	2	1.1
(1,2)	1:88:A:ILE:HG23	1:90:A:HIS:HB3	2	1.1
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	3	1.09
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	6	1.09
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	6	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	6	1.09
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	4	1.09
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	6	1.09
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	5	1.09
(1,1269)	1:167:A:ALA:HB1	1:168:A:PRO:HD2	9	1.09
(1,1269)	1:167:A:ALA:HB2	1:168:A:PRO:HD2	9	1.09
(1,1269)	1:167:A:ALA:HB3	1:168:A:PRO:HD2	9	1.09
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	8	1.09
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	8	1.09
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	8	1.09
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	7	1.09
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	8	1.09
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	7	1.09
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	10	1.09
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	9	1.08
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	9	1.08
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	9	1.08
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	5	1.08
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	7	1.08
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	7	1.08
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	7	1.08
(1,3346)	1:152:B:GLN:HB2	1:169:B:MET:HA	6	1.08
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	5	1.08
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	5	1.08
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	7	1.08
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	6	1.08
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	2	1.08
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	2	1.08
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	2	1.08
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	8	1.08
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	1	1.08
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	2	1.08
(1,4267)	1:167:B:ALA:H	1:169:B:MET:H	9	1.07
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	4	1.07
(1,3566)	1:168:B:PRO:HD2	1:169:B:MET:HA	4	1.07
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	1	1.07
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	3	1.07
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	9	1.07
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	4	1.06
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	4	1.06
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	4	1.06
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	5	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	5	1.06
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	5	1.06
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	2	1.06
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	2	1.06
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	2	1.06
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	3	1.06
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	3	1.06
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	3	1.06
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	3	1.06
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	3	1.06
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	3	1.06
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	2	1.06
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	8	1.06
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	1	1.06
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	2	1.06
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG21	8	1.06
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG22	8	1.06
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG23	8	1.06
(1,1301)	1:169:A:MET:HB3	1:171:A:LYS:HG3	7	1.06
(1,990)	1:148:A:VAL:HA	1:169:A:MET:HB2	4	1.06
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	3	1.06
(1,918)	1:144:A:LEU:HB3	1:147:A:GLY:HA3	8	1.06
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	9	1.06
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	3	1.05
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	3	1.05
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	3	1.05
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	8	1.05
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE1	4	1.05
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE2	4	1.05
(1,722)	1:126:A:GLU:HG2	1:135:A:SER:HA	7	1.05
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	7	1.05
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	7	1.05
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	5	1.04
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	5	1.04
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	5	1.04
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	5	1.04
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	6	1.04
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	6	1.04
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	6	1.04
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	10	1.04
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	4	1.04
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	4	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	4	1.04
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	5	1.04
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	5	1.04
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	5	1.04
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	7	1.04
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB1	8	1.04
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB2	8	1.04
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB3	8	1.04
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB1	1	1.04
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB2	1	1.04
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB3	1	1.04
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	4	1.04
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	8	1.04
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	8	1.04
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	8	1.04
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE1	3	1.04
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE2	3	1.04
(1,4076)	1:152:B:GLN:H	1:170:B:PRO:HD2	1	1.03
(1,3557)	1:168:B:PRO:HA	1:169:B:MET:HG2	7	1.03
(1,3199)	1:144:B:LEU:HB3	1:147:B:GLY:HA3	9	1.03
(1,2285)	1:89:B:ARG:HB3	1:90:B:HIS:HB3	1	1.03
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE2	3	1.03
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	2	1.03
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	2	1.03
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	2	1.03
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	1	1.03
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	1	1.03
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	1	1.03
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	5	1.03
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB1	1	1.03
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB2	1	1.03
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB3	1	1.03
(1,16)	1:93:A:ASP:HA	1:94:A:ARG:HD2	8	1.03
(1,7)	1:90:A:HIS:HB2	1:91:A:THR:HA	9	1.03
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	1	1.02
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	2	1.02
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	2	1.02
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	2	1.02
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	2	1.02
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	2	1.02
(1,1766)	1:149:A:ASP:H	1:169:A:MET:HG3	2	1.02
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	5	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	5	1.02
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	5	1.02
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	10	1.02
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	10	1.02
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	10	1.02
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	4	1.02
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	4	1.02
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	4	1.02
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	7	1.02
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	7	1.02
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE1	6	1.02
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE2	6	1.02
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	3	1.02
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	4	1.01
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	8	1.01
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	8	1.01
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	8	1.01
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	1	1.01
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	1	1.01
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	5	1.01
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	1	1.01
(1,2318)	1:94:B:ARG:HB2	1:96:B:ARG:HA	7	1.01
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG21	5	1.01
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG22	5	1.01
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG23	5	1.01
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	7	1.01
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE1	5	1.01
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE2	5	1.01
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE1	5	1.01
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE2	5	1.01
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE1	5	1.01
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE2	5	1.01
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	2	1.0
(1,3558)	1:168:B:PRO:HA	1:169:B:MET:HG3	7	1.0
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	1	1.0
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	1	1.0
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	1	1.0
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	8	1.0
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	7	1.0
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	7	1.0
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	7	1.0
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	1	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	1	1.0
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	1	1.0
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	1	1.0
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	1	1.0
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	1	1.0
(1,2193)	1:134:B:ILE:HA	1:140:A:ARG:HD2	8	1.0
(1,2061)	1:134:B:ILE:HA	1:140:A:ARG:HD2	8	1.0
(1,4)	1:89:A:ARG:HB3	1:90:A:HIS:HB3	2	1.0
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	10	0.99
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	9	0.99
(1,3566)	1:168:B:PRO:HD2	1:169:B:MET:HA	5	0.99
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	10	0.99
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	10	0.99
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	10	0.99
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	5	0.99
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	9	0.99
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	9	0.99
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	9	0.99
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	3	0.99
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	3	0.99
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	3	0.99
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG21	6	0.99
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG22	6	0.99
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG23	6	0.99
(1,2283)	1:88:B:ILE:HG21	1:90:B:HIS:HB3	4	0.99
(1,2283)	1:88:B:ILE:HG22	1:90:B:HIS:HB3	4	0.99
(1,2283)	1:88:B:ILE:HG23	1:90:B:HIS:HB3	4	0.99
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	7	0.99
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	7	0.99
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	7	0.99
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE1	10	0.99
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE2	10	0.99
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	4	0.99
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	7	0.99
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB1	4	0.99
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB2	4	0.99
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB3	4	0.99
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	8	0.98
(1,3271)	1:148:B:VAL:HA	1:169:B:MET:HB2	5	0.98
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	3	0.98
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	4	0.98
(1,2352)	1:95:B:TRP:HB2	1:168:B:PRO:HB2	7	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	7	0.98
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	7	0.98
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	3	0.98
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD1	8	0.98
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD2	8	0.98
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	8	0.98
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE1	2	0.98
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE2	2	0.98
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE1	2	0.98
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE2	2	0.98
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE1	2	0.98
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE2	2	0.98
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	8	0.98
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	8	0.98
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	8	0.98
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB1	9	0.98
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB2	9	0.98
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB3	9	0.98
(1,4293)	1:172:B:LEU:H	1:171:B:LYS:HA	9	0.97
(1,4283)	1:169:B:MET:H	1:171:B:LYS:HE2	3	0.97
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	1	0.97
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	1	0.97
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG2	3	0.97
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	9	0.97
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	10	0.97
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	10	0.97
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	10	0.97
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	3	0.97
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	3	0.97
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	3	0.97
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	6	0.97
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	6	0.97
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	6	0.97
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	6	0.97
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	6	0.97
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	9	0.97
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	9	0.97
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	9	0.97
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	9	0.97
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	9	0.97
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	9	0.97
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	5	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	5	0.97
(1,2012)	1:172:A:LEU:H	1:171:A:LYS:HA	8	0.97
(1,1012)	1:148:A:VAL:HG11	1:169:A:MET:HB2	4	0.97
(1,1012)	1:148:A:VAL:HG12	1:169:A:MET:HB2	4	0.97
(1,1012)	1:148:A:VAL:HG13	1:169:A:MET:HB2	4	0.97
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	8	0.97
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE1	7	0.97
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE2	7	0.97
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE1	7	0.97
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE2	7	0.97
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE1	7	0.97
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE2	7	0.97
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	9	0.96
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	3	0.96
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	5	0.96
(1,3550)	1:167:B:ALA:HB1	1:168:B:PRO:HD2	3	0.96
(1,3550)	1:167:B:ALA:HB2	1:168:B:PRO:HD2	3	0.96
(1,3550)	1:167:B:ALA:HB3	1:168:B:PRO:HD2	3	0.96
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	8	0.96
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	8	0.96
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	8	0.96
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	9	0.96
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	9	0.96
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	9	0.96
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	9	0.96
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	10	0.96
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	6	0.96
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	6	0.96
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	6	0.96
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	1	0.96
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	1	0.96
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	1	0.96
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	7	0.96
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	7	0.96
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	7	0.96
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	3	0.96
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	8	0.96
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	8	0.96
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	8	0.96
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	10	0.96
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB1	6	0.96
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB2	6	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB3	6	0.96
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	1	0.95
(1,4255)	1:167:B:ALA:H	1:95:B:TRP:HB3	8	0.95
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	2	0.95
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	2	0.95
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	2	0.95
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	2	0.95
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	7	0.95
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	10	0.95
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	3	0.95
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	3	0.95
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	3	0.95
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	4	0.95
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	8	0.95
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	2	0.95
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	2	0.95
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	2	0.95
(1,1012)	1:148:A:VAL:HG11	1:169:A:MET:HB2	3	0.95
(1,1012)	1:148:A:VAL:HG12	1:169:A:MET:HB2	3	0.95
(1,1012)	1:148:A:VAL:HG13	1:169:A:MET:HB2	3	0.95
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	2	0.95
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB1	10	0.95
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB2	10	0.95
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB3	10	0.95
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	8	0.94
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	8	0.94
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	8	0.94
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	6	0.94
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	7	0.94
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	4	0.94
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	4	0.94
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	4	0.94
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	9	0.94
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	5	0.94
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	5	0.94
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	5	0.94
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE1	3	0.94
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE2	3	0.94
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	5	0.93
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	10	0.93
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	2	0.93
(1,2322)	1:94:B:ARG:HB3	1:167:B:ALA:HA	4	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:148:A:VAL:HA	1:169:A:MET:HB2	10	0.93
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	6	0.93
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	6	0.93
(1,724)	1:126:A:GLU:HG2	1:135:A:SER:HB3	6	0.93
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	1	0.93
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	3	0.92
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	1	0.92
(1,3274)	1:148:B:VAL:HA	1:170:B:PRO:HG2	2	0.92
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	3	0.92
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	3	0.92
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	3	0.92
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	5	0.92
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	4	0.92
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	8	0.92
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	8	0.92
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	8	0.92
(1,2194)	1:134:B:ILE:HA	1:140:A:ARG:HD3	4	0.92
(1,2062)	1:134:B:ILE:HA	1:140:A:ARG:HD3	4	0.92
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	4	0.92
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	9	0.92
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	9	0.92
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	9	0.92
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	1	0.92
(1,474)	1:112:A:LYS:HE3	1:114:A:LYS:HB3	1	0.92
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	5	0.92
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	10	0.91
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	4	0.91
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	4	0.91
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	4	0.91
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE1	4	0.91
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE2	4	0.91
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	2	0.91
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	7	0.91
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	7	0.91
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	7	0.91
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	7	0.91
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	7	0.91
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	7	0.91
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	1	0.91
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	3	0.91
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	3	0.91
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	3	0.91
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	5	0.91
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	7	0.91
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	7	0.91
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	7	0.91
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	4	0.91
(1,4267)	1:167:B:ALA:H	1:169:B:MET:H	10	0.9
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	6	0.9
(1,3303)	1:148:B:VAL:HG21	1:170:B:PRO:HG2	2	0.9
(1,3303)	1:148:B:VAL:HG22	1:170:B:PRO:HG2	2	0.9
(1,3303)	1:148:B:VAL:HG23	1:170:B:PRO:HG2	2	0.9
(1,2976)	1:123:B:LYS:HD3	1:137:B:CYS:HB2	10	0.9
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE1	8	0.9
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE2	8	0.9
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	7	0.9
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	8	0.9
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	8	0.9
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	8	0.9
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	5	0.9
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	5	0.9
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	5	0.9
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	5	0.9
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	5	0.9
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	5	0.9
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	5	0.9
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	8	0.9
(1,2009)	1:171:A:LYS:H	1:171:A:LYS:HB2	10	0.9
(1,1916)	1:162:A:THR:H	1:102:A:ASN:HB3	6	0.9
(1,1916)	1:162:A:THR:H	1:102:A:ASN:HB3	9	0.9
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	1	0.9
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	7	0.9
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	8	0.9
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	8	0.9
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	8	0.9
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE1	10	0.9
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE2	10	0.9
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE1	10	0.9
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE2	10	0.9
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE1	10	0.9
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE2	10	0.9
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	4	0.9
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	8	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB1	2	0.9
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB2	2	0.9
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB3	2	0.9
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	4	0.89
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	1	0.89
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	10	0.89
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	10	0.89
(1,1301)	1:169:A:MET:HB3	1:171:A:LYS:HG2	3	0.89
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	10	0.89
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	7	0.89
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	7	0.89
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	7	0.89
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	2	0.89
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	2	0.89
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	2	0.89
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	10	0.89
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	10	0.89
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	10	0.89
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	7	0.89
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	7	0.89
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	7	0.89
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG11	4	0.89
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG12	4	0.89
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG13	4	0.89
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	10	0.89
(1,4086)	1:152:B:GLN:HE21	1:170:B:PRO:HD3	3	0.88
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	7	0.88
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	6	0.88
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	4	0.88
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	6	0.88
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	5	0.88
(1,1018)	1:148:A:VAL:HG21	1:168:A:PRO:HD3	10	0.88
(1,1018)	1:148:A:VAL:HG22	1:168:A:PRO:HD3	10	0.88
(1,1018)	1:148:A:VAL:HG23	1:168:A:PRO:HD3	10	0.88
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD3	4	0.87
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	4	0.87
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	4	0.87
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	4	0.87
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	10	0.87
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	10	0.87
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	10	0.87
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	10	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	10	0.87
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	10	0.87
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	9	0.87
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	4	0.87
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	7	0.87
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	7	0.87
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	7	0.87
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	7	0.87
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	7	0.87
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	7	0.87
(1,2004)	1:171:A:LYS:H	1:169:A:MET:HA	2	0.87
(1,2004)	1:171:A:LYS:H	1:169:A:MET:HA	8	0.87
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	9	0.87
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	9	0.87
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	9	0.87
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	10	0.87
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	10	0.87
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE1	9	0.87
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE2	9	0.87
(1,704)	1:125:A:GLU:HA	1:135:A:SER:HB3	3	0.87
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE1	5	0.87
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE2	5	0.87
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	7	0.87
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	10	0.87
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	10	0.87
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	10	0.87
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE1	6	0.87
(1,254)	1:99:A:LEU:HD21	1:142:A:TYR:HE2	6	0.87
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE1	6	0.87
(1,254)	1:99:A:LEU:HD22	1:142:A:TYR:HE2	6	0.87
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE1	6	0.87
(1,254)	1:99:A:LEU:HD23	1:142:A:TYR:HE2	6	0.87
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	1	0.87
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	4	0.87
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	8	0.87
(1,3763)	1:114:B:LYS:H	1:115:B:ASP:HB2	2	0.86
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	8	0.86
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	8	0.86
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	9	0.86
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	10	0.86
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	4	0.86
(1,2322)	1:94:B:ARG:HB3	1:167:B:ALA:HA	5	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	8	0.86
(1,1012)	1:148:A:VAL:HG11	1:169:A:MET:HB2	10	0.86
(1,1012)	1:148:A:VAL:HG12	1:169:A:MET:HB2	10	0.86
(1,1012)	1:148:A:VAL:HG13	1:169:A:MET:HB2	10	0.86
(1,684)	1:123:A:LYS:HA	1:135:A:SER:HB3	5	0.86
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	2	0.86
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	6	0.86
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	4	0.86
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	4	0.86
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	4	0.86
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	7	0.86
(1,4293)	1:172:B:LEU:H	1:171:B:LYS:HA	3	0.85
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	1	0.85
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	1	0.85
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	1	0.85
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	5	0.85
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	10	0.85
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	10	0.85
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	10	0.85
(1,2567)	1:105:B:ALA:HA	1:108:B:GLU:HB2	5	0.85
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	5	0.85
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	5	0.85
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	10	0.85
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	6	0.85
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	5	0.85
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	6	0.85
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	6	0.85
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	6	0.85
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	6	0.85
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	7	0.85
(1,4076)	1:152:B:GLN:H	1:170:B:PRO:HD3	3	0.84
(1,3566)	1:168:B:PRO:HD2	1:169:B:MET:HA	10	0.84
(1,3293)	1:148:B:VAL:HG11	1:169:B:MET:HB2	5	0.84
(1,3293)	1:148:B:VAL:HG12	1:169:B:MET:HB2	5	0.84
(1,3293)	1:148:B:VAL:HG13	1:169:B:MET:HB2	5	0.84
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	9	0.84
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	3	0.84
(1,2298)	1:93:B:ASP:HA	1:169:B:MET:HG2	8	0.84
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	9	0.84
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	9	0.84
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE1	6	0.84
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE2	6	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:126:A:GLU:HG3	1:133:A:TYR:HA	2	0.84
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	7	0.84
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	7	0.84
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	7	0.84
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	10	0.84
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	10	0.84
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	10	0.84
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	4	0.84
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	4	0.84
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	4	0.84
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	5	0.84
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	9	0.84
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	9	0.84
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	1	0.84
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	7	0.83
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	8	0.83
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	7	0.83
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	7	0.83
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	7	0.83
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	6	0.83
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	6	0.83
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	9	0.83
(1,3003)	1:126:B:GLU:HG2	1:135:B:SER:HA	4	0.83
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	3	0.83
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	3	0.83
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	3	0.83
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	2	0.83
(1,2353)	1:95:B:TRP:HB3	1:168:B:PRO:HB3	7	0.83
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	7	0.83
(1,2290)	1:90:B:HIS:HB3	1:91:B:THR:HA	5	0.83
(1,2012)	1:172:A:LEU:H	1:171:A:LYS:HA	10	0.83
(1,1998)	1:169:A:MET:H	1:169:A:MET:HB2	3	0.83
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	4	0.83
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	2	0.83
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	4	0.83
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	4	0.83
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	4	0.83
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	5	0.83
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	5	0.83
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	5	0.83
(1,7)	1:90:A:HIS:HB2	1:91:A:THR:HA	1	0.83
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	5	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	8	0.82
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	4	0.82
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG11	10	0.82
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG12	10	0.82
(1,3408)	1:155:B:SER:HB3	1:165:B:VAL:HG13	10	0.82
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	8	0.82
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	7	0.82
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	7	0.82
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	7	0.82
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	8	0.82
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	8	0.82
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	8	0.82
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	2	0.82
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE1	7	0.82
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE2	7	0.82
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	5	0.82
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	5	0.82
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	5	0.82
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	10	0.82
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	10	0.82
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	10	0.82
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	2	0.82
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD3	7	0.82
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	8	0.82
(1,827)	1:139:A:THR:HA	1:140:A:ARG:HG2	3	0.82
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE1	2	0.82
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE2	2	0.82
(1,728)	1:126:A:GLU:HG3	1:133:A:TYR:HA	5	0.82
(1,722)	1:126:A:GLU:HG2	1:135:A:SER:HA	5	0.82
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	1	0.82
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	1	0.82
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	1	0.82
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	3	0.82
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	6	0.82
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	3	0.82
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	3	0.82
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	3	0.82
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	6	0.82
(1,1)	1:88:A:ILE:HG21	1:90:A:HIS:HA	7	0.82
(1,1)	1:88:A:ILE:HG22	1:90:A:HIS:HA	7	0.82
(1,1)	1:88:A:ILE:HG23	1:90:A:HIS:HA	7	0.82
(1,4280)	1:169:B:MET:H	1:169:B:MET:HB3	7	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4272)	1:169:B:MET:H	1:95:B:TRP:HA	6	0.81
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	5	0.81
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	2	0.81
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	2	0.81
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	2	0.81
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	7	0.81
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	7	0.81
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	7	0.81
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	10	0.81
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	10	0.81
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	10	0.81
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	4	0.81
(1,2991)	1:126:B:GLU:HA	1:135:B:SER:HB2	4	0.81
(1,2969)	1:123:B:LYS:HB2	1:137:B:CYS:HB3	9	0.81
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE1	1	0.81
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE2	1	0.81
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	8	0.81
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	8	0.81
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	8	0.81
(1,2285)	1:89:B:ARG:HB2	1:90:B:HIS:HB3	10	0.81
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	9	0.81
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	9	0.81
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	9	0.81
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	9	0.81
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	9	0.81
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	9	0.81
(1,1998)	1:169:A:MET:H	1:169:A:MET:HB2	4	0.81
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	4	0.81
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	10	0.81
(1,1482)	1:114:A:LYS:H	1:115:A:ASP:HB2	5	0.81
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	2	0.81
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	1	0.81
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	1	0.81
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	1	0.81
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	7	0.81
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	7	0.81
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	7	0.81
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	2	0.81
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	5	0.81
(1,4288)	1:171:B:LYS:H	1:170:B:PRO:HD3	5	0.8
(1,4197)	1:162:B:THR:H	1:102:B:ASN:HB3	10	0.8
(1,4095)	1:152:B:GLN:HE22	1:170:B:PRO:HD3	2	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	5	0.8
(1,3763)	1:114:B:LYS:H	1:115:B:ASP:HB2	6	0.8
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	3	0.8
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	4	0.8
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	4	0.8
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	4	0.8
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	10	0.8
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	10	0.8
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	10	0.8
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	8	0.8
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	8	0.8
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	8	0.8
(1,2976)	1:123:B:LYS:HD3	1:137:B:CYS:HB2	4	0.8
(1,2538)	1:99:B:LEU:HD21	1:112:B:LYS:HG3	3	0.8
(1,2538)	1:99:B:LEU:HD22	1:112:B:LYS:HG3	3	0.8
(1,2538)	1:99:B:LEU:HD23	1:112:B:LYS:HG3	3	0.8
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	10	0.8
(1,2281)	1:143:A:THR:H	1:132:B:GLY:HA2	10	0.8
(1,2148)	1:143:A:THR:H	1:132:B:GLY:HA2	10	0.8
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	1	0.8
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	1	0.8
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	1	0.8
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	1	0.8
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	1	0.8
(1,688)	1:123:A:LYS:HB2	1:137:A:CYS:HB3	3	0.8
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG21	10	0.8
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG22	10	0.8
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG23	10	0.8
(1,2)	1:88:A:ILE:HG21	1:90:A:HIS:HB3	1	0.8
(1,2)	1:88:A:ILE:HG22	1:90:A:HIS:HB3	1	0.8
(1,2)	1:88:A:ILE:HG23	1:90:A:HIS:HB3	1	0.8
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	3	0.79
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	9	0.79
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	9	0.79
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	9	0.79
(1,3346)	1:152:B:GLN:HB2	1:169:B:MET:HA	4	0.79
(1,3345)	1:152:B:GLN:HB2	1:168:B:PRO:HD3	3	0.79
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	4	0.79
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	10	0.79
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	8	0.79
(1,2969)	1:123:B:LYS:HB2	1:137:B:CYS:HB3	6	0.79
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	6	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	6	0.79
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	6	0.79
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	2	0.79
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	2	0.79
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	2	0.79
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	1	0.79
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	6	0.79
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	6	0.79
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	2	0.79
(1,2009)	1:171:A:LYS:H	1:171:A:LYS:HB3	5	0.79
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	7	0.79
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	7	0.79
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	7	0.79
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	7	0.79
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	9	0.79
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	6	0.79
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	6	0.79
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	6	0.79
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	8	0.79
(1,71)	1:95:A:TRP:HB3	1:168:A:PRO:HB2	10	0.79
(1,1)	1:88:A:ILE:HG21	1:90:A:HIS:HA	6	0.79
(1,1)	1:88:A:ILE:HG22	1:90:A:HIS:HA	6	0.79
(1,1)	1:88:A:ILE:HG23	1:90:A:HIS:HA	6	0.79
(1,4065)	1:152:B:GLN:H	1:149:B:ASP:HB3	5	0.78
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	8	0.78
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	10	0.78
(1,3895)	1:128:B:GLN:HE21	1:128:B:GLN:HB2	10	0.78
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	2	0.78
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	2	0.78
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	2	0.78
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	2	0.78
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	3	0.78
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	10	0.78
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	3	0.78
(1,2007)	1:171:A:LYS:H	1:170:A:PRO:HD3	9	0.78
(1,1799)	1:152:A:GLN:HE21	1:152:A:GLN:HB3	6	0.78
(1,1691)	1:140:A:ARG:H	1:120:A:ILE:HB	9	0.78
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	10	0.78
(1,827)	1:139:A:THR:HA	1:140:A:ARG:HG2	4	0.78
(1,684)	1:123:A:LYS:HA	1:135:A:SER:HB3	2	0.78
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	9	0.78
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	10	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4255)	1:167:B:ALA:H	1:95:B:TRP:HB3	4	0.77
(1,4080)	1:152:B:GLN:HE21	1:152:B:GLN:HB3	3	0.77
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	1	0.77
(1,3346)	1:152:B:GLN:HB2	1:169:B:MET:HA	9	0.77
(1,2976)	1:123:B:LYS:HD2	1:137:B:CYS:HB2	3	0.77
(1,2969)	1:123:B:LYS:HB2	1:137:B:CYS:HB3	5	0.77
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	7	0.77
(1,2322)	1:94:B:ARG:HB3	1:167:B:ALA:HA	10	0.77
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	6	0.77
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	6	0.77
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	6	0.77
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	6	0.77
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	6	0.77
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	6	0.77
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	4	0.77
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	6	0.77
(1,990)	1:148:A:VAL:HA	1:169:A:MET:HB2	5	0.77
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	4	0.77
(1,710)	1:126:A:GLU:HA	1:135:A:SER:HB2	7	0.77
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	10	0.77
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	4	0.77
(1,4272)	1:169:B:MET:H	1:95:B:TRP:HA	5	0.76
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	7	0.76
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	10	0.76
(1,3271)	1:148:B:VAL:HA	1:169:B:MET:HB2	4	0.76
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	1	0.76
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	1	0.76
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	1	0.76
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	7	0.76
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	7	0.76
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	7	0.76
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	6	0.76
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	6	0.76
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	6	0.76
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	7	0.76
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	5	0.76
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	5	0.76
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	5	0.76
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	5	0.76
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	5	0.76
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	5	0.76
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	2	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	5	0.76
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	3	0.76
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	5	0.76
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	3	0.76
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	4	0.76
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE1	8	0.76
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE2	8	0.76
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	5	0.76
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	4	0.76
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	4	0.76
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	4	0.76
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	10	0.76
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	10	0.76
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	10	0.76
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	10	0.76
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	10	0.76
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	10	0.76
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	9	0.76
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	9	0.76
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	9	0.76
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	4	0.76
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	4	0.76
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	4	0.76
(1,99)	1:96:A:ARG:HB3	1:164:A:THR:HB	7	0.76
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	10	0.76
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG2	10	0.75
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	5	0.75
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	5	0.75
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	5	0.75
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	5	0.75
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	5	0.75
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	5	0.75
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	1	0.75
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	1	0.75
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	1	0.75
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	1	0.75
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	3	0.75
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	7	0.75
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	7	0.75
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	7	0.75
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	10	0.75
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	10	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	10	0.75
(1,2284)	1:89:B:ARG:HB3	1:90:B:HIS:HB2	1	0.75
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	3	0.75
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	3	0.75
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	3	0.75
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	6	0.75
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	6	0.75
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	6	0.75
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	3	0.75
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	6	0.75
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	9	0.75
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB1	3	0.74
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB2	3	0.74
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB3	3	0.74
(1,4076)	1:152:B:GLN:H	1:170:B:PRO:HD2	2	0.74
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	4	0.74
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	9	0.74
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	9	0.74
(1,2976)	1:123:B:LYS:HD3	1:137:B:CYS:HB2	1	0.74
(1,2151)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	8	0.74
(1,2151)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	8	0.74
(1,2151)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	8	0.74
(1,2019)	1:97:A:VAL:HG11	1:131:B:HIS:HB2	8	0.74
(1,2019)	1:97:A:VAL:HG12	1:131:B:HIS:HB2	8	0.74
(1,2019)	1:97:A:VAL:HG13	1:131:B:HIS:HB2	8	0.74
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	3	0.74
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	2	0.74
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	3	0.74
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	3	0.74
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	3	0.74
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	10	0.74
(1,385)	1:109:A:LEU:HD21	1:161:A:GLY:HA3	4	0.74
(1,385)	1:109:A:LEU:HD22	1:161:A:GLY:HA3	4	0.74
(1,385)	1:109:A:LEU:HD23	1:161:A:GLY:HA3	4	0.74
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	3	0.74
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	3	0.74
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	3	0.74
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	2	0.74
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	2	0.74
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	2	0.74
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	1	0.74
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	1	0.74
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	3	0.74
(1,8)	1:90:A:HIS:HB2	1:91:A:THR:HG21	4	0.74
(1,8)	1:90:A:HIS:HB2	1:91:A:THR:HG22	4	0.74
(1,8)	1:90:A:HIS:HB2	1:91:A:THR:HG23	4	0.74
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	6	0.73
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	1	0.73
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	2	0.73
(1,2687)	1:110:B:THR:HG21	1:112:B:LYS:HE2	10	0.73
(1,2687)	1:110:B:THR:HG22	1:112:B:LYS:HE2	10	0.73
(1,2687)	1:110:B:THR:HG23	1:112:B:LYS:HE2	10	0.73
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	6	0.73
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	6	0.73
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	6	0.73
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	4	0.73
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	10	0.73
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	6	0.73
(1,1608)	1:128:A:GLN:HE22	1:128:A:GLN:HB2	7	0.73
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	4	0.73
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	4	0.73
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	4	0.73
(1,715)	1:126:A:GLU:HB2	1:135:A:SER:HB3	6	0.73
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	1	0.73
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	1	0.73
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	1	0.73
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	4	0.73
(1,3)	1:89:A:ARG:HB3	1:90:A:HIS:HB2	3	0.73
(1,1)	1:88:A:ILE:HG21	1:90:A:HIS:HA	9	0.73
(1,1)	1:88:A:ILE:HG22	1:90:A:HIS:HA	9	0.73
(1,1)	1:88:A:ILE:HG23	1:90:A:HIS:HA	9	0.73
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	6	0.72
(1,4048)	1:149:B:ASP:H	1:170:B:PRO:HG3	5	0.72
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD1	3	0.72
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD2	3	0.72
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	1	0.72
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	9	0.72
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	5	0.72
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	5	0.72
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	5	0.72
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	3	0.72
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	3	0.72
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	3	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	8	0.72
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	8	0.72
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	8	0.72
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	5	0.72
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	5	0.72
(1,3003)	1:126:B:GLU:HG2	1:135:B:SER:HA	8	0.72
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG21	3	0.72
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG22	3	0.72
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG23	3	0.72
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	3	0.72
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	3	0.72
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	3	0.72
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	3	0.72
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	3	0.72
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	3	0.72
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	3	0.72
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	3	0.72
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	3	0.72
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	3	0.72
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	3	0.72
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	3	0.72
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	1	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	1	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	1	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	1	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	2	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	2	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	2	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	10	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	10	0.72
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	10	0.72
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE1	2	0.72
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE2	2	0.72
(1,405)	1:110:A:THR:HG21	1:112:A:LYS:HD2	1	0.72
(1,405)	1:110:A:THR:HG22	1:112:A:LYS:HD2	1	0.72
(1,405)	1:110:A:THR:HG23	1:112:A:LYS:HD2	1	0.72
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	2	0.72
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	2	0.72
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	2	0.72
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	9	0.72
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	8	0.72
(1,4294)	1:172:B:LEU:H	1:172:B:LEU:HB3	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	10	0.71
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	6	0.71
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	10	0.71
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	8	0.71
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	8	0.71
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	8	0.71
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	9	0.71
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	7	0.71
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	9	0.71
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE1	10	0.71
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE2	10	0.71
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	1	0.71
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	1	0.71
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	1	0.71
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	4	0.71
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	4	0.71
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	4	0.71
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	4	0.71
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	4	0.71
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	4	0.71
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	7	0.71
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	7	0.71
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	7	0.71
(1,2213)	1:134:A:ILE:HA	1:140:B:ARG:HD3	1	0.71
(1,2213)	1:134:A:ILE:HA	1:140:B:ARG:HD3	5	0.71
(1,2081)	1:134:A:ILE:HA	1:140:B:ARG:HD3	1	0.71
(1,2081)	1:134:A:ILE:HA	1:140:B:ARG:HD3	5	0.71
(1,2000)	1:169:A:MET:H	1:169:A:MET:HG3	7	0.71
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	8	0.71
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	8	0.71
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	8	0.71
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	4	0.71
(1,1012)	1:148:A:VAL:HG11	1:169:A:MET:HB2	5	0.71
(1,1012)	1:148:A:VAL:HG12	1:169:A:MET:HB2	5	0.71
(1,1012)	1:148:A:VAL:HG13	1:169:A:MET:HB2	5	0.71
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	10	0.71
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE1	9	0.71
(1,763)	1:128:A:GLN:HG3	1:133:A:TYR:HE2	9	0.71
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	1	0.71
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	1	0.71
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	1	0.71
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	6	0.71
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	6	0.71
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	6	0.71
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	3	0.71
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	3	0.71
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	3	0.71
(1,71)	1:95:A:TRP:HB3	1:168:A:PRO:HB2	7	0.71
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB1	1	0.7
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB2	1	0.7
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB3	1	0.7
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB1	9	0.7
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB2	9	0.7
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB3	9	0.7
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	8	0.7
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	5	0.7
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	5	0.7
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	7	0.7
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	7	0.7
(1,2988)	1:126:B:GLU:HA	1:133:B:TYR:HB3	6	0.7
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	1	0.7
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	7	0.7
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	2	0.7
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	2	0.7
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	2	0.7
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	2	0.7
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	2	0.7
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	2	0.7
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	4	0.7
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	10	0.7
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	10	0.7
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	10	0.7
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	3	0.7
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	5	0.7
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	4	0.7
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	6	0.7
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	9	0.7
(1,9)	1:90:A:HIS:HB3	1:91:A:THR:HA	10	0.7
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	1	0.7
(1,4270)	1:169:B:MET:H	1:94:B:ARG:HB3	6	0.69
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	7	0.69
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	1	0.69
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	1	0.69
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	2	0.69
(1,3096)	1:136:B:ARG:HG3	1:138:B:PHE:HA	10	0.69
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	1	0.69
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	2	0.69
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	2	0.69
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	2	0.69
(1,2545)	1:100:B:ASP:HB2	1:162:B:THR:HB	1	0.69
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	5	0.69
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	4	0.69
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	6	0.69
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	7	0.69
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	7	0.69
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	7	0.69
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	6	0.69
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	5	0.69
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	5	0.69
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	5	0.69
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	1	0.69
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	9	0.69
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	8	0.68
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	9	0.68
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	4	0.68
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE1	1	0.68
(1,3044)	1:128:B:GLN:HG3	1:133:B:TYR:HE2	1	0.68
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	5	0.68
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	5	0.68
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	5	0.68
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG21	9	0.68
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG22	9	0.68
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG23	9	0.68
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG21	10	0.68
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG22	10	0.68
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG23	10	0.68
(1,2619)	1:108:B:GLU:HA	1:123:B:LYS:HD2	1	0.68
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	5	0.68
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	5	0.68
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	5	0.68
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	6	0.68
(1,2007)	1:171:A:LYS:H	1:170:A:PRO:HD3	10	0.68
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	2	0.68
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	2	0.68
(1,1691)	1:140:A:ARG:H	1:120:A:ILE:HB	6	0.68
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	2	0.68
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	8	0.68
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	9	0.68
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	9	0.68
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	9	0.68
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	9	0.68
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	4	0.68
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	7	0.68
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	9	0.68
(1,684)	1:123:A:LYS:HA	1:135:A:SER:HB3	3	0.68
(1,232)	1:99:A:LEU:HD11	1:120:A:ILE:HG12	7	0.68
(1,232)	1:99:A:LEU:HD12	1:120:A:ILE:HG12	7	0.68
(1,232)	1:99:A:LEU:HD13	1:120:A:ILE:HG12	7	0.68
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	7	0.68
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	6	0.67
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	6	0.67
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	6	0.67
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	5	0.67
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	7	0.67
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	4	0.67
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	8	0.67
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	5	0.67
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	5	0.67
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	9	0.67
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	4	0.67
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	7	0.67
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	7	0.67
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	7	0.67
(1,2561)	1:102:B:ASN:HB3	1:161:B:GLY:HA3	1	0.67
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	5	0.67
(1,2322)	1:94:B:ARG:HB3	1:167:B:ALA:HA	1	0.67
(1,1614)	1:128:A:GLN:HE21	1:128:A:GLN:HB2	3	0.67
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	1	0.67
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	5	0.67
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	1	0.67
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	1	0.67
(1,710)	1:126:A:GLU:HA	1:135:A:SER:HB2	9	0.67
(1,695)	1:123:A:LYS:HD3	1:137:A:CYS:HB2	10	0.67
(1,688)	1:123:A:LYS:HB2	1:137:A:CYS:HB3	5	0.67
(1,232)	1:99:A:LEU:HD11	1:120:A:ILE:HG12	6	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,232)	1:99:A:LEU:HD12	1:120:A:ILE:HG12	6	0.67
(1,232)	1:99:A:LEU:HD13	1:120:A:ILE:HG12	6	0.67
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	9	0.67
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	9	0.67
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	9	0.67
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB1	7	0.67
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB2	7	0.67
(1,63)	1:95:A:TRP:HB2	1:167:A:ALA:HB3	7	0.67
(1,4)	1:89:A:ARG:HB3	1:90:A:HIS:HB3	5	0.67
(1,3)	1:89:A:ARG:HB2	1:90:A:HIS:HB2	9	0.67
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	7	0.66
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	8	0.66
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	7	0.66
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	7	0.66
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	7	0.66
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	5	0.66
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	5	0.66
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	5	0.66
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	3	0.66
(1,3009)	1:126:B:GLU:HG3	1:133:B:TYR:HA	4	0.66
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	6	0.66
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	8	0.66
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	7	0.66
(1,2314)	1:94:B:ARG:HA	1:169:B:MET:HB2	2	0.66
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	6	0.66
(1,2157)	1:132:B:GLY:HA2	1:140:A:ARG:HA	10	0.66
(1,2025)	1:132:B:GLY:HA2	1:140:A:ARG:HA	10	0.66
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	7	0.66
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	9	0.66
(1,1920)	1:162:A:THR:H	1:158:A:SER:HB2	4	0.66
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	4	0.66
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	4	0.66
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	4	0.66
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	5	0.66
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	1	0.66
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	6	0.66
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG21	4	0.66
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG22	4	0.66
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG23	4	0.66
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	9	0.66
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	7	0.66
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	7	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	7	0.66
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	2	0.66
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	10	0.66
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	2	0.66
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	3	0.66
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	9	0.66
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	5	0.66
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	5	0.66
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	5	0.66
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	6	0.66
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	6	0.66
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	6	0.66
(1,71)	1:95:A:TRP:HB3	1:168:A:PRO:HB2	4	0.66
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	10	0.65
(1,4285)	1:171:B:LYS:H	1:169:B:MET:HA	9	0.65
(1,4267)	1:167:B:ALA:H	1:169:B:MET:H	8	0.65
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD1	4	0.65
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD2	4	0.65
(1,3904)	1:129:B:ASP:H	1:130:B:GLU:HG3	3	0.65
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD11	8	0.65
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD12	8	0.65
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD13	8	0.65
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	6	0.65
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	6	0.65
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	6	0.65
(1,3346)	1:152:B:GLN:HB2	1:169:B:MET:HA	10	0.65
(1,2996)	1:126:B:GLU:HB2	1:135:B:SER:HB3	8	0.65
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	5	0.65
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	5	0.65
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	3	0.65
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	4	0.65
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	5	0.65
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	4	0.65
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	4	0.65
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	4	0.65
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	9	0.65
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	9	0.65
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	9	0.65
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	4	0.65
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	4	0.65
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	4	0.65
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	9	0.65
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	9	0.65
(1,2004)	1:171:A:LYS:H	1:169:A:MET:HA	5	0.65
(1,1691)	1:140:A:ARG:H	1:120:A:ILE:HB	2	0.65
(1,1277)	1:168:A:PRO:HA	1:169:A:MET:HG3	4	0.65
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	5	0.65
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	5	0.65
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	5	0.65
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	1	0.65
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	4	0.65
(1,710)	1:126:A:GLU:HA	1:135:A:SER:HB2	3	0.65
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	2	0.65
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	2	0.65
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	2	0.65
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	8	0.64
(1,3763)	1:114:B:LYS:H	1:115:B:ASP:HB2	4	0.64
(1,3569)	1:169:B:MET:HA	1:169:B:MET:HG2	6	0.64
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	2	0.64
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	4	0.64
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	4	0.64
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	4	0.64
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	1	0.64
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	1	0.64
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	7	0.64
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	2	0.64
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	2	0.64
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	2	0.64
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	2	0.64
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG21	2	0.64
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG22	2	0.64
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG23	2	0.64
(1,2284)	1:89:B:ARG:HB2	1:90:B:HIS:HB2	10	0.64
(1,2282)	1:88:B:ILE:HG21	1:90:B:HIS:HA	9	0.64
(1,2282)	1:88:B:ILE:HG22	1:90:B:HIS:HA	9	0.64
(1,2282)	1:88:B:ILE:HG23	1:90:B:HIS:HA	9	0.64
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	8	0.64
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	4	0.64
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	4	0.64
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	4	0.64
(1,1322)	1:94:A:ARG:H	1:93:A:ASP:HB2	6	0.64
(1,1288)	1:169:A:MET:HA	1:169:A:MET:HG2	9	0.64
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	1	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	8	0.64
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	3	0.64
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	8	0.64
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	5	0.64
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD3	8	0.64
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	2	0.64
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	2	0.64
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	2	0.64
(1,4255)	1:167:B:ALA:H	1:95:B:TRP:HB3	7	0.63
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	4	0.63
(1,3603)	1:94:B:ARG:H	1:93:B:ASP:HB2	1	0.63
(1,3566)	1:168:B:PRO:HD2	1:169:B:MET:HA	9	0.63
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	2	0.63
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	2	0.63
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	2	0.63
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	4	0.63
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	10	0.63
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	3	0.63
(1,2314)	1:94:B:ARG:HA	1:169:B:MET:HB2	6	0.63
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB1	4	0.63
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB2	4	0.63
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB3	4	0.63
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	3	0.63
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	1	0.63
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG21	6	0.63
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG22	6	0.63
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG23	6	0.63
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	5	0.63
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	7	0.63
(1,695)	1:123:A:LYS:HD2	1:137:A:CYS:HB2	1	0.63
(1,406)	1:110:A:THR:HG21	1:112:A:LYS:HE3	8	0.63
(1,406)	1:110:A:THR:HG22	1:112:A:LYS:HE3	8	0.63
(1,406)	1:110:A:THR:HG23	1:112:A:LYS:HE3	8	0.63
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	10	0.63
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	10	0.63
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	10	0.63
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	7	0.63
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	2	0.63
(1,7)	1:90:A:HIS:HB2	1:91:A:THR:HA	2	0.63
(1,4048)	1:149:B:ASP:H	1:170:B:PRO:HG3	4	0.62
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	7	0.62
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	9	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3569)	1:169:B:MET:HA	1:169:B:MET:HG2	3	0.62
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD11	3	0.62
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD12	3	0.62
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD13	3	0.62
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	10	0.62
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	10	0.62
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	10	0.62
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	6	0.62
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	6	0.62
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	6	0.62
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	9	0.62
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	1	0.62
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	1	0.62
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	1	0.62
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	7	0.62
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	7	0.62
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	7	0.62
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	1	0.62
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	3	0.62
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	3	0.62
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	3	0.62
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	6	0.62
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	6	0.62
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	6	0.62
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	1	0.62
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	1	0.62
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	1	0.62
(1,2513)	1:99:B:LEU:HD11	1:120:B:ILE:HG12	6	0.62
(1,2513)	1:99:B:LEU:HD12	1:120:B:ILE:HG12	6	0.62
(1,2513)	1:99:B:LEU:HD13	1:120:B:ILE:HG12	6	0.62
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	9	0.62
(1,2290)	1:90:B:HIS:HB3	1:91:B:THR:HA	8	0.62
(1,2185)	1:133:A:TYR:HB3	1:141:B:LYS:HD3	10	0.62
(1,2053)	1:133:A:TYR:HB3	1:141:B:LYS:HD3	10	0.62
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD3	2	0.62
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB3	8	0.62
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	1	0.62
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	1	0.62
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	1	0.62
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	3	0.62
(1,1637)	1:131:A:HIS:H	1:130:A:GLU:HG3	9	0.62
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	7	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	7	0.62
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	7	0.62
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	7	0.62
(1,1114)	1:155:A:SER:HB2	1:163:A:LEU:HA	2	0.62
(1,743)	1:127:A:ARG:HB3	1:127:A:ARG:HD2	5	0.62
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	6	0.62
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE1	10	0.62
(1,642)	1:120:A:ILE:HG13	1:142:A:TYR:HE2	10	0.62
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	7	0.62
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	7	0.62
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	7	0.62
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	9	0.62
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	9	0.62
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	9	0.62
(1,31)	1:94:A:ARG:HA	1:168:A:PRO:HD2	2	0.62
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	2	0.61
(1,4080)	1:152:B:GLN:HE21	1:152:B:GLN:HB3	10	0.61
(1,4024)	1:148:B:VAL:H	1:146:B:PRO:HB3	5	0.61
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	2	0.61
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	2	0.61
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	2	0.61
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	5	0.61
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	10	0.61
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	6	0.61
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	8	0.61
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	8	0.61
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	8	0.61
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	7	0.61
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	10	0.61
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	10	0.61
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	10	0.61
(1,3118)	1:140:B:ARG:HA	1:140:B:ARG:HD3	3	0.61
(1,3116)	1:139:B:THR:HG21	1:141:B:LYS:HE2	7	0.61
(1,3116)	1:139:B:THR:HG22	1:141:B:LYS:HE2	7	0.61
(1,3116)	1:139:B:THR:HG23	1:141:B:LYS:HE2	7	0.61
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	2	0.61
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	5	0.61
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	5	0.61
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	5	0.61
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG21	5	0.61
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG22	5	0.61
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG23	5	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG21	8	0.61
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG22	8	0.61
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG23	8	0.61
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	4	0.61
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	4	0.61
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	4	0.61
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	7	0.61
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	5	0.61
(1,2013)	1:172:A:LEU:H	1:172:A:LEU:HB2	10	0.61
(1,1413)	1:108:A:GLU:H	1:106:A:PRO:HB3	7	0.61
(1,1288)	1:169:A:MET:HA	1:169:A:MET:HG2	1	0.61
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	8	0.61
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	8	0.61
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	8	0.61
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	3	0.61
(1,968)	1:146:A:PRO:HB3	1:147:A:GLY:HA3	3	0.61
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	5	0.61
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	7	0.61
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	8	0.61
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	6	0.61
(1,474)	1:112:A:LYS:HE2	1:114:A:LYS:HB3	4	0.61
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD2	10	0.61
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	1	0.61
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	1	0.61
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	1	0.61
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	1	0.61
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	10	0.61
(1,72)	1:95:A:TRP:HB3	1:168:A:PRO:HB3	10	0.61
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	10	0.6
(1,3972)	1:140:B:ARG:H	1:120:B:ILE:HB	2	0.6
(1,3904)	1:129:B:ASP:H	1:130:B:GLU:HG3	1	0.6
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	4	0.6
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	2	0.6
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	2	0.6
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	2	0.6
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	2	0.6
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	5	0.6
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	5	0.6
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	5	0.6
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	4	0.6
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	4	0.6
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	3	0.6
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	3	0.6
(1,2996)	1:126:B:GLU:HB2	1:135:B:SER:HB3	4	0.6
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	8	0.6
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	8	0.6
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	8	0.6
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE1	9	0.6
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE2	9	0.6
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	3	0.6
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	3	0.6
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	3	0.6
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	2	0.6
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	3	0.6
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	6	0.6
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	6	0.6
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	6	0.6
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	8	0.6
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	8	0.6
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	8	0.6
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	6	0.6
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	6	0.6
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	6	0.6
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	8	0.6
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	8	0.6
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	8	0.6
(1,1916)	1:162:A:THR:H	1:102:A:ASN:HB3	4	0.6
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	6	0.6
(1,1656)	1:134:A:ILE:H	1:127:A:ARG:HG3	1	0.6
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	1	0.6
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	10	0.6
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	10	0.6
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	10	0.6
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	9	0.6
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	4	0.6
(1,845)	1:141:A:LYS:HA	1:141:A:LYS:HD2	9	0.6
(1,723)	1:126:A:GLU:HG2	1:135:A:SER:HB2	4	0.6
(1,723)	1:126:A:GLU:HG2	1:135:A:SER:HB2	8	0.6
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	3	0.6
(1,682)	1:123:A:LYS:HA	1:123:A:LYS:HE3	7	0.6
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	3	0.6
(1,4267)	1:167:B:ALA:H	1:169:B:MET:H	7	0.59
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	10	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	7	0.59
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	1	0.59
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	1	0.59
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	1	0.59
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	4	0.59
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	5	0.59
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	5	0.59
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	8	0.59
(1,2907)	1:120:B:ILE:HA	1:120:B:ILE:HG13	4	0.59
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	9	0.59
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	2	0.59
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	2	0.59
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	2	0.59
(1,2625)	1:108:B:GLU:HG2	1:123:B:LYS:HD2	4	0.59
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	9	0.59
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	9	0.59
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	9	0.59
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	7	0.59
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	7	0.59
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	7	0.59
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	8	0.59
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	8	0.59
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	8	0.59
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	8	0.59
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	8	0.59
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	8	0.59
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	1	0.59
(1,2346)	1:95:B:TRP:HB3	1:95:B:TRP:HE3	1	0.59
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	10	0.59
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	10	0.59
(1,1623)	1:129:A:ASP:H	1:130:A:GLU:HG3	9	0.59
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	3	0.59
(1,1277)	1:168:A:PRO:HA	1:169:A:MET:HG3	3	0.59
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD21	10	0.59
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD22	10	0.59
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD23	10	0.59
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	2	0.59
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	2	0.59
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	9	0.59
(1,626)	1:120:A:ILE:HA	1:120:A:ILE:HG13	3	0.59
(1,257)	1:99:A:LEU:HD11	1:112:A:LYS:HG3	6	0.59
(1,257)	1:99:A:LEU:HD12	1:112:A:LYS:HG3	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:99:A:LEU:HD13	1:112:A:LYS:HG3	6	0.59
(1,232)	1:99:A:LEU:HD11	1:120:A:ILE:HG12	9	0.59
(1,232)	1:99:A:LEU:HD12	1:120:A:ILE:HG12	9	0.59
(1,232)	1:99:A:LEU:HD13	1:120:A:ILE:HG12	9	0.59
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	3	0.59
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	3	0.59
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	3	0.59
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB1	9	0.59
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB2	9	0.59
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB3	9	0.59
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD3	10	0.58
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	1	0.58
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	6	0.58
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	4	0.58
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	10	0.58
(1,3249)	1:146:B:PRO:HB3	1:147:B:GLY:HA3	9	0.58
(1,3248)	1:146:B:PRO:HB3	1:147:B:GLY:HA2	6	0.58
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	5	0.58
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	5	0.58
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	5	0.58
(1,3126)	1:141:B:LYS:HA	1:141:B:LYS:HD3	5	0.58
(1,3126)	1:141:B:LYS:HA	1:141:B:LYS:HD2	7	0.58
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	3	0.58
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	6	0.58
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	2	0.58
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	3	0.58
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	7	0.58
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	7	0.58
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	7	0.58
(1,2930)	1:120:B:ILE:HG21	1:140:B:ARG:HA	6	0.58
(1,2930)	1:120:B:ILE:HG22	1:140:B:ARG:HA	6	0.58
(1,2930)	1:120:B:ILE:HG23	1:140:B:ARG:HA	6	0.58
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE2	5	0.58
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	8	0.58
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	8	0.58
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	8	0.58
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	9	0.58
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	9	0.58
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	9	0.58
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	4	0.58
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	4	0.58
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	4	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2561)	1:102:B:ASN:HB3	1:161:B:GLY:HA3	9	0.58
(1,2283)	1:88:B:ILE:HG21	1:90:B:HIS:HB3	8	0.58
(1,2283)	1:88:B:ILE:HG22	1:90:B:HIS:HB3	8	0.58
(1,2283)	1:88:B:ILE:HG23	1:90:B:HIS:HB3	8	0.58
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	7	0.58
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	1	0.58
(1,841)	1:140:A:ARG:HG2	1:142:A:TYR:HE1	8	0.58
(1,841)	1:140:A:ARG:HG2	1:142:A:TYR:HE2	8	0.58
(1,427)	1:111:A:VAL:HG11	1:112:A:LYS:HE3	9	0.58
(1,427)	1:111:A:VAL:HG12	1:112:A:LYS:HE3	9	0.58
(1,427)	1:111:A:VAL:HG13	1:112:A:LYS:HE3	9	0.58
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	1	0.58
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	1	0.58
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	1	0.58
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	2	0.58
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	2	0.58
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	2	0.58
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	8	0.58
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	8	0.58
(1,16)	1:93:A:ASP:HA	1:94:A:ARG:HD2	1	0.58
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB3	1	0.57
(1,4025)	1:148:B:VAL:H	1:146:B:PRO:HG2	5	0.57
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	4	0.57
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	1	0.57
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	1	0.57
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	1	0.57
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	2	0.57
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	2	0.57
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	2	0.57
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	6	0.57
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	6	0.57
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	6	0.57
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	5	0.57
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	8	0.57
(1,3005)	1:126:B:GLU:HG2	1:135:B:SER:HB3	8	0.57
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	3	0.57
(1,2969)	1:123:B:LYS:HB2	1:137:B:CYS:HB3	2	0.57
(1,2907)	1:120:B:ILE:HA	1:120:B:ILE:HG13	8	0.57
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	4	0.57
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	4	0.57
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	4	0.57
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	1	0.57
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	1	0.57
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	8	0.57
(1,2346)	1:95:B:TRP:HB3	1:95:B:TRP:HE3	7	0.57
(1,2193)	1:134:B:ILE:HA	1:140:A:ARG:HD2	10	0.57
(1,2185)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	8	0.57
(1,2061)	1:134:B:ILE:HA	1:140:A:ARG:HD2	10	0.57
(1,2053)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	8	0.57
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	3	0.57
(1,1691)	1:140:A:ARG:H	1:120:A:ILE:HB	7	0.57
(1,1637)	1:131:A:HIS:H	1:130:A:GLU:HG3	7	0.57
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	7	0.57
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	5	0.57
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	9	0.57
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	9	0.57
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	9	0.57
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	5	0.57
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	4	0.57
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	2	0.57
(1,733)	1:126:A:GLU:HG3	1:135:A:SER:HB3	3	0.57
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	5	0.57
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	5	0.57
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	5	0.57
(1,65)	1:95:A:TRP:HB3	1:95:A:TRP:HE3	7	0.57
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB1	7	0.57
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB2	7	0.57
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB3	7	0.57
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	10	0.56
(1,4095)	1:152:B:GLN:HE22	1:170:B:PRO:HD3	3	0.56
(1,4080)	1:152:B:GLN:HE21	1:152:B:GLN:HB3	9	0.56
(1,4024)	1:148:B:VAL:H	1:146:B:PRO:HB3	6	0.56
(1,3972)	1:140:B:ARG:H	1:120:B:ILE:HB	3	0.56
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG3	1	0.56
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD1	2	0.56
(1,3911)	1:129:B:ASP:H	1:133:B:TYR:HD2	2	0.56
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	1	0.56
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	7	0.56
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	6	0.56
(1,3293)	1:148:B:VAL:HG11	1:169:B:MET:HB2	4	0.56
(1,3293)	1:148:B:VAL:HG12	1:169:B:MET:HB2	4	0.56
(1,3293)	1:148:B:VAL:HG13	1:169:B:MET:HB2	4	0.56
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	9	0.56
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	7	0.56
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	5	0.56
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	5	0.56
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	5	0.56
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD2	10	0.56
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD21	8	0.56
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD22	8	0.56
(1,2609)	1:106:B:PRO:HD2	1:157:B:LEU:HD23	8	0.56
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	8	0.56
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	3	0.56
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	10	0.56
(1,2169)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	9	0.56
(1,2037)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	9	0.56
(1,1916)	1:162:A:THR:H	1:102:A:ASN:HB3	2	0.56
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	2	0.56
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	4	0.56
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	7	0.56
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	8	0.56
(1,1114)	1:155:A:SER:HB2	1:163:A:LEU:HA	1	0.56
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	3	0.56
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	2	0.56
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	10	0.56
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	9	0.56
(1,626)	1:120:A:ILE:HA	1:120:A:ILE:HG13	1	0.56
(1,427)	1:111:A:VAL:HG11	1:112:A:LYS:HE3	6	0.56
(1,427)	1:111:A:VAL:HG12	1:112:A:LYS:HE3	6	0.56
(1,427)	1:111:A:VAL:HG13	1:112:A:LYS:HE3	6	0.56
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD3	1	0.56
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	8	0.56
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	8	0.56
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	8	0.56
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	5	0.56
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	5	0.56
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	5	0.56
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	9	0.56
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	9	0.56
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	9	0.56
(1,255)	1:99:A:LEU:HD21	1:109:A:LEU:HG	4	0.56
(1,255)	1:99:A:LEU:HD22	1:109:A:LEU:HG	4	0.56
(1,255)	1:99:A:LEU:HD23	1:109:A:LEU:HG	4	0.56
(1,104)	1:96:A:ARG:HG2	1:166:A:GLU:HA	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	2	0.56
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	2	0.56
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	2	0.56
(1,65)	1:95:A:TRP:HB3	1:95:A:TRP:HE3	4	0.56
(1,33)	1:94:A:ARG:HA	1:169:A:MET:HB2	2	0.56
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	8	0.56
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	6	0.55
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	5	0.55
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	5	0.55
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	5	0.55
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	5	0.55
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD3	6	0.55
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	5	0.55
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	10	0.55
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	3	0.55
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	3	0.55
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	3	0.55
(1,2907)	1:120:B:ILE:HA	1:120:B:ILE:HG13	7	0.55
(1,2687)	1:110:B:THR:HG21	1:112:B:LYS:HE3	5	0.55
(1,2687)	1:110:B:THR:HG22	1:112:B:LYS:HE3	5	0.55
(1,2687)	1:110:B:THR:HG23	1:112:B:LYS:HE3	5	0.55
(1,2687)	1:110:B:THR:HG21	1:112:B:LYS:HE3	6	0.55
(1,2687)	1:110:B:THR:HG22	1:112:B:LYS:HE3	6	0.55
(1,2687)	1:110:B:THR:HG23	1:112:B:LYS:HE3	6	0.55
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	3	0.55
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	3	0.55
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	3	0.55
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	6	0.55
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	6	0.55
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	6	0.55
(1,2322)	1:94:B:ARG:HB3	1:167:B:ALA:HA	3	0.55
(1,2313)	1:94:B:ARG:HA	1:168:B:PRO:HD3	2	0.55
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	7	0.55
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	2	0.55
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	9	0.55
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	10	0.55
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	6	0.55
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	6	0.55
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	6	0.55
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	8	0.55
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	3	0.55
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	9	0.55
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	6	0.55
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	6	0.55
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	6	0.55
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	1	0.55
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	7	0.55
(1,770)	1:129:A:ASP:HB3	1:130:A:GLU:HA	8	0.55
(1,723)	1:126:A:GLU:HG2	1:135:A:SER:HB2	1	0.55
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	1	0.55
(1,626)	1:120:A:ILE:HA	1:120:A:ILE:HG13	8	0.55
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	5	0.55
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	5	0.55
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	5	0.55
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	8	0.55
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	8	0.55
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	8	0.55
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	1	0.55
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	1	0.55
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	1	0.55
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB1	8	0.55
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB2	8	0.55
(1,77)	1:95:A:TRP:HE3	1:167:A:ALA:HB3	8	0.55
(1,4280)	1:169:B:MET:H	1:169:B:MET:HB3	2	0.54
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	7	0.54
(1,4084)	1:152:B:GLN:HE21	1:168:B:PRO:HD2	3	0.54
(1,4036)	1:148:B:VAL:H	1:170:B:PRO:HB2	9	0.54
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	8	0.54
(1,3603)	1:94:B:ARG:H	1:93:B:ASP:HB2	8	0.54
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD3	10	0.54
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	6	0.54
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	6	0.54
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	6	0.54
(1,3137)	1:141:B:LYS:HG2	1:142:B:TYR:HB3	10	0.54
(1,3126)	1:141:B:LYS:HA	1:141:B:LYS:HD2	6	0.54
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	9	0.54
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	9	0.54
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	10	0.54
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	1	0.54
(1,2715)	1:111:B:VAL:HG11	1:120:B:ILE:HG12	6	0.54
(1,2715)	1:111:B:VAL:HG12	1:120:B:ILE:HG12	6	0.54
(1,2715)	1:111:B:VAL:HG13	1:120:B:ILE:HG12	6	0.54
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	9	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	9	0.54
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	9	0.54
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	3	0.54
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	3	0.54
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	3	0.54
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	5	0.54
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	5	0.54
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	5	0.54
(1,2299)	1:93:B:ASP:HB2	1:94:B:ARG:HA	3	0.54
(1,2193)	1:134:B:ILE:HA	1:140:A:ARG:HD2	5	0.54
(1,2185)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	1	0.54
(1,2061)	1:134:B:ILE:HA	1:140:A:ARG:HD2	5	0.54
(1,2053)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	1	0.54
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	7	0.54
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	9	0.54
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	9	0.54
(1,1766)	1:149:A:ASP:H	1:169:A:MET:HG3	7	0.54
(1,1756)	1:148:A:VAL:H	1:170:A:PRO:HG3	7	0.54
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	5	0.54
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	7	0.54
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	3	0.54
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	3	0.54
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	3	0.54
(1,699)	1:125:A:GLU:HA	1:125:A:GLU:HG2	10	0.54
(1,626)	1:120:A:ILE:HA	1:120:A:ILE:HG13	5	0.54
(1,626)	1:120:A:ILE:HA	1:120:A:ILE:HG13	10	0.54
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD11	1	0.54
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD12	1	0.54
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD13	1	0.54
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	8	0.54
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	8	0.54
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	8	0.54
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	6	0.54
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	6	0.54
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	6	0.54
(1,65)	1:95:A:TRP:HB3	1:95:A:TRP:HE3	10	0.54
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	3	0.53
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	5	0.53
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	9	0.53
(1,4025)	1:148:B:VAL:H	1:146:B:PRO:HG2	6	0.53
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	6	0.53
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3491)	1:160:B:GLU:HB2	1:162:B:THR:HB	10	0.53
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	7	0.53
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	7	0.53
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	7	0.53
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	5	0.53
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD21	7	0.53
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD22	7	0.53
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD23	7	0.53
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD11	10	0.53
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD12	10	0.53
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD13	10	0.53
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	1	0.53
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	4	0.53
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	7	0.53
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	7	0.53
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	7	0.53
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	5	0.53
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	5	0.53
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	5	0.53
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	9	0.53
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	10	0.53
(1,2980)	1:125:B:GLU:HA	1:125:B:GLU:HG2	7	0.53
(1,2907)	1:120:B:ILE:HA	1:120:B:ILE:HG13	1	0.53
(1,2708)	1:111:B:VAL:HG11	1:112:B:LYS:HE3	2	0.53
(1,2708)	1:111:B:VAL:HG12	1:112:B:LYS:HE3	2	0.53
(1,2708)	1:111:B:VAL:HG13	1:112:B:LYS:HE3	2	0.53
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	6	0.53
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	6	0.53
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	6	0.53
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	10	0.53
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	10	0.53
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	10	0.53
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	2	0.53
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	10	0.53
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	5	0.53
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	5	0.53
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	5	0.53
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	7	0.53
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	9	0.53
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	9	0.53
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	9	0.53
(1,2000)	1:169:A:MET:H	1:169:A:MET:HG3	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1691)	1:140:A:ARG:H	1:120:A:ILE:HB	4	0.53
(1,1514)	1:118:A:VAL:H	1:119:A:GLU:HG3	1	0.53
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD11	7	0.53
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD12	7	0.53
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD13	7	0.53
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD21	8	0.53
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD22	8	0.53
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD23	8	0.53
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	5	0.53
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	5	0.53
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	5	0.53
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	10	0.53
(1,699)	1:125:A:GLU:HA	1:125:A:GLU:HG2	3	0.53
(1,688)	1:123:A:LYS:HB2	1:137:A:CYS:HB3	8	0.53
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	10	0.53
(1,427)	1:111:A:VAL:HG11	1:112:A:LYS:HE3	1	0.53
(1,427)	1:111:A:VAL:HG12	1:112:A:LYS:HE3	1	0.53
(1,427)	1:111:A:VAL:HG13	1:112:A:LYS:HE3	1	0.53
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	6	0.53
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	6	0.53
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	6	0.53
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	6	0.53
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	6	0.53
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	6	0.53
(1,255)	1:99:A:LEU:HD21	1:109:A:LEU:HG	6	0.53
(1,255)	1:99:A:LEU:HD22	1:109:A:LEU:HG	6	0.53
(1,255)	1:99:A:LEU:HD23	1:109:A:LEU:HG	6	0.53
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	4	0.53
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	2	0.52
(1,4093)	1:152:B:GLN:HE22	1:168:B:PRO:HD3	2	0.52
(1,3895)	1:128:B:GLN:HE21	1:128:B:GLN:HB2	3	0.52
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	5	0.52
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	2	0.52
(1,3612)	1:95:B:TRP:H	1:95:B:TRP:HB2	9	0.52
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD3	5	0.52
(1,3491)	1:160:B:GLU:HB2	1:162:B:THR:HB	8	0.52
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	8	0.52
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	2	0.52
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	2	0.52
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	2	0.52
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD11	5	0.52
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD12	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD13	5	0.52
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	4	0.52
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	4	0.52
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	4	0.52
(1,2975)	1:123:B:LYS:HD3	1:137:B:CYS:HA	7	0.52
(1,2974)	1:123:B:LYS:HG3	1:137:B:CYS:HB3	6	0.52
(1,2971)	1:123:B:LYS:HB3	1:137:B:CYS:HB2	10	0.52
(1,2907)	1:120:B:ILE:HA	1:120:B:ILE:HG13	9	0.52
(1,2790)	1:114:B:LYS:HA	1:114:B:LYS:HB2	5	0.52
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	2	0.52
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	2	0.52
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	2	0.52
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	4	0.52
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD11	1	0.52
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD12	1	0.52
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD13	1	0.52
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	6	0.52
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	9	0.52
(1,2346)	1:95:B:TRP:HB3	1:95:B:TRP:HE3	8	0.52
(1,2200)	1:134:B:ILE:HG21	1:140:A:ARG:HD3	3	0.52
(1,2200)	1:134:B:ILE:HG22	1:140:A:ARG:HD3	3	0.52
(1,2200)	1:134:B:ILE:HG23	1:140:A:ARG:HD3	3	0.52
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	10	0.52
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	10	0.52
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	10	0.52
(1,2068)	1:134:B:ILE:HG21	1:140:A:ARG:HD3	3	0.52
(1,2068)	1:134:B:ILE:HG22	1:140:A:ARG:HD3	3	0.52
(1,2068)	1:134:B:ILE:HG23	1:140:A:ARG:HD3	3	0.52
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	10	0.52
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	10	0.52
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	10	0.52
(1,1642)	1:132:A:GLY:H	1:129:A:ASP:HB2	2	0.52
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	3	0.52
(1,1210)	1:160:A:GLU:HB2	1:162:A:THR:HB	4	0.52
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	6	0.52
(1,694)	1:123:A:LYS:HD3	1:137:A:CYS:HA	4	0.52
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	4	0.52
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	1	0.52
(1,255)	1:99:A:LEU:HD21	1:109:A:LEU:HG	7	0.52
(1,255)	1:99:A:LEU:HD22	1:109:A:LEU:HG	7	0.52
(1,255)	1:99:A:LEU:HD23	1:109:A:LEU:HG	7	0.52
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	6	0.52
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	10	0.52
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	7	0.52
(1,72)	1:95:A:TRP:HB3	1:168:A:PRO:HB3	7	0.52
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	2	0.52
(1,4262)	1:167:B:ALA:H	1:166:B:GLU:HB2	6	0.51
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	7	0.51
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	4	0.51
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	7	0.51
(1,3889)	1:128:B:GLN:HE22	1:128:B:GLN:HB2	10	0.51
(1,3848)	1:123:B:LYS:H	1:109:B:LEU:HG	6	0.51
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	6	0.51
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	6	0.51
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	6	0.51
(1,3613)	1:95:B:TRP:H	1:95:B:TRP:HE3	7	0.51
(1,3604)	1:94:B:ARG:H	1:93:B:ASP:HB3	7	0.51
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	4	0.51
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	1	0.51
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	1	0.51
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	1	0.51
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	10	0.51
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	10	0.51
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	10	0.51
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	8	0.51
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	8	0.51
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	8	0.51
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	4	0.51
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	4	0.51
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	4	0.51
(1,2993)	1:126:B:GLU:HB2	1:133:B:TYR:HB2	4	0.51
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE1	3	0.51
(1,2923)	1:120:B:ILE:HG13	1:142:B:TYR:HE2	3	0.51
(1,2907)	1:120:B:ILE:HA	1:120:B:ILE:HG13	10	0.51
(1,2759)	1:112:B:LYS:HE2	1:121:B:THR:HB	6	0.51
(1,2561)	1:102:B:ASN:HB3	1:161:B:GLY:HA3	3	0.51
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	1	0.51
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	1	0.51
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	8	0.51
(1,2282)	1:88:B:ILE:HG21	1:90:B:HIS:HA	10	0.51
(1,2282)	1:88:B:ILE:HG22	1:90:B:HIS:HA	10	0.51
(1,2282)	1:88:B:ILE:HG23	1:90:B:HIS:HA	10	0.51
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2177)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	5	0.51
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	8	0.51
(1,2045)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	5	0.51
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD3	5	0.51
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	6	0.51
(1,1799)	1:152:A:GLN:HE21	1:152:A:GLN:HB3	7	0.51
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	10	0.51
(1,1193)	1:158:A:SER:HB3	1:160:A:GLU:HB3	2	0.51
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	10	0.51
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	7	0.51
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD21	9	0.51
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD22	9	0.51
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD23	9	0.51
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	8	0.51
(1,722)	1:126:A:GLU:HG2	1:135:A:SER:HA	6	0.51
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	8	0.51
(1,699)	1:125:A:GLU:HA	1:125:A:GLU:HG2	1	0.51
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	6	0.51
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	4	0.51
(1,449)	1:112:A:LYS:HA	1:112:A:LYS:HE3	9	0.51
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	7	0.51
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	4	0.51
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD3	9	0.51
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD21	7	0.51
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD22	7	0.51
(1,328)	1:106:A:PRO:HD2	1:157:A:LEU:HD23	7	0.51
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	6	0.51
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	6	0.51
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	6	0.51
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	3	0.51
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	7	0.51
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	8	0.51
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	6	0.51
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	4	0.51
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	2	0.51
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	2	0.51
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	2	0.51
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG11	1	0.51
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG12	1	0.51
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG13	1	0.51
(1,18)	1:93:A:ASP:HB2	1:94:A:ARG:HA	6	0.51
(1,4269)	1:169:B:MET:H	1:94:B:ARG:HA	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	10	0.5
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB1	7	0.5
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB2	7	0.5
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB3	7	0.5
(1,4095)	1:152:B:GLN:HE22	1:170:B:PRO:HD3	1	0.5
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	10	0.5
(1,4024)	1:148:B:VAL:H	1:146:B:PRO:HB3	8	0.5
(1,3763)	1:114:B:LYS:H	1:115:B:ASP:HB2	7	0.5
(1,3704)	1:108:B:GLU:H	1:123:B:LYS:HG2	2	0.5
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	3	0.5
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD11	6	0.5
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD12	6	0.5
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD13	6	0.5
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	8	0.5
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	7	0.5
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	6	0.5
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	10	0.5
(1,3274)	1:148:B:VAL:HA	1:170:B:PRO:HG2	3	0.5
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	6	0.5
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	1	0.5
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	7	0.5
(1,2993)	1:126:B:GLU:HB2	1:133:B:TYR:HB2	8	0.5
(1,2980)	1:125:B:GLU:HA	1:125:B:GLU:HG2	5	0.5
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	6	0.5
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	7	0.5
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	1	0.5
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	1	0.5
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	1	0.5
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	4	0.5
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	4	0.5
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	4	0.5
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	5	0.5
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	5	0.5
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	5	0.5
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	8	0.5
(1,2473)	1:98:B:SER:HB3	1:99:B:LEU:HD21	3	0.5
(1,2473)	1:98:B:SER:HB3	1:99:B:LEU:HD22	3	0.5
(1,2473)	1:98:B:SER:HB3	1:99:B:LEU:HD23	3	0.5
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	4	0.5
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	4	0.5
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	4	0.5
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2281)	1:143:A:THR:H	1:132:B:GLY:HA2	3	0.5
(1,2148)	1:143:A:THR:H	1:132:B:GLY:HA2	3	0.5
(1,2007)	1:171:A:LYS:H	1:170:A:PRO:HD3	5	0.5
(1,2000)	1:169:A:MET:H	1:169:A:MET:HG3	9	0.5
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD3	6	0.5
(1,1654)	1:134:A:ILE:H	1:127:A:ARG:HB2	3	0.5
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	2	0.5
(1,1331)	1:95:A:TRP:H	1:95:A:TRP:HB2	8	0.5
(1,1322)	1:94:A:ARG:H	1:93:A:ASP:HB2	4	0.5
(1,1193)	1:158:A:SER:HB3	1:160:A:GLU:HB3	4	0.5
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	8	0.5
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	1	0.5
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	1	0.5
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	1	0.5
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	2	0.5
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	2	0.5
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	2	0.5
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	3	0.5
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	6	0.5
(1,712)	1:126:A:GLU:HB3	1:133:A:TYR:HB2	3	0.5
(1,699)	1:125:A:GLU:HA	1:125:A:GLU:HG2	7	0.5
(1,695)	1:123:A:LYS:HD3	1:137:A:CYS:HB2	3	0.5
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	2	0.5
(1,449)	1:112:A:LYS:HA	1:112:A:LYS:HE2	7	0.5
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	1	0.5
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	2	0.5
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	5	0.5
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	9	0.5
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	2	0.5
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	2	0.5
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	2	0.5
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	7	0.5
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	7	0.5
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	7	0.5
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	4	0.5
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	4	0.5
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	4	0.5
(1,18)	1:93:A:ASP:HB2	1:94:A:ARG:HA	4	0.5
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD2	9	0.49
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	8	0.49
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	2	0.49
(1,3460)	1:157:B:LEU:HD21	1:163:B:LEU:HB3	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3460)	1:157:B:LEU:HD22	1:163:B:LEU:HB3	7	0.49
(1,3460)	1:157:B:LEU:HD23	1:163:B:LEU:HB3	7	0.49
(1,3436)	1:157:B:LEU:HB2	1:163:B:LEU:HA	1	0.49
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	2	0.49
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	2	0.49
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	2	0.49
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	2	0.49
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG11	9	0.49
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG12	9	0.49
(1,3240)	1:145:B:PRO:HG3	1:148:B:VAL:HG13	9	0.49
(1,3116)	1:139:B:THR:HG21	1:141:B:LYS:HE2	5	0.49
(1,3116)	1:139:B:THR:HG22	1:141:B:LYS:HE2	5	0.49
(1,3116)	1:139:B:THR:HG23	1:141:B:LYS:HE2	5	0.49
(1,3116)	1:139:B:THR:HG21	1:141:B:LYS:HE2	6	0.49
(1,3116)	1:139:B:THR:HG22	1:141:B:LYS:HE2	6	0.49
(1,3116)	1:139:B:THR:HG23	1:141:B:LYS:HE2	6	0.49
(1,2980)	1:125:B:GLU:HA	1:125:B:GLU:HG2	8	0.49
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	4	0.49
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	4	0.49
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	4	0.49
(1,2790)	1:114:B:LYS:HA	1:114:B:LYS:HB2	3	0.49
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE2	6	0.49
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	2	0.49
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	2	0.49
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	7	0.49
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	7	0.49
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	7	0.49
(1,2194)	1:134:B:ILE:HA	1:140:A:ARG:HD3	5	0.49
(1,2149)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	2	0.49
(1,2149)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	2	0.49
(1,2149)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	2	0.49
(1,2062)	1:134:B:ILE:HA	1:140:A:ARG:HD3	5	0.49
(1,2017)	1:97:B:VAL:HG11	1:131:A:HIS:HB2	2	0.49
(1,2017)	1:97:B:VAL:HG12	1:131:A:HIS:HB2	2	0.49
(1,2017)	1:97:B:VAL:HG13	1:131:A:HIS:HB2	2	0.49
(1,1743)	1:148:A:VAL:H	1:146:A:PRO:HB3	6	0.49
(1,1582)	1:125:A:GLU:H	1:124:A:HIS:HB2	10	0.49
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	7	0.49
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	7	0.49
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	7	0.49
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	8	0.49
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	8	0.49
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	10	0.49
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	10	0.49
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	10	0.49
(1,710)	1:126:A:GLU:HA	1:135:A:SER:HB2	5	0.49
(1,695)	1:123:A:LYS:HD2	1:137:A:CYS:HB2	9	0.49
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	3	0.49
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	3	0.49
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	3	0.49
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	3	0.49
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	1	0.49
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	6	0.49
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	3	0.49
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	3	0.49
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	3	0.49
(1,72)	1:95:A:TRP:HB3	1:168:A:PRO:HB3	4	0.49
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB1	2	0.49
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB2	2	0.49
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB3	2	0.49
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	3	0.48
(1,4267)	1:167:B:ALA:H	1:169:B:MET:H	4	0.48
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD3	8	0.48
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	8	0.48
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	4	0.48
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD21	4	0.48
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD22	4	0.48
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD23	4	0.48
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	7	0.48
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD21	5	0.48
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD22	5	0.48
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD23	5	0.48
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	1	0.48
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	3	0.48
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	1	0.48
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	1	0.48
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	1	0.48
(1,3274)	1:148:B:VAL:HA	1:170:B:PRO:HG2	1	0.48
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	8	0.48
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	8	0.48
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	8	0.48
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	5	0.48
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	5	0.48
(1,3137)	1:141:B:LYS:HG2	1:142:B:TYR:HB3	8	0.48
(1,2970)	1:123:B:LYS:HB3	1:137:B:CYS:HA	10	0.48
(1,2969)	1:123:B:LYS:HB2	1:137:B:CYS:HB3	8	0.48
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	10	0.48
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	10	0.48
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	10	0.48
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	8	0.48
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	8	0.48
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	8	0.48
(1,2753)	1:112:B:LYS:HD2	1:120:B:ILE:HA	1	0.48
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	7	0.48
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	5	0.48
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	6	0.48
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	10	0.48
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	3	0.48
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	3	0.48
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	3	0.48
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	9	0.48
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	9	0.48
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	9	0.48
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	9	0.48
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	10	0.48
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	9	0.48
(1,2185)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	4	0.48
(1,2053)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	4	0.48
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	4	0.48
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	6	0.48
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	10	0.48
(1,1640)	1:132:A:GLY:H	1:128:A:GLN:HG2	5	0.48
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	2	0.48
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	3	0.48
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	7	0.48
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	10	0.48
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	2	0.48
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	2	0.48
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	2	0.48
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	5	0.48
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	5	0.48
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	5	0.48
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	7	0.48
(1,770)	1:129:A:ASP:HB3	1:130:A:GLU:HA	9	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	1:126:A:GLU:HG2	1:133:A:TYR:HB3	10	0.48
(1,688)	1:123:A:LYS:HB2	1:137:A:CYS:HB3	7	0.48
(1,682)	1:123:A:LYS:HA	1:123:A:LYS:HE2	4	0.48
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	3	0.48
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	3	0.48
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	3	0.48
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	5	0.48
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	5	0.48
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	5	0.48
(1,345)	1:108:A:GLU:HG2	1:123:A:LYS:HE2	3	0.48
(1,344)	1:108:A:GLU:HG2	1:123:A:LYS:HD3	8	0.48
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	6	0.48
(1,282)	1:105:A:ALA:HA	1:106:A:PRO:HB2	10	0.48
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	5	0.48
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	5	0.48
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	5	0.48
(1,99)	1:96:A:ARG:HB3	1:164:A:THR:HB	1	0.48
(1,1)	1:88:A:ILE:HG21	1:90:A:HIS:HA	1	0.48
(1,1)	1:88:A:ILE:HG22	1:90:A:HIS:HA	1	0.48
(1,1)	1:88:A:ILE:HG23	1:90:A:HIS:HA	1	0.48
(1,4255)	1:167:B:ALA:H	1:95:B:TRP:HB3	2	0.47
(1,3895)	1:128:B:GLN:HE21	1:128:B:GLN:HB2	6	0.47
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	2	0.47
(1,3612)	1:95:B:TRP:H	1:95:B:TRP:HB2	5	0.47
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	6	0.47
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	6	0.47
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	6	0.47
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	8	0.47
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	8	0.47
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	8	0.47
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	1	0.47
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	7	0.47
(1,2969)	1:123:B:LYS:HB2	1:137:B:CYS:HB3	7	0.47
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	6	0.47
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	6	0.47
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	6	0.47
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG21	1	0.47
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG22	1	0.47
(1,2795)	1:115:B:ASP:HB2	1:143:B:THR:HG23	1	0.47
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	5	0.47
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	1	0.47
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	6	0.47
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	4	0.47
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	4	0.47
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	4	0.47
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	1	0.47
(1,2352)	1:95:B:TRP:HB2	1:168:B:PRO:HB2	10	0.47
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB1	5	0.47
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB2	5	0.47
(1,1843)	1:154:A:SER:H	1:167:A:ALA:HB3	5	0.47
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	7	0.47
(1,1331)	1:95:A:TRP:H	1:95:A:TRP:HB2	5	0.47
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE2	8	0.47
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	6	0.47
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	5	0.47
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	6	0.47
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	6	0.47
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	6	0.47
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	8	0.47
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	8	0.47
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	8	0.47
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	1	0.47
(1,690)	1:123:A:LYS:HB3	1:137:A:CYS:HB2	10	0.47
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	4	0.47
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	4	0.47
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	4	0.47
(1,449)	1:112:A:LYS:HA	1:112:A:LYS:HE2	8	0.47
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	4	0.47
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	4	0.47
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	4	0.47
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	9	0.47
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	9	0.47
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	9	0.47
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	10	0.47
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	10	0.47
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	10	0.47
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	5	0.47
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	5	0.47
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	5	0.47
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	5	0.47
(1,2)	1:88:A:ILE:HG21	1:90:A:HIS:HB3	8	0.47
(1,2)	1:88:A:ILE:HG22	1:90:A:HIS:HB3	8	0.47
(1,2)	1:88:A:ILE:HG23	1:90:A:HIS:HB3	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG3	7	0.46
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG21	10	0.46
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG22	10	0.46
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG23	10	0.46
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	5	0.46
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	10	0.46
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	10	0.46
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	10	0.46
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	6	0.46
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	8	0.46
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	8	0.46
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	8	0.46
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG3	3	0.46
(1,3694)	1:108:B:GLU:H	1:106:B:PRO:HB3	2	0.46
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	9	0.46
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	4	0.46
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	4	0.46
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	4	0.46
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	2	0.46
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	1	0.46
(1,3303)	1:148:B:VAL:HG21	1:170:B:PRO:HG2	1	0.46
(1,3303)	1:148:B:VAL:HG22	1:170:B:PRO:HG2	1	0.46
(1,3303)	1:148:B:VAL:HG23	1:170:B:PRO:HG2	1	0.46
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	6	0.46
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	6	0.46
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	6	0.46
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	6	0.46
(1,3027)	1:128:B:GLN:HA	1:128:B:GLN:HG3	1	0.46
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	3	0.46
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	3	0.46
(1,2930)	1:120:B:ILE:HG21	1:140:B:ARG:HA	5	0.46
(1,2930)	1:120:B:ILE:HG22	1:140:B:ARG:HA	5	0.46
(1,2930)	1:120:B:ILE:HG23	1:140:B:ARG:HA	5	0.46
(1,2893)	1:119:B:GLU:HA	1:141:B:LYS:HE3	9	0.46
(1,2790)	1:114:B:LYS:HA	1:114:B:LYS:HB2	8	0.46
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	1	0.46
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	3	0.46
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD3	8	0.46
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	3	0.46
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	3	0.46
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	3	0.46
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	8	0.46
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	8	0.46
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	3	0.46
(1,2563)	1:105:B:ALA:HA	1:106:B:PRO:HB2	9	0.46
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	4	0.46
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	4	0.46
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	4	0.46
(1,2472)	1:98:B:SER:HB3	1:99:B:LEU:HA	3	0.46
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	5	0.46
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	2	0.46
(1,2352)	1:95:B:TRP:HB2	1:168:B:PRO:HB2	9	0.46
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	7	0.46
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	6	0.46
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	6	0.46
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	6	0.46
(1,2194)	1:134:B:ILE:HA	1:140:A:ARG:HD3	10	0.46
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	6	0.46
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	6	0.46
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	6	0.46
(1,2062)	1:134:B:ILE:HA	1:140:A:ARG:HD3	10	0.46
(1,1916)	1:162:A:THR:H	1:102:A:ASN:HB3	7	0.46
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	3	0.46
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	3	0.46
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	3	0.46
(1,1664)	1:135:A:SER:H	1:134:A:ILE:HG13	5	0.46
(1,1612)	1:128:A:GLN:HE22	1:129:A:ASP:H	7	0.46
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	8	0.46
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	4	0.46
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	7	0.46
(1,1322)	1:94:A:ARG:H	1:93:A:ASP:HB2	9	0.46
(1,1210)	1:160:A:GLU:HB2	1:162:A:THR:HB	7	0.46
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	5	0.46
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG11	9	0.46
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG12	9	0.46
(1,1127)	1:155:A:SER:HB3	1:165:A:VAL:HG13	9	0.46
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	10	0.46
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	7	0.46
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	8	0.46
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	4	0.46
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	4	0.46
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	4	0.46
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	6	0.46
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	6	0.46
(1,834)	1:139:A:THR:HG21	1:140:A:ARG:HG3	4	0.46
(1,834)	1:139:A:THR:HG22	1:140:A:ARG:HG3	4	0.46
(1,834)	1:139:A:THR:HG23	1:140:A:ARG:HG3	4	0.46
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	6	0.46
(1,612)	1:119:A:GLU:HA	1:141:A:LYS:HE3	1	0.46
(1,528)	1:116:A:GLY:HA2	1:148:A:VAL:HB	4	0.46
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	5	0.46
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	9	0.46
(1,107)	1:96:A:ARG:HG2	1:166:A:GLU:HG2	8	0.46
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	3	0.46
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	3	0.46
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	3	0.46
(1,4280)	1:169:B:MET:H	1:169:B:MET:HB3	10	0.45
(1,4231)	1:165:B:VAL:H	1:96:B:ARG:HB2	9	0.45
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	8	0.45
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	7	0.45
(1,3748)	1:113:B:THR:H	1:112:B:LYS:HB2	8	0.45
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	6	0.45
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD22	9	0.45
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	6	0.45
(1,3613)	1:95:B:TRP:H	1:95:B:TRP:HE3	1	0.45
(1,3612)	1:95:B:TRP:H	1:95:B:TRP:HB2	10	0.45
(1,3601)	1:94:B:ARG:H	1:92:B:ALA:HA	5	0.45
(1,3570)	1:169:B:MET:HA	1:169:B:MET:HG3	7	0.45
(1,3460)	1:157:B:LEU:HD21	1:163:B:LEU:HB3	4	0.45
(1,3460)	1:157:B:LEU:HD22	1:163:B:LEU:HB3	4	0.45
(1,3460)	1:157:B:LEU:HD23	1:163:B:LEU:HB3	4	0.45
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	7	0.45
(1,3420)	1:156:B:SER:HB3	1:157:B:LEU:HB3	10	0.45
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	8	0.45
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	4	0.45
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	4	0.45
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	4	0.45
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	5	0.45
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	5	0.45
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	5	0.45
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	9	0.45
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	2	0.45
(1,2957)	1:122:B:GLY:HA3	1:137:B:CYS:HA	8	0.45
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	5	0.45
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	5	0.45
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	6	0.45
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	6	0.45
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	6	0.45
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	5	0.45
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	9	0.45
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	10	0.45
(1,2352)	1:95:B:TRP:HB3	1:168:B:PRO:HB2	1	0.45
(1,2318)	1:94:B:ARG:HB2	1:96:B:ARG:HA	1	0.45
(1,2314)	1:94:B:ARG:HA	1:169:B:MET:HB2	1	0.45
(1,2207)	1:134:B:ILE:HD11	1:140:A:ARG:HG2	2	0.45
(1,2207)	1:134:B:ILE:HD12	1:140:A:ARG:HG2	2	0.45
(1,2207)	1:134:B:ILE:HD13	1:140:A:ARG:HG2	2	0.45
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	7	0.45
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	7	0.45
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	7	0.45
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	8	0.45
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	8	0.45
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	8	0.45
(1,2075)	1:134:B:ILE:HD11	1:140:A:ARG:HG2	2	0.45
(1,2075)	1:134:B:ILE:HD12	1:140:A:ARG:HG2	2	0.45
(1,2075)	1:134:B:ILE:HD13	1:140:A:ARG:HG2	2	0.45
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	7	0.45
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	7	0.45
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	7	0.45
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	8	0.45
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	8	0.45
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	8	0.45
(1,1924)	1:162:A:THR:H	1:160:A:GLU:HB2	2	0.45
(1,1767)	1:149:A:ASP:H	1:170:A:PRO:HG3	4	0.45
(1,1664)	1:135:A:SER:H	1:134:A:ILE:HG13	2	0.45
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	6	0.45
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	7	0.45
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	10	0.45
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	2	0.45
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	8	0.45
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	8	0.45
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	8	0.45
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	9	0.45
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	9	0.45
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	1	0.45
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	1	0.45
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	1	0.45
(1,834)	1:139:A:THR:HG21	1:140:A:ARG:HG3	3	0.45
(1,834)	1:139:A:THR:HG22	1:140:A:ARG:HG3	3	0.45
(1,834)	1:139:A:THR:HG23	1:140:A:ARG:HG3	3	0.45
(1,728)	1:126:A:GLU:HG3	1:133:A:TYR:HA	7	0.45
(1,723)	1:126:A:GLU:HG2	1:135:A:SER:HB2	5	0.45
(1,694)	1:123:A:LYS:HD3	1:137:A:CYS:HA	7	0.45
(1,690)	1:123:A:LYS:HB3	1:137:A:CYS:HB2	4	0.45
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	6	0.45
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	6	0.45
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	6	0.45
(1,528)	1:116:A:GLY:HA2	1:148:A:VAL:HB	1	0.45
(1,472)	1:112:A:LYS:HD2	1:120:A:ILE:HA	9	0.45
(1,455)	1:112:A:LYS:HB2	1:112:A:LYS:HE2	8	0.45
(1,434)	1:111:A:VAL:HG11	1:120:A:ILE:HG12	7	0.45
(1,434)	1:111:A:VAL:HG12	1:120:A:ILE:HG12	7	0.45
(1,434)	1:111:A:VAL:HG13	1:120:A:ILE:HG12	7	0.45
(1,434)	1:111:A:VAL:HG11	1:120:A:ILE:HG12	9	0.45
(1,434)	1:111:A:VAL:HG12	1:120:A:ILE:HG12	9	0.45
(1,434)	1:111:A:VAL:HG13	1:120:A:ILE:HG12	9	0.45
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	5	0.45
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	9	0.45
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	2	0.45
(1,345)	1:108:A:GLU:HG2	1:123:A:LYS:HE2	7	0.45
(1,71)	1:95:A:TRP:HB3	1:168:A:PRO:HB2	9	0.45
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB1	6	0.45
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB2	6	0.45
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB3	6	0.45
(1,4296)	1:173:B:ALA:H	1:172:B:LEU:HG	5	0.44
(1,4272)	1:169:B:MET:H	1:95:B:TRP:HA	4	0.44
(1,4205)	1:162:B:THR:H	1:160:B:GLU:HB2	1	0.44
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	3	0.44
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	3	0.44
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	3	0.44
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	3	0.44
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	8	0.44
(1,3607)	1:94:B:ARG:H	1:168:B:PRO:HA	9	0.44
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD2	3	0.44
(1,3460)	1:157:B:LEU:HD21	1:163:B:LEU:HB3	5	0.44
(1,3460)	1:157:B:LEU:HD22	1:163:B:LEU:HB3	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3460)	1:157:B:LEU:HD23	1:163:B:LEU:HB3	5	0.44
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	9	0.44
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	5	0.44
(1,3345)	1:152:B:GLN:HB2	1:168:B:PRO:HD3	7	0.44
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	7	0.44
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	7	0.44
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	7	0.44
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	2	0.44
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	10	0.44
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	10	0.44
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	10	0.44
(1,2963)	1:123:B:LYS:HA	1:123:B:LYS:HE3	9	0.44
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	2	0.44
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	2	0.44
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	2	0.44
(1,2790)	1:114:B:LYS:HA	1:114:B:LYS:HB2	9	0.44
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	9	0.44
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	9	0.44
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	9	0.44
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	1	0.44
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	1	0.44
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	1	0.44
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	6	0.44
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD2	4	0.44
(1,2551)	1:101:B:VAL:HG11	1:102:B:ASN:HA	5	0.44
(1,2551)	1:101:B:VAL:HG12	1:102:B:ASN:HA	5	0.44
(1,2551)	1:101:B:VAL:HG13	1:102:B:ASN:HA	5	0.44
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	3	0.44
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	6	0.44
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	7	0.44
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	5	0.44
(1,1640)	1:132:A:GLY:H	1:128:A:GLN:HG2	4	0.44
(1,1623)	1:129:A:ASP:H	1:130:A:GLU:HG3	7	0.44
(1,1482)	1:114:A:LYS:H	1:115:A:ASP:HB2	9	0.44
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	6	0.44
(1,1332)	1:95:A:TRP:H	1:95:A:TRP:HE3	10	0.44
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	8	0.44
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	8	0.44
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	8	0.44
(1,1097)	1:154:A:SER:HB3	1:155:A:SER:HA	7	0.44
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	3	0.44
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	3	0.44
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	9	0.44
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	9	0.44
(1,724)	1:126:A:GLU:HG2	1:135:A:SER:HB3	5	0.44
(1,722)	1:126:A:GLU:HG2	1:135:A:SER:HA	9	0.44
(1,718)	1:126:A:GLU:HG2	1:133:A:TYR:HB3	8	0.44
(1,712)	1:126:A:GLU:HB3	1:133:A:TYR:HB2	2	0.44
(1,682)	1:123:A:LYS:HA	1:123:A:LYS:HE3	3	0.44
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	6	0.44
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	6	0.44
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	6	0.44
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	7	0.44
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	7	0.44
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	7	0.44
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	9	0.44
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	9	0.44
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	9	0.44
(1,455)	1:112:A:LYS:HB2	1:112:A:LYS:HE2	7	0.44
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	2	0.44
(1,257)	1:99:A:LEU:HD21	1:112:A:LYS:HG3	1	0.44
(1,257)	1:99:A:LEU:HD22	1:112:A:LYS:HG3	1	0.44
(1,257)	1:99:A:LEU:HD23	1:112:A:LYS:HG3	1	0.44
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	7	0.44
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	3	0.44
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	3	0.44
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD2	4	0.43
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD3	7	0.43
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG21	1	0.43
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG22	1	0.43
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG23	1	0.43
(1,4197)	1:162:B:THR:H	1:102:B:ASN:HB3	2	0.43
(1,4084)	1:152:B:GLN:HE21	1:168:B:PRO:HD2	1	0.43
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	2	0.43
(1,4025)	1:148:B:VAL:H	1:146:B:PRO:HG2	8	0.43
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	10	0.43
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	10	0.43
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	10	0.43
(1,3972)	1:140:B:ARG:H	1:120:B:ILE:HB	5	0.43
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD1	1	0.43
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD2	1	0.43
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	5	0.43
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	7	0.43
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	7	0.43
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	5	0.43
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	6	0.43
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	6	0.43
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	6	0.43
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	8	0.43
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD21	2	0.43
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD22	2	0.43
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD23	2	0.43
(1,3304)	1:149:B:ASP:HA	1:149:B:ASP:HB3	1	0.43
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	1	0.43
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	1	0.43
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	1	0.43
(1,3299)	1:148:B:VAL:HG21	1:168:B:PRO:HD3	10	0.43
(1,3299)	1:148:B:VAL:HG22	1:168:B:PRO:HD3	10	0.43
(1,3299)	1:148:B:VAL:HG23	1:168:B:PRO:HD3	10	0.43
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	1	0.43
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	1	0.43
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	1	0.43
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	2	0.43
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	2	0.43
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	2	0.43
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	7	0.43
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	2	0.43
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	6	0.43
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	2	0.43
(1,2976)	1:123:B:LYS:HD3	1:137:B:CYS:HB2	5	0.43
(1,2976)	1:123:B:LYS:HD3	1:137:B:CYS:HB2	7	0.43
(1,2976)	1:123:B:LYS:HD3	1:137:B:CYS:HB2	9	0.43
(1,2975)	1:123:B:LYS:HD3	1:137:B:CYS:HA	9	0.43
(1,2963)	1:123:B:LYS:HA	1:123:B:LYS:HE3	5	0.43
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	8	0.43
(1,2545)	1:100:B:ASP:HB2	1:162:B:THR:HB	9	0.43
(1,2513)	1:99:B:LEU:HD11	1:120:B:ILE:HG12	2	0.43
(1,2513)	1:99:B:LEU:HD12	1:120:B:ILE:HG12	2	0.43
(1,2513)	1:99:B:LEU:HD13	1:120:B:ILE:HG12	2	0.43
(1,2513)	1:99:B:LEU:HD11	1:120:B:ILE:HG12	5	0.43
(1,2513)	1:99:B:LEU:HD12	1:120:B:ILE:HG12	5	0.43
(1,2513)	1:99:B:LEU:HD13	1:120:B:ILE:HG12	5	0.43
(1,2383)	1:96:B:ARG:HB3	1:166:B:GLU:HB3	6	0.43
(1,2314)	1:94:B:ARG:HA	1:169:B:MET:HB2	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	5	0.43
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	5	0.43
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	5	0.43
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	5	0.43
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	5	0.43
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	5	0.43
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	3	0.43
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	8	0.43
(1,1799)	1:152:A:GLN:HE21	1:152:A:GLN:HB3	3	0.43
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	9	0.43
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	8	0.43
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	1	0.43
(1,1288)	1:169:A:MET:HA	1:169:A:MET:HG2	6	0.43
(1,1260)	1:166:A:GLU:HG3	1:168:A:PRO:HD3	1	0.43
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	9	0.43
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	9	0.43
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	9	0.43
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	6	0.43
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD11	6	0.43
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD12	6	0.43
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD13	6	0.43
(1,1085)	1:153:A:VAL:HG21	1:155:A:SER:HB3	1	0.43
(1,1085)	1:153:A:VAL:HG22	1:155:A:SER:HB3	1	0.43
(1,1085)	1:153:A:VAL:HG23	1:155:A:SER:HB3	1	0.43
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	5	0.43
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	1	0.43
(1,694)	1:123:A:LYS:HD3	1:137:A:CYS:HA	2	0.43
(1,694)	1:123:A:LYS:HD2	1:137:A:CYS:HA	6	0.43
(1,682)	1:123:A:LYS:HA	1:123:A:LYS:HE3	8	0.43
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	4	0.43
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	4	0.43
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	4	0.43
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	8	0.43
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	8	0.43
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	8	0.43
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	8	0.43
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	6	0.43
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	7	0.43
(1,405)	1:110:A:THR:HG21	1:112:A:LYS:HD3	2	0.43
(1,405)	1:110:A:THR:HG22	1:112:A:LYS:HD3	2	0.43
(1,405)	1:110:A:THR:HG23	1:112:A:LYS:HD3	2	0.43
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	7	0.43
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	7	0.43
(1,370)	1:109:A:LEU:HD11	1:122:A:GLY:HA3	5	0.43
(1,370)	1:109:A:LEU:HD12	1:122:A:GLY:HA3	5	0.43
(1,370)	1:109:A:LEU:HD13	1:122:A:GLY:HA3	5	0.43
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	1	0.43
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	1	0.43
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	1	0.43
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD21	1	0.43
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD22	1	0.43
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD23	1	0.43
(1,247)	1:99:A:LEU:HD21	1:140:A:ARG:HG3	3	0.43
(1,247)	1:99:A:LEU:HD22	1:140:A:ARG:HG3	3	0.43
(1,247)	1:99:A:LEU:HD23	1:140:A:ARG:HG3	3	0.43
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	8	0.43
(1,71)	1:95:A:TRP:HB2	1:168:A:PRO:HB2	5	0.43
(1,71)	1:95:A:TRP:HB2	1:168:A:PRO:HB2	8	0.43
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	9	0.43
(1,7)	1:90:A:HIS:HB2	1:91:A:THR:HA	8	0.43
(1,4197)	1:162:B:THR:H	1:102:B:ASN:HB3	8	0.42
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	6	0.42
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	3	0.42
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	3	0.42
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	3	0.42
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	2	0.42
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	2	0.42
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	2	0.42
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	4	0.42
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	4	0.42
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	4	0.42
(1,3904)	1:129:B:ASP:H	1:130:B:GLU:HG3	6	0.42
(1,3904)	1:129:B:ASP:H	1:130:B:GLU:HG3	9	0.42
(1,3895)	1:128:B:GLN:HE21	1:128:B:GLN:HB2	7	0.42
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	10	0.42
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD21	7	0.42
(1,3491)	1:160:B:GLU:HB2	1:162:B:THR:HB	2	0.42
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	3	0.42
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	3	0.42
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	3	0.42
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	4	0.42
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	4	0.42
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	9	0.42
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	9	0.42
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	9	0.42
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	3	0.42
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	9	0.42
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	4	0.42
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	1	0.42
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	10	0.42
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	3	0.42
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	3	0.42
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	3	0.42
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	3	0.42
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	8	0.42
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	6	0.42
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD11	4	0.42
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD12	4	0.42
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD13	4	0.42
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD11	4	0.42
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD12	4	0.42
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD13	4	0.42
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD11	4	0.42
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD12	4	0.42
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD13	4	0.42
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	5	0.42
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	5	0.42
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	5	0.42
(1,2468)	1:98:B:SER:HB2	1:164:B:THR:HB	8	0.42
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	6	0.42
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	7	0.42
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	2	0.42
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	2	0.42
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	2	0.42
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	4	0.42
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	4	0.42
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	4	0.42
(1,2177)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	2	0.42
(1,2157)	1:132:B:GLY:HA2	1:140:A:ARG:HA	5	0.42
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	2	0.42
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	2	0.42
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	2	0.42
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	4	0.42
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	4	0.42
(1,2045)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	2	0.42
(1,2025)	1:132:B:GLY:HA2	1:140:A:ARG:HA	5	0.42
(1,2009)	1:171:A:LYS:H	1:171:A:LYS:HB2	9	0.42
(1,2008)	1:171:A:LYS:H	1:171:A:LYS:HA	9	0.42
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD3	3	0.42
(1,1974)	1:167:A:ALA:H	1:95:A:TRP:HB3	10	0.42
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	10	0.42
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	5	0.42
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	5	0.42
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	5	0.42
(1,1637)	1:131:A:HIS:H	1:130:A:GLU:HG2	8	0.42
(1,1623)	1:129:A:ASP:H	1:130:A:GLU:HG3	2	0.42
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	4	0.42
(1,1552)	1:121:A:THR:H	1:120:A:ILE:HG12	10	0.42
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	9	0.42
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD21	5	0.42
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD22	5	0.42
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD23	5	0.42
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	3	0.42
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	1	0.42
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	1	0.42
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	1	0.42
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	9	0.42
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	9	0.42
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	9	0.42
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	4	0.42
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	4	0.42
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	4	0.42
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	6	0.42
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	6	0.42
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	6	0.42
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	7	0.42
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	7	0.42
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	7	0.42
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	3	0.42
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	3	0.42
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	3	0.42
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	1	0.42
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	10	0.42
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	3	0.42
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:126:A:GLU:HG2	1:135:A:SER:HA	3	0.42
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	5	0.42
(1,695)	1:123:A:LYS:HD3	1:137:A:CYS:HB2	2	0.42
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	10	0.42
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	10	0.42
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	10	0.42
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	4	0.42
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	4	0.42
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	4	0.42
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	7	0.42
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	9	0.42
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	9	0.42
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	9	0.42
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	2	0.42
(1,71)	1:95:A:TRP:HB3	1:168:A:PRO:HB2	6	0.42
(1,49)	1:94:A:ARG:HD3	1:168:A:PRO:HA	8	0.42
(1,41)	1:94:A:ARG:HB3	1:167:A:ALA:HA	4	0.42
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG21	1	0.42
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG22	1	0.42
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG23	1	0.42
(1,4285)	1:171:B:LYS:H	1:169:B:MET:HA	6	0.41
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE1	8	0.41
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE2	8	0.41
(1,3603)	1:94:B:ARG:H	1:93:B:ASP:HB2	7	0.41
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD3	8	0.41
(1,3255)	1:147:B:GLY:HA2	1:148:B:VAL:HG11	9	0.41
(1,3255)	1:147:B:GLY:HA2	1:148:B:VAL:HG12	9	0.41
(1,3255)	1:147:B:GLY:HA2	1:148:B:VAL:HG13	9	0.41
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	8	0.41
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	8	0.41
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	8	0.41
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	9	0.41
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	9	0.41
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	9	0.41
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	6	0.41
(1,3092)	1:136:B:ARG:HA	1:136:B:ARG:HG2	10	0.41
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	9	0.41
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	2	0.41
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	2	0.41
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	2	0.41
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	8	0.41
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	2	0.41
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	2	0.41
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	2	0.41
(1,2447)	1:97:B:VAL:HG21	1:118:B:VAL:HB	2	0.41
(1,2447)	1:97:B:VAL:HG22	1:118:B:VAL:HB	2	0.41
(1,2447)	1:97:B:VAL:HG23	1:118:B:VAL:HB	2	0.41
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG21	5	0.41
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG22	5	0.41
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG23	5	0.41
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	3	0.41
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB1	9	0.41
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB2	9	0.41
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB3	9	0.41
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	2	0.41
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	10	0.41
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	10	0.41
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	10	0.41
(1,2213)	1:134:A:ILE:HA	1:140:B:ARG:HD3	10	0.41
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	6	0.41
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	6	0.41
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	6	0.41
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	10	0.41
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	10	0.41
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	10	0.41
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	10	0.41
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	10	0.41
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	10	0.41
(1,2081)	1:134:A:ILE:HA	1:140:B:ARG:HD3	10	0.41
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	6	0.41
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	6	0.41
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	6	0.41
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	10	0.41
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	10	0.41
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	10	0.41
(1,2008)	1:171:A:LYS:H	1:171:A:LYS:HA	10	0.41
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	8	0.41
(1,1812)	1:152:A:GLN:HE22	1:168:A:PRO:HD3	1	0.41
(1,1756)	1:148:A:VAL:H	1:170:A:PRO:HG3	2	0.41
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD21	3	0.41
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD22	3	0.41
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD23	3	0.41
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD21	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1332)	1:95:A:TRP:H	1:95:A:TRP:HE3	7	0.41
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD11	5	0.41
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD12	5	0.41
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD13	5	0.41
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	5	0.41
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	5	0.41
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	5	0.41
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	3	0.41
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	3	0.41
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	3	0.41
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	8	0.41
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	8	0.41
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	8	0.41
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	2	0.41
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	2	0.41
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	2	0.41
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	3	0.41
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	3	0.41
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	3	0.41
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	5	0.41
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	5	0.41
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	5	0.41
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	7	0.41
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	7	0.41
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	7	0.41
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	9	0.41
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	9	0.41
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	9	0.41
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	3	0.41
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	3	0.41
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	3	0.41
(1,845)	1:141:A:LYS:HA	1:141:A:LYS:HD3	7	0.41
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	3	0.41
(1,695)	1:123:A:LYS:HD2	1:137:A:CYS:HB2	6	0.41
(1,694)	1:123:A:LYS:HD3	1:137:A:CYS:HA	5	0.41
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	3	0.41
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	5	0.41
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	5	0.41
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	5	0.41
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	5	0.41
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	6	0.41
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	6	0.41
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	9	0.41
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	10	0.41
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	8	0.41
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	8	0.41
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	8	0.41
(1,270)	1:101:A:VAL:HG11	1:102:A:ASN:HA	8	0.41
(1,270)	1:101:A:VAL:HG12	1:102:A:ASN:HA	8	0.41
(1,270)	1:101:A:VAL:HG13	1:102:A:ASN:HA	8	0.41
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	6	0.41
(1,4262)	1:167:B:ALA:H	1:166:B:GLU:HB2	4	0.4
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	2	0.4
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	7	0.4
(1,4037)	1:148:B:VAL:H	1:170:B:PRO:HG3	6	0.4
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	7	0.4
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	7	0.4
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	7	0.4
(1,3902)	1:129:B:ASP:H	1:129:B:ASP:HB2	3	0.4
(1,3847)	1:123:B:LYS:H	1:109:B:LEU:HB2	6	0.4
(1,3806)	1:119:B:GLU:H	1:114:B:LYS:HB3	10	0.4
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	8	0.4
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	8	0.4
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	8	0.4
(1,3612)	1:95:B:TRP:H	1:95:B:TRP:HB2	2	0.4
(1,3612)	1:95:B:TRP:H	1:95:B:TRP:HB2	3	0.4
(1,3601)	1:94:B:ARG:H	1:92:B:ALA:HA	1	0.4
(1,3566)	1:168:B:PRO:HD2	1:169:B:MET:HA	8	0.4
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	4	0.4
(1,3460)	1:157:B:LEU:HD21	1:163:B:LEU:HB3	2	0.4
(1,3460)	1:157:B:LEU:HD22	1:163:B:LEU:HB3	2	0.4
(1,3460)	1:157:B:LEU:HD23	1:163:B:LEU:HB3	2	0.4
(1,3303)	1:148:B:VAL:HG21	1:170:B:PRO:HG2	3	0.4
(1,3303)	1:148:B:VAL:HG22	1:170:B:PRO:HG2	3	0.4
(1,3303)	1:148:B:VAL:HG23	1:170:B:PRO:HG2	3	0.4
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	10	0.4
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	10	0.4
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	10	0.4
(1,3126)	1:141:B:LYS:HA	1:141:B:LYS:HD3	9	0.4
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	2	0.4
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	2	0.4
(1,2976)	1:123:B:LYS:HD2	1:137:B:CYS:HB2	8	0.4
(1,2975)	1:123:B:LYS:HD3	1:137:B:CYS:HA	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE2	10	0.4
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	2	0.4
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	4	0.4
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	2	0.4
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	2	0.4
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	2	0.4
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG21	10	0.4
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG22	10	0.4
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG23	10	0.4
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	6	0.4
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	6	0.4
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	6	0.4
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	5	0.4
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	5	0.4
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	5	0.4
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	5	0.4
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	5	0.4
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	5	0.4
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	7	0.4
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	7	0.4
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	7	0.4
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB1	7	0.4
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB2	7	0.4
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB3	7	0.4
(1,2328)	1:94:B:ARG:HG3	1:168:B:PRO:HB3	7	0.4
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	1	0.4
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	9	0.4
(1,1950)	1:165:A:VAL:H	1:96:A:ARG:HB2	5	0.4
(1,1924)	1:162:A:THR:H	1:160:A:GLU:HB2	4	0.4
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	4	0.4
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	4	0.4
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	2	0.4
(1,1331)	1:95:A:TRP:H	1:95:A:TRP:HB2	3	0.4
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	1	0.4
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	1	0.4
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	1	0.4
(1,1114)	1:155:A:SER:HB2	1:163:A:LEU:HA	6	0.4
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	4	0.4
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	4	0.4
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	4	0.4
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	1	0.4
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	1	0.4
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	8	0.4
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	8	0.4
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	8	0.4
(1,917)	1:144:A:LEU:HB3	1:147:A:GLY:HA2	10	0.4
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	5	0.4
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	5	0.4
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	5	0.4
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	1	0.4
(1,455)	1:112:A:LYS:HB2	1:112:A:LYS:HE2	3	0.4
(1,449)	1:112:A:LYS:HA	1:112:A:LYS:HE2	3	0.4
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	3	0.4
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	3	0.4
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	3	0.4
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	8	0.4
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	4	0.4
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	8	0.4
(1,348)	1:108:A:GLU:HG3	1:123:A:LYS:HE3	6	0.4
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	10	0.4
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	10	0.4
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	10	0.4
(1,99)	1:96:A:ARG:HB3	1:164:A:THR:HB	5	0.4
(1,51)	1:95:A:TRP:HA	1:95:A:TRP:HB2	1	0.4
(1,51)	1:95:A:TRP:HA	1:95:A:TRP:HB2	9	0.4
(1,50)	1:94:A:ARG:HD2	1:168:A:PRO:HB2	8	0.4
(1,16)	1:93:A:ASP:HA	1:94:A:ARG:HD2	6	0.4
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	4	0.39
(1,4037)	1:148:B:VAL:H	1:170:B:PRO:HG3	9	0.39
(1,3910)	1:129:B:ASP:H	1:133:B:TYR:HB2	4	0.39
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	4	0.39
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	4	0.39
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	9	0.39
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	9	0.39
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	9	0.39
(1,3612)	1:95:B:TRP:H	1:95:B:TRP:HB2	4	0.39
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	8	0.39
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	5	0.39
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	5	0.39
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	5	0.39
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	5	0.39
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	5	0.39
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	3	0.39
(1,3395)	1:155:B:SER:HB2	1:163:B:LEU:HA	6	0.39
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG21	6	0.39
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG22	6	0.39
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG23	6	0.39
(1,3128)	1:141:B:LYS:HA	1:141:B:LYS:HE3	9	0.39
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	4	0.39
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	2	0.39
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	2	0.39
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	6	0.39
(1,2935)	1:120:B:ILE:HD11	1:140:B:ARG:HD2	6	0.39
(1,2935)	1:120:B:ILE:HD12	1:140:B:ARG:HD2	6	0.39
(1,2935)	1:120:B:ILE:HD13	1:140:B:ARG:HD2	6	0.39
(1,2790)	1:114:B:LYS:HA	1:114:B:LYS:HB2	4	0.39
(1,2736)	1:112:B:LYS:HB2	1:112:B:LYS:HE2	6	0.39
(1,2708)	1:111:B:VAL:HG11	1:112:B:LYS:HE3	3	0.39
(1,2708)	1:111:B:VAL:HG12	1:112:B:LYS:HE3	3	0.39
(1,2708)	1:111:B:VAL:HG13	1:112:B:LYS:HE3	3	0.39
(1,2666)	1:109:B:LEU:HD21	1:161:B:GLY:HA3	3	0.39
(1,2666)	1:109:B:LEU:HD22	1:161:B:GLY:HA3	3	0.39
(1,2666)	1:109:B:LEU:HD23	1:161:B:GLY:HA3	3	0.39
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	1	0.39
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	9	0.39
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD21	1	0.39
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD22	1	0.39
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD23	1	0.39
(1,2332)	1:95:B:TRP:HA	1:95:B:TRP:HB2	6	0.39
(1,2299)	1:93:B:ASP:HB2	1:94:B:ARG:HA	10	0.39
(1,2288)	1:90:B:HIS:HB2	1:91:B:THR:HA	2	0.39
(1,2002)	1:169:A:MET:H	1:171:A:LYS:HE3	1	0.39
(1,1899)	1:160:A:GLU:H	1:160:A:GLU:HG3	3	0.39
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	5	0.39
(1,1816)	1:153:A:VAL:H	1:149:A:ASP:HB2	3	0.39
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD22	1	0.39
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	9	0.39
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD11	2	0.39
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD12	2	0.39
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD13	2	0.39
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	10	0.39
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	10	0.39
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	10	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	5	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	5	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	7	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	7	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	7	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	9	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	9	0.39
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	9	0.39
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	4	0.39
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	4	0.39
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	4	0.39
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	4	0.39
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	7	0.39
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	9	0.39
(1,406)	1:110:A:THR:HG21	1:112:A:LYS:HE3	7	0.39
(1,406)	1:110:A:THR:HG22	1:112:A:LYS:HE3	7	0.39
(1,406)	1:110:A:THR:HG23	1:112:A:LYS:HE3	7	0.39
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	2	0.39
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	2	0.39
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	2	0.39
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	4	0.39
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	5	0.39
(1,264)	1:100:A:ASP:HB2	1:162:A:THR:HB	2	0.39
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	3	0.39
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	10	0.39
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	10	0.39
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	10	0.39
(1,71)	1:95:A:TRP:HB3	1:168:A:PRO:HB2	2	0.39
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG11	9	0.39
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG12	9	0.39
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG13	9	0.39
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	2	0.39
(1,4289)	1:171:B:LYS:H	1:171:B:LYS:HA	5	0.38
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	3	0.38
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	10	0.38
(1,4095)	1:152:B:GLN:HE22	1:170:B:PRO:HD3	7	0.38
(1,3848)	1:123:B:LYS:H	1:109:B:LEU:HG	8	0.38
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	3	0.38
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	10	0.38
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	3	0.38
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	3	0.38
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	4	0.38
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD21	2	0.38
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD22	2	0.38
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD23	2	0.38
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	4	0.38
(1,3345)	1:152:B:GLN:HB2	1:168:B:PRO:HD3	8	0.38
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG11	9	0.38
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG12	9	0.38
(1,3193)	1:144:B:LEU:HB2	1:148:B:VAL:HG13	9	0.38
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	8	0.38
(1,3107)	1:139:B:THR:HA	1:140:B:ARG:HB2	5	0.38
(1,3092)	1:136:B:ARG:HA	1:136:B:ARG:HG2	8	0.38
(1,3014)	1:126:B:GLU:HG3	1:135:B:SER:HB3	6	0.38
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	1	0.38
(1,2976)	1:123:B:LYS:HD2	1:137:B:CYS:HB2	2	0.38
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	1	0.38
(1,2651)	1:109:B:LEU:HD11	1:122:B:GLY:HA3	9	0.38
(1,2651)	1:109:B:LEU:HD12	1:122:B:GLY:HA3	9	0.38
(1,2651)	1:109:B:LEU:HD13	1:122:B:GLY:HA3	9	0.38
(1,2626)	1:108:B:GLU:HG2	1:123:B:LYS:HE2	5	0.38
(1,2617)	1:108:B:GLU:HA	1:108:B:GLU:HG2	9	0.38
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	2	0.38
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	5	0.38
(1,2568)	1:105:B:ALA:HA	1:108:B:GLU:HB3	10	0.38
(1,2529)	1:99:B:LEU:HD21	1:140:B:ARG:HD2	2	0.38
(1,2529)	1:99:B:LEU:HD22	1:140:B:ARG:HD2	2	0.38
(1,2529)	1:99:B:LEU:HD23	1:140:B:ARG:HD2	2	0.38
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	9	0.38
(1,2331)	1:94:B:ARG:HD3	1:168:B:PRO:HB2	8	0.38
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	10	0.38
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	1	0.38
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	1	0.38
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	1	0.38
(1,2185)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	3	0.38
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	1	0.38
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	1	0.38
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	1	0.38
(1,2053)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	3	0.38
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	1	0.38
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	2	0.38
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD3	9	0.38
(1,1799)	1:152:A:GLN:HE21	1:152:A:GLN:HB3	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	6	0.38
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	6	0.38
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	6	0.38
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	5	0.38
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	9	0.38
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD22	5	0.38
(1,1326)	1:94:A:ARG:H	1:168:A:PRO:HA	1	0.38
(1,1288)	1:169:A:MET:HA	1:169:A:MET:HG2	7	0.38
(1,1197)	1:158:A:SER:HB3	1:159:A:PRO:HD3	5	0.38
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	2	0.38
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	2	0.38
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	2	0.38
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	4	0.38
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	4	0.38
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	4	0.38
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	5	0.38
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	5	0.38
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	5	0.38
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD1	8	0.38
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD2	8	0.38
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD1	8	0.38
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD2	8	0.38
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD1	8	0.38
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD2	8	0.38
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	6	0.38
(1,718)	1:126:A:GLU:HG2	1:133:A:TYR:HB3	4	0.38
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	2	0.38
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	4	0.38
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	3	0.38
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	3	0.38
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	3	0.38
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	4	0.38
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	4	0.38
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	4	0.38
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	4	0.38
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	4	0.38
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	4	0.38
(1,362)	1:109:A:LEU:HB3	1:121:A:THR:HB	1	0.38
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	3	0.38
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	1	0.38
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	2	0.38
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD21	5	0.38
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD22	5	0.38
(1,277)	1:102:A:ASN:HB2	1:157:A:LEU:HD23	5	0.38
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	3	0.38
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	3	0.38
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	3	0.38
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	1	0.38
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	1	0.38
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	1	0.38
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	7	0.38
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG21	8	0.38
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG22	8	0.38
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG23	8	0.38
(1,51)	1:95:A:TRP:HA	1:95:A:TRP:HB2	6	0.38
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD2	2	0.37
(1,4095)	1:152:B:GLN:HE22	1:170:B:PRO:HD3	4	0.37
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	5	0.37
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	5	0.37
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	5	0.37
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE1	5	0.37
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE2	5	0.37
(1,3902)	1:129:B:ASP:H	1:129:B:ASP:HB2	7	0.37
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	5	0.37
(1,3474)	1:158:B:SER:HB3	1:160:B:GLU:HB3	8	0.37
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	2	0.37
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	10	0.37
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	9	0.37
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	6	0.37
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	6	0.37
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	6	0.37
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	8	0.37
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	8	0.37
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	8	0.37
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	3	0.37
(1,3137)	1:141:B:LYS:HG2	1:142:B:TYR:HB3	1	0.37
(1,3137)	1:141:B:LYS:HG2	1:142:B:TYR:HB3	2	0.37
(1,3122)	1:140:B:ARG:HG2	1:142:B:TYR:HE1	2	0.37
(1,3122)	1:140:B:ARG:HG2	1:142:B:TYR:HE2	2	0.37
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	3	0.37
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	5	0.37
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	8	0.37
(1,2783)	1:113:B:THR:HG21	1:150:B:PRO:HB3	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2783)	1:113:B:THR:HG22	1:150:B:PRO:HB3	1	0.37
(1,2783)	1:113:B:THR:HG23	1:150:B:PRO:HB3	1	0.37
(1,2736)	1:112:B:LYS:HB2	1:112:B:LYS:HE2	10	0.37
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	8	0.37
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	8	0.37
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	8	0.37
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	10	0.37
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	7	0.37
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	7	0.37
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	7	0.37
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	2	0.37
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	2	0.37
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	2	0.37
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	4	0.37
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	10	0.37
(1,2385)	1:96:B:ARG:HG2	1:166:B:GLU:HA	10	0.37
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	9	0.37
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	9	0.37
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	9	0.37
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	9	0.37
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	9	0.37
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	9	0.37
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	10	0.37
(1,2169)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	10	0.37
(1,2037)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	10	0.37
(1,1998)	1:169:A:MET:H	1:169:A:MET:HB2	10	0.37
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	7	0.37
(1,1940)	1:164:A:THR:H	1:162:A:THR:HG21	2	0.37
(1,1940)	1:164:A:THR:H	1:162:A:THR:HG22	2	0.37
(1,1940)	1:164:A:THR:H	1:162:A:THR:HG23	2	0.37
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	4	0.37
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	10	0.37
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	7	0.37
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	7	0.37
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	7	0.37
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	8	0.37
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	8	0.37
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	8	0.37
(1,1197)	1:158:A:SER:HB3	1:159:A:PRO:HD3	1	0.37
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	7	0.37
(1,1097)	1:154:A:SER:HB3	1:155:A:SER:HA	1	0.37
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	1	0.37
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	1	0.37
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	2	0.37
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	2	0.37
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	2	0.37
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	9	0.37
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	9	0.37
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	9	0.37
(1,928)	1:144:A:LEU:HD11	1:145:A:PRO:HB3	10	0.37
(1,928)	1:144:A:LEU:HD12	1:145:A:PRO:HB3	10	0.37
(1,928)	1:144:A:LEU:HD13	1:145:A:PRO:HB3	10	0.37
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	6	0.37
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	5	0.37
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE1	5	0.37
(1,731)	1:126:A:GLU:HG3	1:133:A:TYR:HE2	5	0.37
(1,728)	1:126:A:GLU:HG3	1:133:A:TYR:HA	9	0.37
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	9	0.37
(1,652)	1:120:A:ILE:HD11	1:140:A:ARG:HB2	10	0.37
(1,652)	1:120:A:ILE:HD12	1:140:A:ARG:HB2	10	0.37
(1,652)	1:120:A:ILE:HD13	1:140:A:ARG:HB2	10	0.37
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	1	0.37
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	5	0.37
(1,589)	1:118:A:VAL:HG11	1:148:A:VAL:HB	6	0.37
(1,589)	1:118:A:VAL:HG12	1:148:A:VAL:HB	6	0.37
(1,589)	1:118:A:VAL:HG13	1:148:A:VAL:HB	6	0.37
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	8	0.37
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	8	0.37
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	8	0.37
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	5	0.37
(1,356)	1:109:A:LEU:HA	1:122:A:GLY:HA2	7	0.37
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	4	0.37
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG21	9	0.37
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG22	9	0.37
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG23	9	0.37
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	8	0.37
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	8	0.37
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	8	0.37
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	7	0.37
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	7	0.37
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	7	0.37
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	7	0.37
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	7	0.37
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	7	0.37
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	7	0.37
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	7	0.37
(1,232)	1:99:A:LEU:HD11	1:120:A:ILE:HG12	4	0.37
(1,232)	1:99:A:LEU:HD12	1:120:A:ILE:HG12	4	0.37
(1,232)	1:99:A:LEU:HD13	1:120:A:ILE:HG12	4	0.37
(1,184)	1:98:A:SER:HB2	1:162:A:THR:HG21	3	0.37
(1,184)	1:98:A:SER:HB2	1:162:A:THR:HG22	3	0.37
(1,184)	1:98:A:SER:HB2	1:162:A:THR:HG23	3	0.37
(1,166)	1:97:A:VAL:HG21	1:118:A:VAL:HB	1	0.37
(1,166)	1:97:A:VAL:HG22	1:118:A:VAL:HB	1	0.37
(1,166)	1:97:A:VAL:HG23	1:118:A:VAL:HB	1	0.37
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	7	0.37
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	7	0.37
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	7	0.37
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	6	0.37
(1,51)	1:95:A:TRP:HA	1:95:A:TRP:HB2	2	0.37
(1,33)	1:94:A:ARG:HA	1:169:A:MET:HB2	1	0.37
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	4	0.37
(1,4293)	1:172:B:LEU:H	1:171:B:LYS:HA	2	0.36
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB1	7	0.36
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB2	7	0.36
(1,4274)	1:169:B:MET:H	1:167:B:ALA:HB3	7	0.36
(1,4191)	1:161:B:GLY:H	1:160:B:GLU:HG3	9	0.36
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	6	0.36
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	9	0.36
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD22	1	0.36
(1,3492)	1:160:B:GLU:HG2	1:162:B:THR:HB	9	0.36
(1,3436)	1:157:B:LEU:HB2	1:163:B:LEU:HA	9	0.36
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	1	0.36
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	2	0.36
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	6	0.36
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	6	0.36
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	6	0.36
(1,3139)	1:141:B:LYS:HG3	1:141:B:LYS:HE2	10	0.36
(1,3060)	1:131:B:HIS:HA	1:131:B:HIS:HE1	9	0.36
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	6	0.36
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	7	0.36
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	3	0.36
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	6	0.36
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	6	0.36
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	3	0.36
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	3	0.36
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	3	0.36
(1,2738)	1:112:B:LYS:HB2	1:120:B:ILE:HA	8	0.36
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	9	0.36
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	4	0.36
(1,2637)	1:109:B:LEU:HA	1:122:B:GLY:HA2	8	0.36
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG21	6	0.36
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG22	6	0.36
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG23	6	0.36
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	1	0.36
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	1	0.36
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	1	0.36
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	8	0.36
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	8	0.36
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	8	0.36
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	10	0.36
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	10	0.36
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	10	0.36
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	8	0.36
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	3	0.36
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	3	0.36
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	3	0.36
(1,2314)	1:94:B:ARG:HA	1:169:B:MET:HB2	8	0.36
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	5	0.36
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	5	0.36
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	5	0.36
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	5	0.36
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	5	0.36
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	5	0.36
(1,1974)	1:167:A:ALA:H	1:95:A:TRP:HB3	5	0.36
(1,1916)	1:162:A:THR:H	1:102:A:ASN:HB3	3	0.36
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	1	0.36
(1,1642)	1:132:A:GLY:H	1:129:A:ASP:HB2	3	0.36
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	10	0.36
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	10	0.36
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	10	0.36
(1,1332)	1:95:A:TRP:H	1:95:A:TRP:HE3	4	0.36
(1,1321)	1:94:A:ARG:H	1:93:A:ASP:HA	8	0.36
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG21	10	0.36
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG22	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1319)	1:94:A:ARG:H	1:91:A:THR:HG23	10	0.36
(1,1280)	1:168:A:PRO:HB2	1:170:A:PRO:HD3	8	0.36
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	3	0.36
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	3	0.36
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	3	0.36
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	5	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	7	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	7	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	7	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	9	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	9	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	9	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	10	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	10	0.36
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	10	0.36
(1,1097)	1:154:A:SER:HB3	1:155:A:SER:HA	9	0.36
(1,990)	1:148:A:VAL:HA	1:169:A:MET:HB2	6	0.36
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	1	0.36
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	1	0.36
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	1	0.36
(1,847)	1:141:A:LYS:HA	1:141:A:LYS:HE3	7	0.36
(1,826)	1:139:A:THR:HA	1:140:A:ARG:HB2	1	0.36
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD1	1	0.36
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD2	1	0.36
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD1	1	0.36
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD2	1	0.36
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD1	1	0.36
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD2	1	0.36
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	4	0.36
(1,695)	1:123:A:LYS:HD3	1:137:A:CYS:HB2	5	0.36
(1,694)	1:123:A:LYS:HD3	1:137:A:CYS:HA	3	0.36
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	9	0.36
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	9	0.36
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	9	0.36
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	9	0.36
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	9	0.36
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	9	0.36
(1,336)	1:108:A:GLU:HA	1:108:A:GLU:HG2	2	0.36
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	2	0.36
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	5	0.36
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	9	0.36
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	2	0.36
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	2	0.36
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	2	0.36
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	3	0.36
(1,4290)	1:171:B:LYS:H	1:171:B:LYS:HB3	4	0.35
(1,4084)	1:152:B:GLN:HE21	1:168:B:PRO:HD2	10	0.35
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	9	0.35
(1,3915)	1:131:B:HIS:H	1:129:B:ASP:HB3	2	0.35
(1,3847)	1:123:B:LYS:H	1:109:B:LEU:HB2	9	0.35
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	7	0.35
(1,3474)	1:158:B:SER:HB3	1:160:B:GLU:HB3	3	0.35
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	6	0.35
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	5	0.35
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	4	0.35
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	4	0.35
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	4	0.35
(1,3304)	1:149:B:ASP:HA	1:149:B:ASP:HB3	5	0.35
(1,3252)	1:146:B:PRO:HG2	1:147:B:GLY:HA2	8	0.35
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	5	0.35
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	3	0.35
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	3	0.35
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	3	0.35
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	10	0.35
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	10	0.35
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	10	0.35
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	10	0.35
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	10	0.35
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	10	0.35
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	8	0.35
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	10	0.35
(1,2971)	1:123:B:LYS:HB3	1:137:B:CYS:HB2	1	0.35
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	10	0.35
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	10	0.35
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	10	0.35
(1,2755)	1:112:B:LYS:HE2	1:114:B:LYS:HB3	4	0.35
(1,2754)	1:112:B:LYS:HE3	1:114:B:LYS:HB2	5	0.35
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	9	0.35
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	5	0.35
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	2	0.35
(1,2629)	1:108:B:GLU:HG3	1:123:B:LYS:HE2	9	0.35
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	6	0.35
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	5	0.35
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	5	0.35
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	8	0.35
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	8	0.35
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	8	0.35
(1,2536)	1:99:B:LEU:HD21	1:109:B:LEU:HG	6	0.35
(1,2536)	1:99:B:LEU:HD22	1:109:B:LEU:HG	6	0.35
(1,2536)	1:99:B:LEU:HD23	1:109:B:LEU:HG	6	0.35
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB1	6	0.35
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB2	6	0.35
(1,2344)	1:95:B:TRP:HB2	1:167:B:ALA:HB3	6	0.35
(1,2299)	1:93:B:ASP:HB2	1:94:B:ARG:HA	4	0.35
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	4	0.35
(1,2286)	1:90:B:HIS:HA	1:91:B:THR:HA	8	0.35
(1,2213)	1:134:A:ILE:HA	1:140:B:ARG:HD3	8	0.35
(1,2081)	1:134:A:ILE:HA	1:140:B:ARG:HD3	8	0.35
(1,1816)	1:153:A:VAL:H	1:149:A:ASP:HB2	9	0.35
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	10	0.35
(1,1423)	1:108:A:GLU:H	1:123:A:LYS:HG2	3	0.35
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	4	0.35
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	5	0.35
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	5	0.35
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	5	0.35
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	5	0.35
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	9	0.35
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	9	0.35
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	9	0.35
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	9	0.35
(1,1193)	1:158:A:SER:HB3	1:160:A:GLU:HB3	8	0.35
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	6	0.35
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	6	0.35
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	6	0.35
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	8	0.35
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	10	0.35
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	1	0.35
(1,858)	1:141:A:LYS:HG3	1:141:A:LYS:HE2	10	0.35
(1,841)	1:140:A:ARG:HG2	1:142:A:TYR:HE1	4	0.35
(1,841)	1:140:A:ARG:HG2	1:142:A:TYR:HE2	4	0.35
(1,826)	1:139:A:THR:HA	1:140:A:ARG:HB2	5	0.35
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	3	0.35
(1,718)	1:126:A:GLU:HG2	1:133:A:TYR:HB3	1	0.35
(1,718)	1:126:A:GLU:HG2	1:133:A:TYR:HB3	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:120:A:ILE:HD11	1:140:A:ARG:HD2	9	0.35
(1,654)	1:120:A:ILE:HD12	1:140:A:ARG:HD2	9	0.35
(1,654)	1:120:A:ILE:HD13	1:140:A:ARG:HD2	9	0.35
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	10	0.35
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	10	0.35
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	10	0.35
(1,457)	1:112:A:LYS:HB2	1:120:A:ILE:HA	3	0.35
(1,338)	1:108:A:GLU:HA	1:123:A:LYS:HD2	7	0.35
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	6	0.35
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	6	0.35
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	6	0.35
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	6	0.35
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	2	0.35
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	2	0.35
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	2	0.35
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	10	0.35
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	10	0.35
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	10	0.35
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	3	0.35
(1,71)	1:95:A:TRP:HB2	1:168:A:PRO:HB2	3	0.35
(1,9)	1:90:A:HIS:HB3	1:91:A:THR:HA	2	0.35
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	9	0.35
(1,4182)	1:161:B:GLY:H	1:102:B:ASN:HB2	3	0.34
(1,4051)	1:151:B:THR:H	1:149:B:ASP:HB2	5	0.34
(1,4024)	1:148:B:VAL:H	1:146:B:PRO:HB3	4	0.34
(1,3902)	1:129:B:ASP:H	1:129:B:ASP:HB2	2	0.34
(1,3833)	1:121:B:THR:H	1:120:B:ILE:HG12	9	0.34
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD21	9	0.34
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD22	9	0.34
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD23	9	0.34
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	1	0.34
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	1	0.34
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	1	0.34
(1,3491)	1:160:B:GLU:HB2	1:162:B:THR:HB	6	0.34
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	5	0.34
(1,3460)	1:157:B:LEU:HD21	1:163:B:LEU:HB3	3	0.34
(1,3460)	1:157:B:LEU:HD22	1:163:B:LEU:HB3	3	0.34
(1,3460)	1:157:B:LEU:HD23	1:163:B:LEU:HB3	3	0.34
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	9	0.34
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	9	0.34
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	9	0.34
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD21	9	0.34
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD22	9	0.34
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD23	9	0.34
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	6	0.34
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	6	0.34
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	7	0.34
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	7	0.34
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	7	0.34
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	7	0.34
(1,3302)	1:148:B:VAL:HG21	1:169:B:MET:HB3	1	0.34
(1,3302)	1:148:B:VAL:HG22	1:169:B:MET:HB3	1	0.34
(1,3302)	1:148:B:VAL:HG23	1:169:B:MET:HB3	1	0.34
(1,3252)	1:146:B:PRO:HG2	1:147:B:GLY:HA2	4	0.34
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	4	0.34
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	10	0.34
(1,2971)	1:123:B:LYS:HB3	1:137:B:CYS:HB2	4	0.34
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	10	0.34
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	10	0.34
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	10	0.34
(1,2686)	1:110:B:THR:HG21	1:112:B:LYS:HD3	4	0.34
(1,2686)	1:110:B:THR:HG22	1:112:B:LYS:HD3	4	0.34
(1,2686)	1:110:B:THR:HG23	1:112:B:LYS:HD3	4	0.34
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	10	0.34
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	10	0.34
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	10	0.34
(1,2629)	1:108:B:GLU:HG3	1:123:B:LYS:HE2	5	0.34
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD11	9	0.34
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD12	9	0.34
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD13	9	0.34
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	6	0.34
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	6	0.34
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	6	0.34
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB1	3	0.34
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB2	3	0.34
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB3	3	0.34
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	7	0.34
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	8	0.34
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	8	0.34
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	8	0.34
(1,2200)	1:134:B:ILE:HG21	1:140:A:ARG:HD3	4	0.34
(1,2200)	1:134:B:ILE:HG22	1:140:A:ARG:HD3	4	0.34
(1,2200)	1:134:B:ILE:HG23	1:140:A:ARG:HD3	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2177)	1:133:B:TYR:HB3	1:141:A:LYS:HD3	10	0.34
(1,2169)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	6	0.34
(1,2169)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	7	0.34
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	8	0.34
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	8	0.34
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	8	0.34
(1,2068)	1:134:B:ILE:HG21	1:140:A:ARG:HD3	4	0.34
(1,2068)	1:134:B:ILE:HG22	1:140:A:ARG:HD3	4	0.34
(1,2068)	1:134:B:ILE:HG23	1:140:A:ARG:HD3	4	0.34
(1,2045)	1:133:B:TYR:HB3	1:141:A:LYS:HD3	10	0.34
(1,2037)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	6	0.34
(1,2037)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	7	0.34
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	1	0.34
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	4	0.34
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD2	8	0.34
(1,1805)	1:152:A:GLN:HE21	1:170:A:PRO:HD3	7	0.34
(1,1654)	1:134:A:ILE:H	1:127:A:ARG:HB2	6	0.34
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD1	5	0.34
(1,1630)	1:129:A:ASP:H	1:133:A:TYR:HD2	5	0.34
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	7	0.34
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	10	0.34
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD11	3	0.34
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD12	3	0.34
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD13	3	0.34
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD21	8	0.34
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	4	0.34
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	4	0.34
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	4	0.34
(1,1321)	1:94:A:ARG:H	1:93:A:ASP:HA	5	0.34
(1,1193)	1:158:A:SER:HB3	1:160:A:GLU:HB3	6	0.34
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	4	0.34
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD11	1	0.34
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD12	1	0.34
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD13	1	0.34
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	8	0.34
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	2	0.34
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	4	0.34
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	5	0.34
(1,1065)	1:152:A:GLN:HB2	1:169:A:MET:HA	9	0.34
(1,847)	1:141:A:LYS:HA	1:141:A:LYS:HE3	1	0.34
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	2	0.34
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:126:A:GLU:HG2	1:135:A:SER:HA	2	0.34
(1,694)	1:123:A:LYS:HD2	1:137:A:CYS:HA	10	0.34
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	4	0.34
(1,688)	1:123:A:LYS:HB2	1:137:A:CYS:HB3	9	0.34
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD1	4	0.34
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD2	4	0.34
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD1	4	0.34
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD2	4	0.34
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD1	4	0.34
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD2	4	0.34
(1,478)	1:112:A:LYS:HE3	1:121:A:THR:HB	9	0.34
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	4	0.34
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	8	0.34
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD11	5	0.34
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD12	5	0.34
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD13	5	0.34
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	9	0.34
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	9	0.34
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	9	0.34
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	4	0.34
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	4	0.34
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	4	0.34
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	2	0.34
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	2	0.34
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	2	0.34
(1,102)	1:96:A:ARG:HB3	1:166:A:GLU:HB3	2	0.34
(1,99)	1:96:A:ARG:HB3	1:164:A:THR:HB	9	0.34
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	1	0.34
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	1	0.34
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	1	0.34
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	1	0.34
(1,69)	1:95:A:TRP:HB3	1:166:A:GLU:HB2	6	0.34
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG21	9	0.33
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG22	9	0.33
(1,4221)	1:164:B:THR:H	1:162:B:THR:HG23	9	0.33
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	9	0.33
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	2	0.33
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	1	0.33
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	1	0.33
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	1	0.33
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	6	0.33
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	6	0.33
(1,3935)	1:134:B:ILE:H	1:127:B:ARG:HB2	2	0.33
(1,3907)	1:129:B:ASP:H	1:132:B:GLY:HA3	8	0.33
(1,3847)	1:123:B:LYS:H	1:109:B:LEU:HB2	2	0.33
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	5	0.33
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	5	0.33
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	5	0.33
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	4	0.33
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	4	0.33
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	4	0.33
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	8	0.33
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	8	0.33
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	8	0.33
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	3	0.33
(1,3252)	1:146:B:PRO:HG2	1:147:B:GLY:HA2	5	0.33
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	6	0.33
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	1	0.33
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	1	0.33
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	1	0.33
(1,3120)	1:140:B:ARG:HB2	1:140:B:ARG:HD2	4	0.33
(1,3060)	1:131:B:HIS:HA	1:131:B:HIS:HE1	3	0.33
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	7	0.33
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	7	0.33
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	7	0.33
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	8	0.33
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	8	0.33
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	8	0.33
(1,2753)	1:112:B:LYS:HD3	1:120:B:ILE:HA	8	0.33
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE3	1	0.33
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	3	0.33
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	3	0.33
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	3	0.33
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	8	0.33
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	8	0.33
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	8	0.33
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	2	0.33
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	2	0.33
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	2	0.33
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	10	0.33
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	10	0.33
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	10	0.33
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD11	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD12	10	0.33
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD13	10	0.33
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	10	0.33
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	9	0.33
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD3	2	0.33
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	7	0.33
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	7	0.33
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	7	0.33
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	7	0.33
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	10	0.33
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	10	0.33
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	10	0.33
(1,2568)	1:105:B:ALA:HA	1:108:B:GLU:HB3	3	0.33
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	1	0.33
(1,2447)	1:97:B:VAL:HG21	1:118:B:VAL:HB	9	0.33
(1,2447)	1:97:B:VAL:HG22	1:118:B:VAL:HB	9	0.33
(1,2447)	1:97:B:VAL:HG23	1:118:B:VAL:HB	9	0.33
(1,2299)	1:93:B:ASP:HB2	1:94:B:ARG:HA	1	0.33
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	8	0.33
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	7	0.33
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	7	0.33
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	7	0.33
(1,2150)	1:97:B:VAL:HG21	1:131:A:HIS:HB3	9	0.33
(1,2150)	1:97:B:VAL:HG22	1:131:A:HIS:HB3	9	0.33
(1,2150)	1:97:B:VAL:HG23	1:131:A:HIS:HB3	9	0.33
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	7	0.33
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	7	0.33
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	7	0.33
(1,2018)	1:97:B:VAL:HG21	1:131:A:HIS:HB3	9	0.33
(1,2018)	1:97:B:VAL:HG22	1:131:A:HIS:HB3	9	0.33
(1,2018)	1:97:B:VAL:HG23	1:131:A:HIS:HB3	9	0.33
(1,1847)	1:155:A:SER:H	1:154:A:SER:HB2	9	0.33
(1,1634)	1:131:A:HIS:H	1:129:A:ASP:HB3	3	0.33
(1,1621)	1:129:A:ASP:H	1:129:A:ASP:HB2	6	0.33
(1,1587)	1:126:A:GLU:H	1:125:A:GLU:HG2	2	0.33
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	4	0.33
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	1	0.33
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	6	0.33
(1,1179)	1:157:A:LEU:HD21	1:163:A:LEU:HB3	8	0.33
(1,1179)	1:157:A:LEU:HD22	1:163:A:LEU:HB3	8	0.33
(1,1179)	1:157:A:LEU:HD23	1:163:A:LEU:HB3	8	0.33
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD21	4	0.33
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD22	4	0.33
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD23	4	0.33
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	3	0.33
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	2	0.33
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	9	0.33
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD1	3	0.33
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD2	3	0.33
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD1	3	0.33
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD2	3	0.33
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD1	3	0.33
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD2	3	0.33
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD1	4	0.33
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD2	4	0.33
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD1	4	0.33
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD2	4	0.33
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD1	4	0.33
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD2	4	0.33
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE1	7	0.33
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE2	7	0.33
(1,707)	1:126:A:GLU:HA	1:133:A:TYR:HB3	2	0.33
(1,703)	1:125:A:GLU:HA	1:135:A:SER:HB2	4	0.33
(1,695)	1:123:A:LYS:HD3	1:137:A:CYS:HB2	7	0.33
(1,612)	1:119:A:GLU:HA	1:141:A:LYS:HE3	7	0.33
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	4	0.33
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	4	0.33
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	4	0.33
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	4	0.33
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	4	0.33
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	4	0.33
(1,528)	1:116:A:GLY:HA2	1:148:A:VAL:HB	7	0.33
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	4	0.33
(1,434)	1:111:A:VAL:HG11	1:120:A:ILE:HG12	6	0.33
(1,434)	1:111:A:VAL:HG12	1:120:A:ILE:HG12	6	0.33
(1,434)	1:111:A:VAL:HG13	1:120:A:ILE:HG12	6	0.33
(1,406)	1:110:A:THR:HG21	1:112:A:LYS:HE3	3	0.33
(1,406)	1:110:A:THR:HG22	1:112:A:LYS:HE3	3	0.33
(1,406)	1:110:A:THR:HG23	1:112:A:LYS:HE3	3	0.33
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	9	0.33
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	9	0.33
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	9	0.33
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	4	0.33
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	4	0.33
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	9	0.33
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	9	0.33
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	9	0.33
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	9	0.33
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	9	0.33
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	9	0.33
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	9	0.33
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	9	0.33
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	9	0.33
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	1	0.33
(1,166)	1:97:A:VAL:HG21	1:118:A:VAL:HB	9	0.33
(1,166)	1:97:A:VAL:HG22	1:118:A:VAL:HB	9	0.33
(1,166)	1:97:A:VAL:HG23	1:118:A:VAL:HB	9	0.33
(1,102)	1:96:A:ARG:HB3	1:166:A:GLU:HB3	9	0.33
(1,99)	1:96:A:ARG:HB3	1:164:A:THR:HB	2	0.33
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	9	0.33
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	4	0.33
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	2	0.33
(1,4290)	1:171:B:LYS:H	1:171:B:LYS:HB2	5	0.32
(1,4281)	1:169:B:MET:H	1:169:B:MET:HG3	9	0.32
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB1	10	0.32
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB2	10	0.32
(1,4268)	1:169:B:MET:H	1:92:B:ALA:HB3	10	0.32
(1,4255)	1:167:B:ALA:H	1:95:B:TRP:HB3	1	0.32
(1,4205)	1:162:B:THR:H	1:160:B:GLU:HB2	9	0.32
(1,4197)	1:162:B:THR:H	1:102:B:ASN:HB3	6	0.32
(1,4128)	1:155:B:SER:H	1:154:B:SER:HB2	7	0.32
(1,3955)	1:137:B:CYS:H	1:136:B:ARG:HB3	9	0.32
(1,3847)	1:123:B:LYS:H	1:109:B:LEU:HB2	3	0.32
(1,3847)	1:123:B:LYS:H	1:109:B:LEU:HB2	5	0.32
(1,3827)	1:120:B:ILE:H	1:142:B:TYR:H	2	0.32
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	4	0.32
(1,3825)	1:120:B:ILE:H	1:140:B:ARG:HG2	2	0.32
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	1	0.32
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD21	1	0.32
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD22	1	0.32
(1,3653)	1:102:B:ASN:HD21	1:157:B:LEU:HD23	1	0.32
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD21	4	0.32
(1,3613)	1:95:B:TRP:H	1:95:B:TRP:HE3	8	0.32
(1,3604)	1:94:B:ARG:H	1:93:B:ASP:HB3	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3602)	1:94:B:ARG:H	1:93:B:ASP:HA	4	0.32
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	6	0.32
(1,3561)	1:168:B:PRO:HB2	1:170:B:PRO:HD3	9	0.32
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	1	0.32
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	4	0.32
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	7	0.32
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	7	0.32
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	7	0.32
(1,3096)	1:136:B:ARG:HG3	1:138:B:PHE:HA	9	0.32
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	10	0.32
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	10	0.32
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	1	0.32
(1,2929)	1:120:B:ILE:HG21	1:139:B:THR:HA	10	0.32
(1,2929)	1:120:B:ILE:HG22	1:139:B:THR:HA	10	0.32
(1,2929)	1:120:B:ILE:HG23	1:139:B:THR:HA	10	0.32
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	7	0.32
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	2	0.32
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	2	0.32
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	2	0.32
(1,2617)	1:108:B:GLU:HA	1:108:B:GLU:HG2	5	0.32
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	4	0.32
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	7	0.32
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	3	0.32
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	3	0.32
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	3	0.32
(1,2447)	1:97:B:VAL:HG21	1:118:B:VAL:HB	6	0.32
(1,2447)	1:97:B:VAL:HG22	1:118:B:VAL:HB	6	0.32
(1,2447)	1:97:B:VAL:HG23	1:118:B:VAL:HB	6	0.32
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	1	0.32
(1,2282)	1:88:B:ILE:HG21	1:90:B:HIS:HA	1	0.32
(1,2282)	1:88:B:ILE:HG22	1:90:B:HIS:HA	1	0.32
(1,2282)	1:88:B:ILE:HG23	1:90:B:HIS:HA	1	0.32
(1,1974)	1:167:A:ALA:H	1:95:A:TRP:HB3	7	0.32
(1,1894)	1:160:A:GLU:H	1:159:A:PRO:HG2	2	0.32
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG21	2	0.32
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG22	2	0.32
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG23	2	0.32
(1,1814)	1:152:A:GLN:HE22	1:170:A:PRO:HD3	2	0.32
(1,1794)	1:152:A:GLN:H	1:168:A:PRO:HD3	1	0.32
(1,1756)	1:148:A:VAL:H	1:170:A:PRO:HG3	9	0.32
(1,1664)	1:135:A:SER:H	1:134:A:ILE:HG13	1	0.32
(1,1621)	1:129:A:ASP:H	1:129:A:ASP:HB2	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	3	0.32
(1,1322)	1:94:A:ARG:H	1:93:A:ASP:HB2	7	0.32
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD21	9	0.32
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD22	9	0.32
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD23	9	0.32
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD21	10	0.32
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD22	10	0.32
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD23	10	0.32
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	3	0.32
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	7	0.32
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	6	0.32
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG3	6	0.32
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	8	0.32
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	8	0.32
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	8	0.32
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	4	0.32
(1,835)	1:139:A:THR:HG21	1:141:A:LYS:HE2	9	0.32
(1,835)	1:139:A:THR:HG22	1:141:A:LYS:HE2	9	0.32
(1,835)	1:139:A:THR:HG23	1:141:A:LYS:HE2	9	0.32
(1,715)	1:126:A:GLU:HB2	1:135:A:SER:HB3	7	0.32
(1,693)	1:123:A:LYS:HG3	1:137:A:CYS:HB3	10	0.32
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD1	9	0.32
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD2	9	0.32
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD1	9	0.32
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD2	9	0.32
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD1	9	0.32
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD2	9	0.32
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	3	0.32
(1,635)	1:120:A:ILE:HB	1:140:A:ARG:HD2	10	0.32
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	1	0.32
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	1	0.32
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	6	0.32
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	5	0.32
(1,42)	1:94:A:ARG:HB3	1:168:A:PRO:HA	1	0.32
(1,7)	1:90:A:HIS:HB2	1:91:A:THR:HA	6	0.32
(1,4205)	1:162:B:THR:H	1:160:B:GLU:HB2	10	0.31
(1,4128)	1:155:B:SER:H	1:154:B:SER:HB2	4	0.31
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	4	0.31
(1,4065)	1:152:B:GLN:H	1:149:B:ASP:HB3	3	0.31
(1,3935)	1:134:B:ILE:H	1:127:B:ARG:HB2	3	0.31
(1,3862)	1:125:B:GLU:H	1:108:B:GLU:HG3	4	0.31
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	5	0.31
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	10	0.31
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	10	0.31
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	10	0.31
(1,3492)	1:160:B:GLU:HG2	1:162:B:THR:HB	1	0.31
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	1	0.31
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	7	0.31
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	4	0.31
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	8	0.31
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	5	0.31
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	10	0.31
(1,3209)	1:144:B:LEU:HD11	1:145:B:PRO:HB3	3	0.31
(1,3209)	1:144:B:LEU:HD12	1:145:B:PRO:HB3	3	0.31
(1,3209)	1:144:B:LEU:HD13	1:145:B:PRO:HB3	3	0.31
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	4	0.31
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	4	0.31
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	4	0.31
(1,3139)	1:141:B:LYS:HG3	1:141:B:LYS:HE2	1	0.31
(1,3139)	1:141:B:LYS:HG3	1:141:B:LYS:HE2	2	0.31
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	1	0.31
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	5	0.31
(1,3018)	1:127:B:ARG:HA	1:127:B:ARG:HD3	1	0.31
(1,3018)	1:127:B:ARG:HA	1:127:B:ARG:HD3	2	0.31
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE1	10	0.31
(1,3012)	1:126:B:GLU:HG3	1:133:B:TYR:HE2	10	0.31
(1,2975)	1:123:B:LYS:HD2	1:137:B:CYS:HA	3	0.31
(1,2975)	1:123:B:LYS:HD2	1:137:B:CYS:HA	4	0.31
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG21	4	0.31
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG22	4	0.31
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG23	4	0.31
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG21	8	0.31
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG22	8	0.31
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG23	8	0.31
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG11	10	0.31
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG12	10	0.31
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG13	10	0.31
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	5	0.31
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	5	0.31
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	5	0.31
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD11	1	0.31
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD12	1	0.31
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD13	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	9	0.31
(1,2601)	1:106:B:PRO:HB2	1:106:B:PRO:HD3	3	0.31
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	1	0.31
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	1	0.31
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	1	0.31
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	3	0.31
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	3	0.31
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	3	0.31
(1,2377)	1:96:B:ARG:HB2	1:166:B:GLU:HB2	5	0.31
(1,2353)	1:95:B:TRP:HB2	1:168:B:PRO:HB3	9	0.31
(1,2352)	1:95:B:TRP:HB2	1:168:B:PRO:HB2	5	0.31
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	6	0.31
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	6	0.31
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	6	0.31
(1,2330)	1:94:B:ARG:HD3	1:168:B:PRO:HA	8	0.31
(1,2329)	1:94:B:ARG:HD2	1:168:B:PRO:HA	7	0.31
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	1	0.31
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	1	0.31
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	1	0.31
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	1	0.31
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	1	0.31
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	1	0.31
(1,1998)	1:169:A:MET:H	1:169:A:MET:HB2	5	0.31
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD2	4	0.31
(1,1902)	1:161:A:GLY:H	1:102:A:ASN:HB3	2	0.31
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	9	0.31
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	9	0.31
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	9	0.31
(1,1640)	1:132:A:GLY:H	1:128:A:GLN:HG2	1	0.31
(1,1634)	1:131:A:HIS:H	1:129:A:ASP:HB3	7	0.31
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	3	0.31
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	8	0.31
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	1	0.31
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	1	0.31
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	1	0.31
(1,1323)	1:94:A:ARG:H	1:93:A:ASP:HB3	4	0.31
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	6	0.31
(1,1163)	1:157:A:LEU:HG	1:161:A:GLY:HA3	8	0.31
(1,1085)	1:153:A:VAL:HG11	1:155:A:SER:HB3	6	0.31
(1,1085)	1:153:A:VAL:HG12	1:155:A:SER:HB3	6	0.31
(1,1085)	1:153:A:VAL:HG13	1:155:A:SER:HB3	6	0.31
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	2	0.31
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	2	0.31
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	2	0.31
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG11	10	0.31
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG12	10	0.31
(1,974)	1:147:A:GLY:HA2	1:148:A:VAL:HG13	10	0.31
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG11	6	0.31
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG12	6	0.31
(1,959)	1:145:A:PRO:HG3	1:148:A:VAL:HG13	6	0.31
(1,930)	1:144:A:LEU:HD11	1:148:A:VAL:HA	10	0.31
(1,930)	1:144:A:LEU:HD12	1:148:A:VAL:HA	10	0.31
(1,930)	1:144:A:LEU:HD13	1:148:A:VAL:HA	10	0.31
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	10	0.31
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	10	0.31
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	10	0.31
(1,827)	1:139:A:THR:HA	1:140:A:ARG:HG2	9	0.31
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	4	0.31
(1,746)	1:128:A:GLN:HA	1:128:A:GLN:HG3	2	0.31
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	2	0.31
(1,694)	1:123:A:LYS:HD2	1:137:A:CYS:HA	1	0.31
(1,648)	1:120:A:ILE:HG21	1:139:A:THR:HA	1	0.31
(1,648)	1:120:A:ILE:HG22	1:139:A:THR:HA	1	0.31
(1,648)	1:120:A:ILE:HG23	1:139:A:THR:HA	1	0.31
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG21	1	0.31
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG22	1	0.31
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG23	1	0.31
(1,528)	1:116:A:GLY:HA2	1:148:A:VAL:HB	2	0.31
(1,427)	1:111:A:VAL:HG11	1:112:A:LYS:HE3	10	0.31
(1,427)	1:111:A:VAL:HG12	1:112:A:LYS:HE3	10	0.31
(1,427)	1:111:A:VAL:HG13	1:112:A:LYS:HE3	10	0.31
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	4	0.31
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD3	6	0.31
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	3	0.31
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	5	0.31
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	3	0.31
(1,320)	1:106:A:PRO:HB2	1:106:A:PRO:HD3	10	0.31
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	5	0.31
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	5	0.31
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	5	0.31
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	3	0.31
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	7	0.31
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	7	0.31
(1,4280)	1:169:B:MET:H	1:169:B:MET:HB3	8	0.3
(1,4205)	1:162:B:THR:H	1:160:B:GLU:HB2	2	0.3
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	1	0.3
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	1	0.3
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	1	0.3
(1,3915)	1:131:B:HIS:H	1:129:B:ASP:HB3	7	0.3
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	8	0.3
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	2	0.3
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	2	0.3
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	2	0.3
(1,3491)	1:160:B:GLU:HB2	1:162:B:THR:HB	7	0.3
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	3	0.3
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	9	0.3
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD11	9	0.3
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD12	9	0.3
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD13	9	0.3
(1,3400)	1:155:B:SER:HB2	1:165:B:VAL:HA	5	0.3
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	7	0.3
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	7	0.3
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	2	0.3
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	10	0.3
(1,3018)	1:127:B:ARG:HA	1:127:B:ARG:HD3	7	0.3
(1,2996)	1:126:B:GLU:HB2	1:135:B:SER:HB3	7	0.3
(1,2977)	1:123:B:LYS:HD3	1:137:B:CYS:HB3	10	0.3
(1,2975)	1:123:B:LYS:HD2	1:137:B:CYS:HA	1	0.3
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG21	1	0.3
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG22	1	0.3
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG23	1	0.3
(1,2891)	1:119:B:GLU:HA	1:141:B:LYS:HD3	6	0.3
(1,2783)	1:113:B:THR:HG21	1:150:B:PRO:HB3	7	0.3
(1,2783)	1:113:B:THR:HG22	1:150:B:PRO:HB3	7	0.3
(1,2783)	1:113:B:THR:HG23	1:150:B:PRO:HB3	7	0.3
(1,2736)	1:112:B:LYS:HB2	1:112:B:LYS:HE3	8	0.3
(1,2715)	1:111:B:VAL:HG11	1:120:B:ILE:HG12	5	0.3
(1,2715)	1:111:B:VAL:HG12	1:120:B:ILE:HG12	5	0.3
(1,2715)	1:111:B:VAL:HG13	1:120:B:ILE:HG12	5	0.3
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD11	7	0.3
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD12	7	0.3
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD13	7	0.3
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	5	0.3
(1,2626)	1:108:B:GLU:HG2	1:123:B:LYS:HE3	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	3	0.3
(1,2539)	1:99:B:LEU:HD21	1:120:B:ILE:HA	10	0.3
(1,2539)	1:99:B:LEU:HD22	1:120:B:ILE:HA	10	0.3
(1,2539)	1:99:B:LEU:HD23	1:120:B:ILE:HA	10	0.3
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	4	0.3
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	4	0.3
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	4	0.3
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE1	6	0.3
(1,2535)	1:99:B:LEU:HD21	1:142:B:TYR:HE2	6	0.3
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE1	6	0.3
(1,2535)	1:99:B:LEU:HD22	1:142:B:TYR:HE2	6	0.3
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE1	6	0.3
(1,2535)	1:99:B:LEU:HD23	1:142:B:TYR:HE2	6	0.3
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG21	3	0.3
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG22	3	0.3
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG23	3	0.3
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG21	3	0.3
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG22	3	0.3
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG23	3	0.3
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG21	3	0.3
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG22	3	0.3
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG23	3	0.3
(1,2447)	1:97:B:VAL:HG21	1:118:B:VAL:HB	5	0.3
(1,2447)	1:97:B:VAL:HG22	1:118:B:VAL:HB	5	0.3
(1,2447)	1:97:B:VAL:HG23	1:118:B:VAL:HB	5	0.3
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	9	0.3
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	9	0.3
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	9	0.3
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	7	0.3
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	7	0.3
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	7	0.3
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	8	0.3
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	8	0.3
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	8	0.3
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	5	0.3
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	5	0.3
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	5	0.3
(1,2312)	1:94:B:ARG:HA	1:168:B:PRO:HD2	2	0.3
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB1	2	0.3
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB2	2	0.3
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB3	2	0.3
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	6	0.3
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	6	0.3
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	6	0.3
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	6	0.3
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	6	0.3
(1,1915)	1:162:A:THR:H	1:102:A:ASN:HB2	10	0.3
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	2	0.3
(1,1847)	1:155:A:SER:H	1:154:A:SER:HB2	7	0.3
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	8	0.3
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	8	0.3
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	8	0.3
(1,1654)	1:134:A:ILE:H	1:127:A:ARG:HB2	2	0.3
(1,1598)	1:128:A:GLN:H	1:127:A:ARG:HG2	7	0.3
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	9	0.3
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	6	0.3
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	8	0.3
(1,1411)	1:108:A:GLU:H	1:105:A:ALA:HA	6	0.3
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	2	0.3
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	3	0.3
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	2	0.3
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	2	0.3
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	2	0.3
(1,1219)	1:162:A:THR:HA	1:162:A:THR:HG21	2	0.3
(1,1219)	1:162:A:THR:HA	1:162:A:THR:HG22	2	0.3
(1,1219)	1:162:A:THR:HA	1:162:A:THR:HG23	2	0.3
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	10	0.3
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	1	0.3
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD11	4	0.3
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD12	4	0.3
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD13	4	0.3
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	3	0.3
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	3	0.3
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	3	0.3
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	1	0.3
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	10	0.3
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	8	0.3
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	8	0.3
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	8	0.3
(1,1012)	1:148:A:VAL:HG11	1:169:A:MET:HB2	2	0.3
(1,1012)	1:148:A:VAL:HG12	1:169:A:MET:HB2	2	0.3
(1,1012)	1:148:A:VAL:HG13	1:169:A:MET:HB2	2	0.3
(1,920)	1:144:A:LEU:HB3	1:148:A:VAL:HG21	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:144:A:LEU:HB3	1:148:A:VAL:HG22	6	0.3
(1,920)	1:144:A:LEU:HB3	1:148:A:VAL:HG23	6	0.3
(1,777)	1:131:A:HIS:HA	1:131:A:HIS:HB3	2	0.3
(1,723)	1:126:A:GLU:HG2	1:135:A:SER:HB2	10	0.3
(1,699)	1:125:A:GLU:HA	1:125:A:GLU:HG2	9	0.3
(1,690)	1:123:A:LYS:HB3	1:137:A:CYS:HB2	6	0.3
(1,684)	1:123:A:LYS:HA	1:135:A:SER:HB3	4	0.3
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	8	0.3
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	8	0.3
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	8	0.3
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	8	0.3
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	1	0.3
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	1	0.3
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	1	0.3
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	7	0.3
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	7	0.3
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	7	0.3
(1,427)	1:111:A:VAL:HG11	1:112:A:LYS:HE3	2	0.3
(1,427)	1:111:A:VAL:HG12	1:112:A:LYS:HE3	2	0.3
(1,427)	1:111:A:VAL:HG13	1:112:A:LYS:HE3	2	0.3
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	2	0.3
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	2	0.3
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	2	0.3
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	9	0.3
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	7	0.3
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	10	0.3
(1,258)	1:99:A:LEU:HD21	1:120:A:ILE:HA	1	0.3
(1,258)	1:99:A:LEU:HD22	1:120:A:ILE:HA	1	0.3
(1,258)	1:99:A:LEU:HD23	1:120:A:ILE:HA	1	0.3
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	4	0.3
(1,80)	1:96:A:ARG:HA	1:96:A:ARG:HD2	7	0.3
(1,19)	1:93:A:ASP:HB2	1:94:A:ARG:HG2	2	0.3
(1,5)	1:90:A:HIS:HA	1:91:A:THR:HA	6	0.3
(1,3972)	1:140:B:ARG:H	1:120:B:ILE:HB	6	0.29
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG2	4	0.29
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	1	0.29
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	2	0.29
(1,3748)	1:113:B:THR:H	1:112:B:LYS:HB2	2	0.29
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	7	0.29
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	7	0.29
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	5	0.29
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	7	0.29
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	7	0.29
(1,3599)	1:171:B:LYS:HA	1:171:B:LYS:HD3	1	0.29
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	5	0.29
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	1	0.29
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	7	0.29
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	2	0.29
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	2	0.29
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	2	0.29
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG21	4	0.29
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG22	4	0.29
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG23	4	0.29
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	5	0.29
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	5	0.29
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	5	0.29
(1,3139)	1:141:B:LYS:HG3	1:141:B:LYS:HE2	8	0.29
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD1	7	0.29
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD2	7	0.29
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD1	7	0.29
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD2	7	0.29
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD1	7	0.29
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD2	7	0.29
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	7	0.29
(1,2977)	1:123:B:LYS:HD3	1:137:B:CYS:HB3	1	0.29
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	10	0.29
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	10	0.29
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	10	0.29
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG21	10	0.29
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG22	10	0.29
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG23	10	0.29
(1,2715)	1:111:B:VAL:HG11	1:120:B:ILE:HG12	2	0.29
(1,2715)	1:111:B:VAL:HG12	1:120:B:ILE:HG12	2	0.29
(1,2715)	1:111:B:VAL:HG13	1:120:B:ILE:HG12	2	0.29
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	4	0.29
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	4	0.29
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	4	0.29
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD11	8	0.29
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD12	8	0.29
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD13	8	0.29
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD11	9	0.29
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD12	9	0.29
(1,2608)	1:106:B:PRO:HG3	1:157:B:LEU:HD13	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	1	0.29
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	8	0.29
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	10	0.29
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	10	0.29
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	10	0.29
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	7	0.29
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	7	0.29
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	7	0.29
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG11	6	0.29
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG12	6	0.29
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG13	6	0.29
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG11	6	0.29
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG12	6	0.29
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG13	6	0.29
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG11	6	0.29
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG12	6	0.29
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG13	6	0.29
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	2	0.29
(1,2383)	1:96:B:ARG:HB3	1:166:B:GLU:HB3	2	0.29
(1,2383)	1:96:B:ARG:HB3	1:166:B:GLU:HB3	4	0.29
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB1	10	0.29
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB2	10	0.29
(1,2358)	1:95:B:TRP:HE3	1:167:B:ALA:HB3	10	0.29
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	1	0.29
(1,2285)	1:89:B:ARG:HB3	1:90:B:HIS:HB3	5	0.29
(1,2284)	1:89:B:ARG:HB3	1:90:B:HIS:HB2	9	0.29
(1,1998)	1:169:A:MET:H	1:169:A:MET:HB2	8	0.29
(1,1847)	1:155:A:SER:H	1:154:A:SER:HB2	4	0.29
(1,1650)	1:132:A:GLY:H	1:133:A:TYR:HD1	1	0.29
(1,1650)	1:132:A:GLY:H	1:133:A:TYR:HD2	1	0.29
(1,1621)	1:129:A:ASP:H	1:129:A:ASP:HB2	1	0.29
(1,1500)	1:117:A:VAL:H	1:115:A:ASP:HB2	10	0.29
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	7	0.29
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD11	10	0.29
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD12	10	0.29
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD13	10	0.29
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD21	1	0.29
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD22	1	0.29
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD23	1	0.29
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG21	6	0.29
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG22	6	0.29
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG23	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:171:A:LYS:HA	1:171:A:LYS:HD3	8	0.29
(1,1276)	1:168:A:PRO:HA	1:169:A:MET:HG2	9	0.29
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD21	8	0.29
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD22	8	0.29
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD23	8	0.29
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	1	0.29
(1,1197)	1:158:A:SER:HB3	1:159:A:PRO:HD3	9	0.29
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	5	0.29
(1,1149)	1:157:A:LEU:HA	1:163:A:LEU:HB3	1	0.29
(1,1149)	1:157:A:LEU:HA	1:163:A:LEU:HB3	6	0.29
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	9	0.29
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	3	0.29
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	3	0.29
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	3	0.29
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	3	0.29
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	7	0.29
(1,1065)	1:152:A:GLN:HB2	1:169:A:MET:HA	7	0.29
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	2	0.29
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	6	0.29
(1,1012)	1:148:A:VAL:HG11	1:169:A:MET:HB2	6	0.29
(1,1012)	1:148:A:VAL:HG12	1:169:A:MET:HB2	6	0.29
(1,1012)	1:148:A:VAL:HG13	1:169:A:MET:HB2	6	0.29
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	6	0.29
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	6	0.29
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	6	0.29
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	6	0.29
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG11	8	0.29
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG12	8	0.29
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG13	8	0.29
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG11	8	0.29
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG12	8	0.29
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG13	8	0.29
(1,847)	1:141:A:LYS:HA	1:141:A:LYS:HE3	6	0.29
(1,808)	1:135:A:SER:HA	1:135:A:SER:HB2	5	0.29
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	7	0.29
(1,688)	1:123:A:LYS:HB2	1:137:A:CYS:HB3	2	0.29
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	10	0.29
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	10	0.29
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	10	0.29
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	10	0.29
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	10	0.29
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	10	0.29
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	10	0.29
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	10	0.29
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	8	0.29
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	8	0.29
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	8	0.29
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	6	0.29
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	6	0.29
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	6	0.29
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD2	7	0.29
(1,324)	1:106:A:PRO:HB3	1:107:A:ASP:HA	9	0.29
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	3	0.29
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	3	0.29
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	3	0.29
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	7	0.29
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	7	0.29
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	7	0.29
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	10	0.29
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	7	0.29
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	7	0.29
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	7	0.29
(1,102)	1:96:A:ARG:HB3	1:166:A:GLU:HB3	1	0.29
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	2	0.29
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	2	0.29
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	2	0.29
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	8	0.29
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	8	0.29
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	8	0.29
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE1	1	0.28
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE2	1	0.28
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE1	2	0.28
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE2	2	0.28
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	3	0.28
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	7	0.28
(1,3748)	1:113:B:THR:H	1:112:B:LYS:HB2	3	0.28
(1,3748)	1:113:B:THR:H	1:112:B:LYS:HB2	9	0.28
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	1	0.28
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	6	0.28
(1,3654)	1:102:B:ASN:HD21	1:161:B:GLY:HA2	6	0.28
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD21	5	0.28
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	4	0.28
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	4	0.28
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	1	0.28
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	1	0.28
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	1	0.28
(1,3454)	1:157:B:LEU:HD11	1:163:B:LEU:HB3	9	0.28
(1,3454)	1:157:B:LEU:HD12	1:163:B:LEU:HB3	9	0.28
(1,3454)	1:157:B:LEU:HD13	1:163:B:LEU:HB3	9	0.28
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	1	0.28
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	1	0.28
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	1	0.28
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	2	0.28
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	3	0.28
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	8	0.28
(1,3252)	1:146:B:PRO:HG2	1:147:B:GLY:HA2	6	0.28
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	1	0.28
(1,3211)	1:144:B:LEU:HD11	1:148:B:VAL:HA	7	0.28
(1,3211)	1:144:B:LEU:HD12	1:148:B:VAL:HA	7	0.28
(1,3211)	1:144:B:LEU:HD13	1:148:B:VAL:HA	7	0.28
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG21	5	0.28
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG22	5	0.28
(1,3201)	1:144:B:LEU:HB3	1:148:B:VAL:HG23	5	0.28
(1,3138)	1:141:B:LYS:HG2	1:143:B:THR:HA	3	0.28
(1,3137)	1:141:B:LYS:HG2	1:142:B:TYR:HB3	3	0.28
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD1	9	0.28
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD2	9	0.28
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD1	9	0.28
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD2	9	0.28
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD1	9	0.28
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD2	9	0.28
(1,3053)	1:130:B:GLU:HA	1:130:B:GLU:HG2	4	0.28
(1,3003)	1:126:B:GLU:HG2	1:135:B:SER:HA	1	0.28
(1,3003)	1:126:B:GLU:HG2	1:135:B:SER:HA	5	0.28
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	9	0.28
(1,2935)	1:120:B:ILE:HD11	1:140:B:ARG:HD2	2	0.28
(1,2935)	1:120:B:ILE:HD12	1:140:B:ARG:HD2	2	0.28
(1,2935)	1:120:B:ILE:HD13	1:140:B:ARG:HD2	2	0.28
(1,2928)	1:120:B:ILE:HG21	1:122:B:GLY:HA3	6	0.28
(1,2928)	1:120:B:ILE:HG22	1:122:B:GLY:HA3	6	0.28
(1,2928)	1:120:B:ILE:HG23	1:122:B:GLY:HA3	6	0.28
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	4	0.28
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	1	0.28
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	1	0.28
(1,2738)	1:112:B:LYS:HB2	1:120:B:ILE:HA	1	0.28
(1,2736)	1:112:B:LYS:HB2	1:112:B:LYS:HE3	5	0.28
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	5	0.28
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	5	0.28
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	5	0.28
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	2	0.28
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	2	0.28
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	2	0.28
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	5	0.28
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	4	0.28
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	1	0.28
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	1	0.28
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	1	0.28
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	2	0.28
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	4	0.28
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	4	0.28
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	4	0.28
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	6	0.28
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	6	0.28
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	6	0.28
(1,2353)	1:95:B:TRP:HB2	1:168:B:PRO:HB3	5	0.28
(1,2353)	1:95:B:TRP:HB2	1:168:B:PRO:HB3	10	0.28
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	9	0.28
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	9	0.28
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	9	0.28
(1,2318)	1:94:B:ARG:HB2	1:96:B:ARG:HA	2	0.28
(1,2282)	1:88:B:ILE:HG21	1:90:B:HIS:HA	5	0.28
(1,2282)	1:88:B:ILE:HG22	1:90:B:HIS:HA	5	0.28
(1,2282)	1:88:B:ILE:HG23	1:90:B:HIS:HA	5	0.28
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	7	0.28
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	7	0.28
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	7	0.28
(1,2207)	1:134:B:ILE:HD11	1:140:A:ARG:HG2	9	0.28
(1,2207)	1:134:B:ILE:HD12	1:140:A:ARG:HG2	9	0.28
(1,2207)	1:134:B:ILE:HD13	1:140:A:ARG:HG2	9	0.28
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	7	0.28
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	7	0.28
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	7	0.28
(1,2075)	1:134:B:ILE:HD11	1:140:A:ARG:HG2	9	0.28
(1,2075)	1:134:B:ILE:HD12	1:140:A:ARG:HG2	9	0.28
(1,2075)	1:134:B:ILE:HD13	1:140:A:ARG:HG2	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD2	10	0.28
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	8	0.28
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	3	0.28
(1,1847)	1:155:A:SER:H	1:154:A:SER:HB2	10	0.28
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	9	0.28
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	6	0.28
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	6	0.28
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	6	0.28
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	10	0.28
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	8	0.28
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	8	0.28
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	6	0.28
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	6	0.28
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	6	0.28
(1,1323)	1:94:A:ARG:H	1:93:A:ASP:HB3	6	0.28
(1,1314)	1:170:A:PRO:HB3	1:170:A:PRO:HD3	6	0.28
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	4	0.28
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	7	0.28
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	8	0.28
(1,1280)	1:168:A:PRO:HB2	1:170:A:PRO:HD3	2	0.28
(1,1102)	1:155:A:SER:HA	1:155:A:SER:HB3	7	0.28
(1,1097)	1:154:A:SER:HB3	1:155:A:SER:HA	5	0.28
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	6	0.28
(1,990)	1:148:A:VAL:HA	1:169:A:MET:HB2	2	0.28
(1,958)	1:145:A:PRO:HG3	1:146:A:PRO:HD2	6	0.28
(1,845)	1:141:A:LYS:HA	1:141:A:LYS:HD3	6	0.28
(1,831)	1:139:A:THR:HB	1:141:A:LYS:HE2	8	0.28
(1,826)	1:139:A:THR:HA	1:140:A:ARG:HB2	9	0.28
(1,718)	1:126:A:GLU:HG2	1:133:A:TYR:HB3	6	0.28
(1,687)	1:123:A:LYS:HB2	1:137:A:CYS:HB2	10	0.28
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG21	3	0.28
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG22	3	0.28
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG23	3	0.28
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	3	0.28
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	3	0.28
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	3	0.28
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	3	0.28
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	3	0.28
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	3	0.28
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	3	0.28
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	3	0.28
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	7	0.28
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	7	0.28
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	7	0.28
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	7	0.28
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	7	0.28
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	7	0.28
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	7	0.28
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	7	0.28
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	7	0.28
(1,427)	1:111:A:VAL:HG11	1:112:A:LYS:HE3	4	0.28
(1,427)	1:111:A:VAL:HG12	1:112:A:LYS:HE3	4	0.28
(1,427)	1:111:A:VAL:HG13	1:112:A:LYS:HE3	4	0.28
(1,427)	1:111:A:VAL:HG11	1:112:A:LYS:HE3	5	0.28
(1,427)	1:111:A:VAL:HG12	1:112:A:LYS:HE3	5	0.28
(1,427)	1:111:A:VAL:HG13	1:112:A:LYS:HE3	5	0.28
(1,336)	1:108:A:GLU:HA	1:108:A:GLU:HG2	4	0.28
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG21	6	0.28
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG22	6	0.28
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG23	6	0.28
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	10	0.28
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	10	0.28
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	10	0.28
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	10	0.28
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	10	0.28
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	10	0.28
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	10	0.28
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	10	0.28
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	10	0.28
(1,232)	1:99:A:LEU:HD11	1:120:A:ILE:HG12	8	0.28
(1,232)	1:99:A:LEU:HD12	1:120:A:ILE:HG12	8	0.28
(1,232)	1:99:A:LEU:HD13	1:120:A:ILE:HG12	8	0.28
(1,102)	1:96:A:ARG:HB3	1:166:A:GLU:HB3	7	0.28
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	5	0.28
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	5	0.28
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	5	0.28
(1,9)	1:90:A:HIS:HB3	1:91:A:THR:HA	7	0.28
(1,4263)	1:167:B:ALA:H	1:166:B:GLU:HB3	6	0.27
(1,4262)	1:167:B:ALA:H	1:166:B:GLU:HB2	5	0.27
(1,4025)	1:148:B:VAL:H	1:146:B:PRO:HG2	4	0.27
(1,3935)	1:134:B:ILE:H	1:127:B:ARG:HB2	7	0.27
(1,3902)	1:129:B:ASP:H	1:129:B:ASP:HB2	8	0.27
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	1	0.27
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD21	3	0.27
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD22	3	0.27
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD23	3	0.27
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD21	3	0.27
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	10	0.27
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	10	0.27
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	10	0.27
(1,3566)	1:168:B:PRO:HD2	1:169:B:MET:HA	2	0.27
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	10	0.27
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	9	0.27
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	1	0.27
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD21	7	0.27
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD22	7	0.27
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD23	7	0.27
(1,3395)	1:155:B:SER:HB2	1:163:B:LEU:HA	5	0.27
(1,3383)	1:155:B:SER:HA	1:155:B:SER:HB3	10	0.27
(1,3345)	1:152:B:GLN:HB2	1:168:B:PRO:HD3	6	0.27
(1,3274)	1:148:B:VAL:HA	1:170:B:PRO:HG2	10	0.27
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	7	0.27
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	7	0.27
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	7	0.27
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	5	0.27
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	5	0.27
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	5	0.27
(1,3092)	1:136:B:ARG:HA	1:136:B:ARG:HG2	4	0.27
(1,2975)	1:123:B:LYS:HD2	1:137:B:CYS:HA	10	0.27
(1,2931)	1:120:B:ILE:HG21	1:142:B:TYR:HD1	2	0.27
(1,2931)	1:120:B:ILE:HG21	1:142:B:TYR:HD2	2	0.27
(1,2931)	1:120:B:ILE:HG22	1:142:B:TYR:HD1	2	0.27
(1,2931)	1:120:B:ILE:HG22	1:142:B:TYR:HD2	2	0.27
(1,2931)	1:120:B:ILE:HG23	1:142:B:TYR:HD1	2	0.27
(1,2931)	1:120:B:ILE:HG23	1:142:B:TYR:HD2	2	0.27
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	1	0.27
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	1	0.27
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	1	0.27
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	9	0.27
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	9	0.27
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	9	0.27
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG21	7	0.27
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG22	7	0.27
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG23	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG21	9	0.27
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG22	9	0.27
(1,2919)	1:120:B:ILE:HG12	1:120:B:ILE:HG23	9	0.27
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD11	4	0.27
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD12	4	0.27
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD13	4	0.27
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	1	0.27
(1,2625)	1:108:B:GLU:HG2	1:123:B:LYS:HD2	5	0.27
(1,2619)	1:108:B:GLU:HA	1:123:B:LYS:HD2	10	0.27
(1,2613)	1:107:B:ASP:HA	1:108:B:GLU:HG3	6	0.27
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	9	0.27
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	9	0.27
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	9	0.27
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	5	0.27
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	5	0.27
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	5	0.27
(1,2332)	1:95:B:TRP:HA	1:95:B:TRP:HB2	8	0.27
(1,2313)	1:94:B:ARG:HA	1:168:B:PRO:HD3	1	0.27
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG21	8	0.27
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG22	8	0.27
(1,2287)	1:90:B:HIS:HA	1:91:B:THR:HG23	8	0.27
(1,2281)	1:143:A:THR:H	1:132:B:GLY:HA2	6	0.27
(1,2213)	1:134:A:ILE:HA	1:140:B:ARG:HD3	6	0.27
(1,2207)	1:134:B:ILE:HD11	1:140:A:ARG:HG2	1	0.27
(1,2207)	1:134:B:ILE:HD12	1:140:A:ARG:HG2	1	0.27
(1,2207)	1:134:B:ILE:HD13	1:140:A:ARG:HG2	1	0.27
(1,2192)	1:134:B:ILE:HA	1:140:A:ARG:HG3	4	0.27
(1,2152)	1:97:A:VAL:HG11	1:131:B:HIS:HB3	5	0.27
(1,2152)	1:97:A:VAL:HG12	1:131:B:HIS:HB3	5	0.27
(1,2152)	1:97:A:VAL:HG13	1:131:B:HIS:HB3	5	0.27
(1,2148)	1:143:A:THR:H	1:132:B:GLY:HA2	6	0.27
(1,2081)	1:134:A:ILE:HA	1:140:B:ARG:HD3	6	0.27
(1,2075)	1:134:B:ILE:HD11	1:140:A:ARG:HG2	1	0.27
(1,2075)	1:134:B:ILE:HD12	1:140:A:ARG:HG2	1	0.27
(1,2075)	1:134:B:ILE:HD13	1:140:A:ARG:HG2	1	0.27
(1,2060)	1:134:B:ILE:HA	1:140:A:ARG:HG3	4	0.27
(1,2020)	1:97:A:VAL:HG11	1:131:B:HIS:HB3	5	0.27
(1,2020)	1:97:A:VAL:HG12	1:131:B:HIS:HB3	5	0.27
(1,2020)	1:97:A:VAL:HG13	1:131:B:HIS:HB3	5	0.27
(1,2009)	1:171:A:LYS:H	1:171:A:LYS:HB2	6	0.27
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	9	0.27
(1,1703)	1:142:A:TYR:H	1:141:A:LYS:HG3	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1703)	1:142:A:TYR:H	1:141:A:LYS:HG3	7	0.27
(1,1626)	1:129:A:ASP:H	1:132:A:GLY:HA3	9	0.27
(1,1584)	1:125:A:GLU:H	1:126:A:GLU:H	2	0.27
(1,1580)	1:125:A:GLU:H	1:108:A:GLU:HG2	7	0.27
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	3	0.27
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	4	0.27
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	1	0.27
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	1	0.27
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	5	0.27
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD11	8	0.27
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD12	8	0.27
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD13	8	0.27
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	7	0.27
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	7	0.27
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	7	0.27
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	6	0.27
(1,1191)	1:158:A:SER:HB2	1:160:A:GLU:HG2	6	0.27
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	9	0.27
(1,1168)	1:157:A:LEU:HD11	1:161:A:GLY:HA3	3	0.27
(1,1168)	1:157:A:LEU:HD12	1:161:A:GLY:HA3	3	0.27
(1,1168)	1:157:A:LEU:HD13	1:161:A:GLY:HA3	3	0.27
(1,1097)	1:154:A:SER:HB3	1:155:A:SER:HA	6	0.27
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	10	0.27
(1,917)	1:144:A:LEU:HB3	1:147:A:GLY:HA2	1	0.27
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	2	0.27
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	2	0.27
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	2	0.27
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	7	0.27
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	7	0.27
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	7	0.27
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	5	0.27
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	5	0.27
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	5	0.27
(1,837)	1:140:A:ARG:HA	1:140:A:ARG:HD3	8	0.27
(1,808)	1:135:A:SER:HA	1:135:A:SER:HB2	2	0.27
(1,782)	1:131:A:HIS:HB2	1:132:A:GLY:HA2	8	0.27
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	1	0.27
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	8	0.27
(1,715)	1:126:A:GLU:HB2	1:135:A:SER:HB3	9	0.27
(1,689)	1:123:A:LYS:HB3	1:137:A:CYS:HA	8	0.27
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	3	0.27
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	3	0.27
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	5	0.27
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	5	0.27
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	5	0.27
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	10	0.27
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	10	0.27
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	10	0.27
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG21	5	0.27
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG22	5	0.27
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG23	5	0.27
(1,455)	1:112:A:LYS:HB2	1:112:A:LYS:HE3	9	0.27
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	8	0.27
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	6	0.27
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	9	0.27
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	9	0.27
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	9	0.27
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	8	0.27
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	8	0.27
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	8	0.27
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	8	0.27
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	8	0.27
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	8	0.27
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	8	0.27
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	8	0.27
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	8	0.27
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	2	0.27
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	2	0.27
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	2	0.27
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	2	0.27
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	2	0.27
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	2	0.27
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	2	0.27
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	2	0.27
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	2	0.27
(1,99)	1:96:A:ARG:HB3	1:164:A:THR:HB	10	0.27
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	4	0.27
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	4	0.27
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	4	0.27
(1,72)	1:95:A:TRP:HB3	1:168:A:PRO:HB3	6	0.27
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG11	7	0.27
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG12	7	0.27
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG13	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:95:A:TRP:HA	1:95:A:TRP:HB2	4	0.27
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	1	0.26
(1,3915)	1:131:B:HIS:H	1:129:B:ASP:HB3	9	0.26
(1,3907)	1:129:B:ASP:H	1:132:B:GLY:HA3	3	0.26
(1,3862)	1:125:B:GLU:H	1:108:B:GLU:HG3	5	0.26
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	9	0.26
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	10	0.26
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	3	0.26
(1,3672)	1:105:B:ALA:H	1:108:B:GLU:HB3	2	0.26
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD21	8	0.26
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD22	8	0.26
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD23	8	0.26
(1,3602)	1:94:B:ARG:H	1:93:B:ASP:HA	9	0.26
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG21	1	0.26
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG22	1	0.26
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG23	1	0.26
(1,3595)	1:170:B:PRO:HB3	1:170:B:PRO:HD3	9	0.26
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD11	1	0.26
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD12	1	0.26
(1,3437)	1:157:B:LEU:HB2	1:163:B:LEU:HD13	1	0.26
(1,3346)	1:152:B:GLN:HB2	1:169:B:MET:HA	5	0.26
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	9	0.26
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	9	0.26
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	9	0.26
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	10	0.26
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	10	0.26
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	10	0.26
(1,3295)	1:148:B:VAL:HG11	1:170:B:PRO:HG3	1	0.26
(1,3295)	1:148:B:VAL:HG12	1:170:B:PRO:HG3	1	0.26
(1,3295)	1:148:B:VAL:HG13	1:170:B:PRO:HG3	1	0.26
(1,3295)	1:148:B:VAL:HG11	1:170:B:PRO:HG3	3	0.26
(1,3295)	1:148:B:VAL:HG12	1:170:B:PRO:HG3	3	0.26
(1,3295)	1:148:B:VAL:HG13	1:170:B:PRO:HG3	3	0.26
(1,3295)	1:148:B:VAL:HG11	1:170:B:PRO:HG3	9	0.26
(1,3295)	1:148:B:VAL:HG12	1:170:B:PRO:HG3	9	0.26
(1,3295)	1:148:B:VAL:HG13	1:170:B:PRO:HG3	9	0.26
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	3	0.26
(1,3096)	1:136:B:ARG:HG3	1:138:B:PHE:HA	8	0.26
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	3	0.26
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	5	0.26
(1,3054)	1:130:B:GLU:HA	1:130:B:GLU:HG3	3	0.26
(1,3003)	1:126:B:GLU:HG2	1:135:B:SER:HA	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2930)	1:120:B:ILE:HG21	1:140:B:ARG:HA	3	0.26
(1,2930)	1:120:B:ILE:HG22	1:140:B:ARG:HA	3	0.26
(1,2930)	1:120:B:ILE:HG23	1:140:B:ARG:HA	3	0.26
(1,2929)	1:120:B:ILE:HG21	1:139:B:THR:HA	1	0.26
(1,2929)	1:120:B:ILE:HG22	1:139:B:THR:HA	1	0.26
(1,2929)	1:120:B:ILE:HG23	1:139:B:THR:HA	1	0.26
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	9	0.26
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	4	0.26
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	4	0.26
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	4	0.26
(1,2708)	1:111:B:VAL:HG11	1:112:B:LYS:HE3	1	0.26
(1,2708)	1:111:B:VAL:HG12	1:112:B:LYS:HE3	1	0.26
(1,2708)	1:111:B:VAL:HG13	1:112:B:LYS:HE3	1	0.26
(1,2687)	1:110:B:THR:HG21	1:112:B:LYS:HE3	8	0.26
(1,2687)	1:110:B:THR:HG22	1:112:B:LYS:HE3	8	0.26
(1,2687)	1:110:B:THR:HG23	1:112:B:LYS:HE3	8	0.26
(1,2686)	1:110:B:THR:HG21	1:112:B:LYS:HD3	2	0.26
(1,2686)	1:110:B:THR:HG22	1:112:B:LYS:HD3	2	0.26
(1,2686)	1:110:B:THR:HG23	1:112:B:LYS:HD3	2	0.26
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	4	0.26
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	6	0.26
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	9	0.26
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	9	0.26
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	9	0.26
(1,2625)	1:108:B:GLU:HG2	1:123:B:LYS:HD2	1	0.26
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD21	8	0.26
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD22	8	0.26
(1,2616)	1:107:B:ASP:HA	1:157:B:LEU:HD23	8	0.26
(1,2592)	1:106:B:PRO:HA	1:109:B:LEU:HB2	10	0.26
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	1	0.26
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	4	0.26
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	4	0.26
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	4	0.26
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG21	1	0.26
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG22	1	0.26
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG23	1	0.26
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	2	0.26
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	2	0.26
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	2	0.26
(1,2352)	1:95:B:TRP:HB2	1:168:B:PRO:HB2	4	0.26
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	4	0.26
(1,2283)	1:88:B:ILE:HG21	1:90:B:HIS:HB3	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2283)	1:88:B:ILE:HG22	1:90:B:HIS:HB3	3	0.26
(1,2283)	1:88:B:ILE:HG23	1:90:B:HIS:HB3	3	0.26
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	3	0.26
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	3	0.26
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	3	0.26
(1,2169)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	5	0.26
(1,2152)	1:97:A:VAL:HG11	1:131:B:HIS:HB3	9	0.26
(1,2152)	1:97:A:VAL:HG12	1:131:B:HIS:HB3	9	0.26
(1,2152)	1:97:A:VAL:HG13	1:131:B:HIS:HB3	9	0.26
(1,2150)	1:97:B:VAL:HG11	1:131:A:HIS:HB3	3	0.26
(1,2150)	1:97:B:VAL:HG12	1:131:A:HIS:HB3	3	0.26
(1,2150)	1:97:B:VAL:HG13	1:131:A:HIS:HB3	3	0.26
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	3	0.26
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	3	0.26
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	3	0.26
(1,2037)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	5	0.26
(1,2020)	1:97:A:VAL:HG11	1:131:B:HIS:HB3	9	0.26
(1,2020)	1:97:A:VAL:HG12	1:131:B:HIS:HB3	9	0.26
(1,2020)	1:97:A:VAL:HG13	1:131:B:HIS:HB3	9	0.26
(1,2018)	1:97:B:VAL:HG11	1:131:A:HIS:HB3	3	0.26
(1,2018)	1:97:B:VAL:HG12	1:131:A:HIS:HB3	3	0.26
(1,2018)	1:97:B:VAL:HG13	1:131:A:HIS:HB3	3	0.26
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD11	8	0.26
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD12	8	0.26
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD13	8	0.26
(1,1915)	1:162:A:THR:H	1:102:A:ASN:HB2	8	0.26
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG21	5	0.26
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG22	5	0.26
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG23	5	0.26
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	5	0.26
(1,1626)	1:129:A:ASP:H	1:132:A:GLY:HA3	7	0.26
(1,1598)	1:128:A:GLN:H	1:127:A:ARG:HG2	3	0.26
(1,1525)	1:119:A:GLU:H	1:114:A:LYS:HB3	3	0.26
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	7	0.26
(1,1459)	1:112:A:LYS:H	1:112:A:LYS:HE3	1	0.26
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	2	0.26
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	3	0.26
(1,1399)	1:107:A:ASP:H	1:106:A:PRO:HB2	10	0.26
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	9	0.26
(1,1302)	1:169:A:MET:HB2	1:171:A:LYS:HE3	2	0.26
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	2	0.26
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	4	0.26
(1,1179)	1:157:A:LEU:HD21	1:163:A:LEU:HB3	9	0.26
(1,1179)	1:157:A:LEU:HD22	1:163:A:LEU:HB3	9	0.26
(1,1179)	1:157:A:LEU:HD23	1:163:A:LEU:HB3	9	0.26
(1,1179)	1:157:A:LEU:HD21	1:163:A:LEU:HB3	10	0.26
(1,1179)	1:157:A:LEU:HD22	1:163:A:LEU:HB3	10	0.26
(1,1179)	1:157:A:LEU:HD23	1:163:A:LEU:HB3	10	0.26
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	5	0.26
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	5	0.26
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	5	0.26
(1,1168)	1:157:A:LEU:HD11	1:161:A:GLY:HA3	1	0.26
(1,1168)	1:157:A:LEU:HD12	1:161:A:GLY:HA3	1	0.26
(1,1168)	1:157:A:LEU:HD13	1:161:A:GLY:HA3	1	0.26
(1,1168)	1:157:A:LEU:HD11	1:161:A:GLY:HA3	10	0.26
(1,1168)	1:157:A:LEU:HD12	1:161:A:GLY:HA3	10	0.26
(1,1168)	1:157:A:LEU:HD13	1:161:A:GLY:HA3	10	0.26
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD11	3	0.26
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD12	3	0.26
(1,1156)	1:157:A:LEU:HB2	1:163:A:LEU:HD13	3	0.26
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	8	0.26
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	1	0.26
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	4	0.26
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	6	0.26
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	9	0.26
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG11	6	0.26
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG12	6	0.26
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG13	6	0.26
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	10	0.26
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	10	0.26
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	10	0.26
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	5	0.26
(1,831)	1:139:A:THR:HB	1:141:A:LYS:HE2	6	0.26
(1,808)	1:135:A:SER:HA	1:135:A:SER:HB2	3	0.26
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	8	0.26
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	8	0.26
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	8	0.26
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	10	0.26
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	10	0.26
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	10	0.26
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	10	0.26
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	10	0.26
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	10	0.26
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	4	0.26
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	4	0.26
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	4	0.26
(1,478)	1:112:A:LYS:HE2	1:121:A:THR:HB	7	0.26
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	2	0.26
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD2	4	0.26
(1,337)	1:108:A:GLU:HA	1:108:A:GLU:HG3	6	0.26
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD11	4	0.26
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD12	4	0.26
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD13	4	0.26
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD11	7	0.26
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD12	7	0.26
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD13	7	0.26
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	7	0.26
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	7	0.26
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	7	0.26
(1,166)	1:97:A:VAL:HG21	1:118:A:VAL:HB	2	0.26
(1,166)	1:97:A:VAL:HG22	1:118:A:VAL:HB	2	0.26
(1,166)	1:97:A:VAL:HG23	1:118:A:VAL:HB	2	0.26
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	9	0.26
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	9	0.26
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	9	0.26
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG11	5	0.26
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG12	5	0.26
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG13	5	0.26
(1,51)	1:95:A:TRP:HA	1:95:A:TRP:HB2	7	0.26
(1,18)	1:93:A:ASP:HB2	1:94:A:ARG:HA	3	0.26
(1,9)	1:90:A:HIS:HB3	1:91:A:THR:HA	5	0.26
(1,4281)	1:169:B:MET:H	1:169:B:MET:HG3	8	0.25
(1,4279)	1:169:B:MET:H	1:169:B:MET:HB2	9	0.25
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	1	0.25
(1,4048)	1:149:B:ASP:H	1:170:B:PRO:HG3	10	0.25
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD21	3	0.25
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD22	3	0.25
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD23	3	0.25
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD21	9	0.25
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD22	9	0.25
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD23	9	0.25
(1,3936)	1:134:B:ILE:H	1:127:B:ARG:HG2	8	0.25
(1,3908)	1:129:B:ASP:H	1:132:B:GLY:H	4	0.25
(1,3904)	1:129:B:ASP:H	1:130:B:GLU:HG3	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3896)	1:128:B:GLN:HE21	1:128:B:GLN:HB3	1	0.25
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD1	6	0.25
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD2	6	0.25
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	8	0.25
(1,3748)	1:113:B:THR:H	1:112:B:LYS:HB2	7	0.25
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD11	10	0.25
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD12	10	0.25
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD13	10	0.25
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD21	7	0.25
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD22	7	0.25
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD23	7	0.25
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD11	7	0.25
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD12	7	0.25
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD13	7	0.25
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD22	8	0.25
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	6	0.25
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	6	0.25
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	6	0.25
(1,3605)	1:94:B:ARG:H	1:94:B:ARG:HG3	7	0.25
(1,3604)	1:94:B:ARG:H	1:93:B:ASP:HB3	2	0.25
(1,3436)	1:157:B:LEU:HB2	1:163:B:LEU:HA	8	0.25
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	1	0.25
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	6	0.25
(1,3302)	1:148:B:VAL:HG21	1:169:B:MET:HB3	3	0.25
(1,3302)	1:148:B:VAL:HG22	1:169:B:MET:HB3	3	0.25
(1,3302)	1:148:B:VAL:HG23	1:169:B:MET:HB3	3	0.25
(1,3302)	1:148:B:VAL:HG21	1:169:B:MET:HB3	10	0.25
(1,3302)	1:148:B:VAL:HG22	1:169:B:MET:HB3	10	0.25
(1,3302)	1:148:B:VAL:HG23	1:169:B:MET:HB3	10	0.25
(1,3295)	1:148:B:VAL:HG11	1:170:B:PRO:HG3	2	0.25
(1,3295)	1:148:B:VAL:HG12	1:170:B:PRO:HG3	2	0.25
(1,3295)	1:148:B:VAL:HG13	1:170:B:PRO:HG3	2	0.25
(1,3295)	1:148:B:VAL:HG11	1:170:B:PRO:HG3	10	0.25
(1,3295)	1:148:B:VAL:HG12	1:170:B:PRO:HG3	10	0.25
(1,3295)	1:148:B:VAL:HG13	1:170:B:PRO:HG3	10	0.25
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	1	0.25
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG2	2	0.25
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	8	0.25
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	10	0.25
(1,3164)	1:142:B:TYR:HD1	1:165:B:VAL:HG21	2	0.25
(1,3164)	1:142:B:TYR:HD1	1:165:B:VAL:HG22	2	0.25
(1,3164)	1:142:B:TYR:HD1	1:165:B:VAL:HG23	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3164)	1:142:B:TYR:HD2	1:165:B:VAL:HG21	2	0.25
(1,3164)	1:142:B:TYR:HD2	1:165:B:VAL:HG22	2	0.25
(1,3164)	1:142:B:TYR:HD2	1:165:B:VAL:HG23	2	0.25
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD1	2	0.25
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD2	2	0.25
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD1	2	0.25
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD2	2	0.25
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD1	2	0.25
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD2	2	0.25
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	1	0.25
(1,3058)	1:131:B:HIS:HA	1:131:B:HIS:HB3	4	0.25
(1,2968)	1:123:B:LYS:HB2	1:137:B:CYS:HB2	4	0.25
(1,2965)	1:123:B:LYS:HA	1:135:B:SER:HB3	10	0.25
(1,2935)	1:120:B:ILE:HD11	1:140:B:ARG:HD2	5	0.25
(1,2935)	1:120:B:ILE:HD12	1:140:B:ARG:HD2	5	0.25
(1,2935)	1:120:B:ILE:HD13	1:140:B:ARG:HD2	5	0.25
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	7	0.25
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	7	0.25
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	7	0.25
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	1	0.25
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	1	0.25
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	1	0.25
(1,2716)	1:111:B:VAL:HG11	1:120:B:ILE:HG13	10	0.25
(1,2716)	1:111:B:VAL:HG12	1:120:B:ILE:HG13	10	0.25
(1,2716)	1:111:B:VAL:HG13	1:120:B:ILE:HG13	10	0.25
(1,2708)	1:111:B:VAL:HG11	1:112:B:LYS:HE3	7	0.25
(1,2708)	1:111:B:VAL:HG12	1:112:B:LYS:HE3	7	0.25
(1,2708)	1:111:B:VAL:HG13	1:112:B:LYS:HE3	7	0.25
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	7	0.25
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	7	0.25
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	7	0.25
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	10	0.25
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	10	0.25
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	10	0.25
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	10	0.25
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	10	0.25
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	10	0.25
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	10	0.25
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	10	0.25
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	10	0.25
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	1	0.25
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	1	0.25
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD2	7	0.25
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	2	0.25
(1,2605)	1:106:B:PRO:HB3	1:107:B:ASP:HA	10	0.25
(1,2568)	1:105:B:ALA:HA	1:108:B:GLU:HB3	5	0.25
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	5	0.25
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	8	0.25
(1,2529)	1:99:B:LEU:HD21	1:140:B:ARG:HD2	8	0.25
(1,2529)	1:99:B:LEU:HD22	1:140:B:ARG:HD2	8	0.25
(1,2529)	1:99:B:LEU:HD23	1:140:B:ARG:HD2	8	0.25
(1,2393)	1:96:B:ARG:HD3	1:164:B:THR:HA	1	0.25
(1,2383)	1:96:B:ARG:HB3	1:166:B:GLU:HB3	1	0.25
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	4	0.25
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	1	0.25
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	1	0.25
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	1	0.25
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	10	0.25
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	10	0.25
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	10	0.25
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	7	0.25
(1,2353)	1:95:B:TRP:HB3	1:168:B:PRO:HB3	1	0.25
(1,2353)	1:95:B:TRP:HB3	1:168:B:PRO:HB3	6	0.25
(1,2352)	1:95:B:TRP:HB3	1:168:B:PRO:HB2	6	0.25
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	4	0.25
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	4	0.25
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	4	0.25
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	9	0.25
(1,2322)	1:94:B:ARG:HB3	1:167:B:ALA:HA	2	0.25
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	9	0.25
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	9	0.25
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	9	0.25
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	1	0.25
(1,2185)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	2	0.25
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	9	0.25
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	9	0.25
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	9	0.25
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	1	0.25
(1,2053)	1:133:A:TYR:HB3	1:141:B:LYS:HD2	2	0.25
(1,2015)	1:173:A:ALA:H	1:172:A:LEU:HG	9	0.25
(1,1910)	1:161:A:GLY:H	1:160:A:GLU:HG3	2	0.25
(1,1654)	1:134:A:ILE:H	1:127:A:ARG:HB2	4	0.25
(1,1637)	1:131:A:HIS:H	1:130:A:GLU:HG2	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1634)	1:131:A:HIS:H	1:129:A:ASP:HB3	1	0.25
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD1	10	0.25
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD2	10	0.25
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB1	6	0.25
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB2	6	0.25
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB3	6	0.25
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	3	0.25
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	3	0.25
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	3	0.25
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	6	0.25
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD21	5	0.25
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD22	5	0.25
(1,1372)	1:102:A:ASN:HD21	1:157:A:LEU:HD23	5	0.25
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG21	1	0.25
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG22	1	0.25
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG23	1	0.25
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG21	3	0.25
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG22	3	0.25
(1,1344)	1:97:A:VAL:H	1:165:A:VAL:HG23	3	0.25
(1,1327)	1:94:A:ARG:H	1:169:A:MET:HG2	6	0.25
(1,1210)	1:160:A:GLU:HB2	1:162:A:THR:HB	9	0.25
(1,1173)	1:157:A:LEU:HD11	1:163:A:LEU:HB3	9	0.25
(1,1173)	1:157:A:LEU:HD12	1:163:A:LEU:HB3	9	0.25
(1,1173)	1:157:A:LEU:HD13	1:163:A:LEU:HB3	9	0.25
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	3	0.25
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	3	0.25
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	3	0.25
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	10	0.25
(1,862)	1:141:A:LYS:HG3	1:142:A:TYR:HB3	1	0.25
(1,827)	1:139:A:THR:HA	1:140:A:ARG:HG2	1	0.25
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD1	7	0.25
(1,797)	1:134:A:ILE:HG21	1:133:A:TYR:HD2	7	0.25
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD1	7	0.25
(1,797)	1:134:A:ILE:HG22	1:133:A:TYR:HD2	7	0.25
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD1	7	0.25
(1,797)	1:134:A:ILE:HG23	1:133:A:TYR:HD2	7	0.25
(1,749)	1:128:A:GLN:HA	1:133:A:TYR:HE1	5	0.25
(1,749)	1:128:A:GLN:HA	1:133:A:TYR:HE2	5	0.25
(1,716)	1:126:A:GLU:HG2	1:127:A:ARG:HG2	2	0.25
(1,701)	1:125:A:GLU:HA	1:126:A:GLU:HG2	9	0.25
(1,699)	1:125:A:GLU:HA	1:125:A:GLU:HG2	6	0.25
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	5	0.25
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	5	0.25
(1,649)	1:120:A:ILE:HG21	1:140:A:ARG:HA	7	0.25
(1,649)	1:120:A:ILE:HG22	1:140:A:ARG:HA	7	0.25
(1,649)	1:120:A:ILE:HG23	1:140:A:ARG:HA	7	0.25
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	1	0.25
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	1	0.25
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	1	0.25
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	5	0.25
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	5	0.25
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	5	0.25
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	5	0.25
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	5	0.25
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	5	0.25
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	5	0.25
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	5	0.25
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	5	0.25
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	2	0.25
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	2	0.25
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	2	0.25
(1,434)	1:111:A:VAL:HG11	1:120:A:ILE:HG12	4	0.25
(1,434)	1:111:A:VAL:HG12	1:120:A:ILE:HG12	4	0.25
(1,434)	1:111:A:VAL:HG13	1:120:A:ILE:HG12	4	0.25
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	10	0.25
(1,405)	1:110:A:THR:HG21	1:112:A:LYS:HD3	10	0.25
(1,405)	1:110:A:THR:HG22	1:112:A:LYS:HD3	10	0.25
(1,405)	1:110:A:THR:HG23	1:112:A:LYS:HD3	10	0.25
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	7	0.25
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	7	0.25
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	7	0.25
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD11	1	0.25
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD12	1	0.25
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD13	1	0.25
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	6	0.25
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	6	0.25
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	6	0.25
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	4	0.25
(1,344)	1:108:A:GLU:HG2	1:123:A:LYS:HD3	1	0.25
(1,344)	1:108:A:GLU:HG2	1:123:A:LYS:HD2	3	0.25
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	1	0.25
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	1	0.25
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	7	0.25
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG21	2	0.25
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG22	2	0.25
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG23	2	0.25
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG21	2	0.25
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG22	2	0.25
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG23	2	0.25
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG21	2	0.25
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG22	2	0.25
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG23	2	0.25
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	2	0.25
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	10	0.25
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	10	0.25
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	10	0.25
(1,102)	1:96:A:ARG:HB3	1:166:A:GLU:HB3	5	0.25
(1,72)	1:95:A:TRP:HB2	1:168:A:PRO:HB3	8	0.25
(1,19)	1:93:A:ASP:HB2	1:94:A:ARG:HG2	7	0.25
(1,4262)	1:167:B:ALA:H	1:166:B:GLU:HB2	10	0.24
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD2	5	0.24
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG21	1	0.24
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG22	1	0.24
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG23	1	0.24
(1,4128)	1:155:B:SER:H	1:154:B:SER:HB2	3	0.24
(1,3925)	1:132:B:GLY:H	1:130:B:GLU:HG3	10	0.24
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG3	6	0.24
(1,3910)	1:129:B:ASP:H	1:133:B:TYR:HB2	1	0.24
(1,3904)	1:129:B:ASP:H	1:130:B:GLU:HG2	4	0.24
(1,3865)	1:125:B:GLU:H	1:126:B:GLU:H	4	0.24
(1,3865)	1:125:B:GLU:H	1:126:B:GLU:H	9	0.24
(1,3848)	1:123:B:LYS:H	1:109:B:LEU:HG	4	0.24
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	9	0.24
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	10	0.24
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	6	0.24
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG21	1	0.24
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG22	1	0.24
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG23	1	0.24
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	1	0.24
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD21	4	0.24
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD22	4	0.24
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD23	4	0.24
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	2	0.24
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	2	0.24
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	1	0.24
(1,3138)	1:141:B:LYS:HG2	1:143:B:THR:HA	4	0.24
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	6	0.24
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	3	0.24
(1,3004)	1:126:B:GLU:HG2	1:135:B:SER:HB2	8	0.24
(1,2991)	1:126:B:GLU:HA	1:135:B:SER:HB2	8	0.24
(1,2975)	1:123:B:LYS:HD2	1:137:B:CYS:HA	2	0.24
(1,2918)	1:120:B:ILE:HB	1:142:B:TYR:HE1	9	0.24
(1,2918)	1:120:B:ILE:HB	1:142:B:TYR:HE2	9	0.24
(1,2894)	1:119:B:GLU:HB3	1:121:B:THR:HB	8	0.24
(1,2738)	1:112:B:LYS:HB2	1:120:B:ILE:HA	10	0.24
(1,2686)	1:110:B:THR:HG21	1:112:B:LYS:HD3	5	0.24
(1,2686)	1:110:B:THR:HG22	1:112:B:LYS:HD3	5	0.24
(1,2686)	1:110:B:THR:HG23	1:112:B:LYS:HD3	5	0.24
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	6	0.24
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	6	0.24
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	6	0.24
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD11	9	0.24
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD12	9	0.24
(1,2645)	1:109:B:LEU:HG	1:120:B:ILE:HD13	9	0.24
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	6	0.24
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	6	0.24
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	6	0.24
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	10	0.24
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	10	0.24
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	10	0.24
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	3	0.24
(1,2617)	1:108:B:GLU:HA	1:108:B:GLU:HG2	4	0.24
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	2	0.24
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	2	0.24
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	2	0.24
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	5	0.24
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	5	0.24
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	5	0.24
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	7	0.24
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	7	0.24
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	7	0.24
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG21	5	0.24
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG22	5	0.24
(1,2364)	1:96:B:ARG:HA	1:97:B:VAL:HG23	5	0.24
(1,2322)	1:94:B:ARG:HB3	1:167:B:ALA:HA	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	1	0.24
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	1	0.24
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	1	0.24
(1,2215)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	5	0.24
(1,2215)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	9	0.24
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	5	0.24
(1,2192)	1:134:B:ILE:HA	1:140:A:ARG:HG3	3	0.24
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	1	0.24
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	1	0.24
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	1	0.24
(1,2083)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	5	0.24
(1,2083)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	9	0.24
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	5	0.24
(1,2060)	1:134:B:ILE:HA	1:140:A:ARG:HG3	3	0.24
(1,2007)	1:171:A:LYS:H	1:170:A:PRO:HD3	6	0.24
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	6	0.24
(1,1978)	1:167:A:ALA:H	1:96:A:ARG:HD3	1	0.24
(1,1884)	1:158:A:SER:H	1:158:A:SER:HB3	2	0.24
(1,1805)	1:152:A:GLN:HE21	1:170:A:PRO:HD3	8	0.24
(1,1796)	1:152:A:GLN:HE21	1:149:A:ASP:HB2	4	0.24
(1,1796)	1:152:A:GLN:HE21	1:149:A:ASP:HB2	8	0.24
(1,1657)	1:134:A:ILE:H	1:133:A:TYR:HB3	4	0.24
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD1	2	0.24
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD2	2	0.24
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	2	0.24
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	4	0.24
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD21	6	0.24
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD21	9	0.24
(1,1280)	1:168:A:PRO:HB2	1:170:A:PRO:HD3	7	0.24
(1,1211)	1:160:A:GLU:HG2	1:162:A:THR:HB	2	0.24
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	5	0.24
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD21	1	0.24
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD22	1	0.24
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD23	1	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD21	1	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD22	1	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD23	1	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD21	6	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD22	6	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD23	6	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD21	8	0.24
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD22	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:155:A:SER:HB3	1:157:A:LEU:HD23	8	0.24
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	8	0.24
(1,1065)	1:152:A:GLN:HB2	1:169:A:MET:HA	8	0.24
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	2	0.24
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	2	0.24
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	2	0.24
(1,862)	1:141:A:LYS:HG3	1:142:A:TYR:HB3	9	0.24
(1,858)	1:141:A:LYS:HG3	1:141:A:LYS:HE2	5	0.24
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE1	5	0.24
(1,754)	1:128:A:GLN:HB2	1:133:A:TYR:HE2	5	0.24
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	7	0.24
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	7	0.24
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	7	0.24
(1,654)	1:120:A:ILE:HD11	1:140:A:ARG:HD2	7	0.24
(1,654)	1:120:A:ILE:HD12	1:140:A:ARG:HD2	7	0.24
(1,654)	1:120:A:ILE:HD13	1:140:A:ARG:HD2	7	0.24
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG21	8	0.24
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG22	8	0.24
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG23	8	0.24
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG21	10	0.24
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG22	10	0.24
(1,638)	1:120:A:ILE:HG12	1:120:A:ILE:HG23	10	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	2	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	2	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	2	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	2	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	2	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	2	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	2	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	2	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	2	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	8	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	8	0.24
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	8	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	8	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	8	0.24
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	8	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	8	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	8	0.24
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	8	0.24
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	1	0.24
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	1	0.24
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	1	0.24
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	1	0.24
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	1	0.24
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	8	0.24
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	8	0.24
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	8	0.24
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	8	0.24
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	8	0.24
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	8	0.24
(1,528)	1:116:A:GLY:HA2	1:148:A:VAL:HB	8	0.24
(1,373)	1:109:A:LEU:HD11	1:161:A:GLY:HA3	6	0.24
(1,373)	1:109:A:LEU:HD12	1:161:A:GLY:HA3	6	0.24
(1,373)	1:109:A:LEU:HD13	1:161:A:GLY:HA3	6	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	1	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	1	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	1	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	2	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	2	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	2	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	7	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	7	0.24
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	7	0.24
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD2	5	0.24
(1,272)	1:101:A:VAL:HG21	1:120:A:ILE:HD11	10	0.24
(1,272)	1:101:A:VAL:HG21	1:120:A:ILE:HD12	10	0.24
(1,272)	1:101:A:VAL:HG21	1:120:A:ILE:HD13	10	0.24
(1,272)	1:101:A:VAL:HG22	1:120:A:ILE:HD11	10	0.24
(1,272)	1:101:A:VAL:HG22	1:120:A:ILE:HD12	10	0.24
(1,272)	1:101:A:VAL:HG22	1:120:A:ILE:HD13	10	0.24
(1,272)	1:101:A:VAL:HG23	1:120:A:ILE:HD11	10	0.24
(1,272)	1:101:A:VAL:HG23	1:120:A:ILE:HD12	10	0.24
(1,272)	1:101:A:VAL:HG23	1:120:A:ILE:HD13	10	0.24
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	4	0.24
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	4	0.24
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	4	0.24
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	5	0.24
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	5	0.24
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	5	0.24
(1,247)	1:99:A:LEU:HD21	1:140:A:ARG:HG3	4	0.24
(1,247)	1:99:A:LEU:HD22	1:140:A:ARG:HG3	4	0.24
(1,247)	1:99:A:LEU:HD23	1:140:A:ARG:HG3	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	5	0.24
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	5	0.24
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	5	0.24
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	6	0.24
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	6	0.24
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	6	0.24
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	8	0.24
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	8	0.24
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	8	0.24
(1,80)	1:96:A:ARG:HA	1:96:A:ARG:HD3	6	0.24
(1,79)	1:96:A:ARG:HA	1:96:A:ARG:HG3	3	0.24
(1,51)	1:95:A:TRP:HA	1:95:A:TRP:HB2	10	0.24
(1,20)	1:93:A:ASP:HB3	1:94:A:ARG:HA	5	0.24
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG21	2	0.23
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG22	2	0.23
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG23	2	0.23
(1,4196)	1:162:B:THR:H	1:102:B:ASN:HB2	7	0.23
(1,4191)	1:161:B:GLY:H	1:160:B:GLU:HG3	1	0.23
(1,4052)	1:151:B:THR:H	1:149:B:ASP:HB3	1	0.23
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG11	9	0.23
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG12	9	0.23
(1,4011)	1:144:B:LEU:H	1:148:B:VAL:HG13	9	0.23
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD11	1	0.23
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD12	1	0.23
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD13	1	0.23
(1,3902)	1:129:B:ASP:H	1:129:B:ASP:HB2	9	0.23
(1,3893)	1:128:B:GLN:HE22	1:129:B:ASP:H	6	0.23
(1,3848)	1:123:B:LYS:H	1:109:B:LEU:HG	7	0.23
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	10	0.23
(1,3763)	1:114:B:LYS:H	1:115:B:ASP:HB2	5	0.23
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	10	0.23
(1,3664)	1:102:B:ASN:HD22	1:161:B:GLY:HA3	3	0.23
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD11	4	0.23
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD12	4	0.23
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD13	4	0.23
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD11	5	0.23
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD12	5	0.23
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD13	5	0.23
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	1	0.23
(1,3557)	1:168:B:PRO:HA	1:169:B:MET:HG2	3	0.23
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG21	9	0.23
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG22	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3500)	1:162:B:THR:HA	1:162:B:THR:HG23	9	0.23
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD21	6	0.23
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD22	6	0.23
(1,3499)	1:161:B:GLY:HA3	1:163:B:LEU:HD23	6	0.23
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	3	0.23
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	9	0.23
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	5	0.23
(1,3366)	1:153:B:VAL:HG11	1:155:B:SER:HB3	5	0.23
(1,3366)	1:153:B:VAL:HG12	1:155:B:SER:HB3	5	0.23
(1,3366)	1:153:B:VAL:HG13	1:155:B:SER:HB3	5	0.23
(1,3366)	1:153:B:VAL:HG11	1:155:B:SER:HB3	6	0.23
(1,3366)	1:153:B:VAL:HG12	1:155:B:SER:HB3	6	0.23
(1,3366)	1:153:B:VAL:HG13	1:155:B:SER:HB3	6	0.23
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	4	0.23
(1,3295)	1:148:B:VAL:HG11	1:170:B:PRO:HG3	7	0.23
(1,3295)	1:148:B:VAL:HG12	1:170:B:PRO:HG3	7	0.23
(1,3295)	1:148:B:VAL:HG13	1:170:B:PRO:HG3	7	0.23
(1,3252)	1:146:B:PRO:HG2	1:147:B:GLY:HA2	1	0.23
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	7	0.23
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	7	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	1	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	1	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	1	0.23
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	1	0.23
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	1	0.23
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	1	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	1	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	1	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	1	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	4	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	4	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	4	0.23
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	4	0.23
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	4	0.23
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	4	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	4	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	4	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	4	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	6	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	6	0.23
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	6	0.23
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	6	0.23
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	6	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	6	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	6	0.23
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	6	0.23
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	4	0.23
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	4	0.23
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	4	0.23
(1,3139)	1:141:B:LYS:HG3	1:141:B:LYS:HE2	3	0.23
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	4	0.23
(1,3116)	1:139:B:THR:HG21	1:141:B:LYS:HE2	2	0.23
(1,3116)	1:139:B:THR:HG22	1:141:B:LYS:HE2	2	0.23
(1,3116)	1:139:B:THR:HG23	1:141:B:LYS:HE2	2	0.23
(1,3003)	1:126:B:GLU:HG2	1:135:B:SER:HA	10	0.23
(1,2982)	1:125:B:GLU:HA	1:126:B:GLU:HG2	4	0.23
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	3	0.23
(1,2930)	1:120:B:ILE:HG21	1:140:B:ARG:HA	2	0.23
(1,2930)	1:120:B:ILE:HG22	1:140:B:ARG:HA	2	0.23
(1,2930)	1:120:B:ILE:HG23	1:140:B:ARG:HA	2	0.23
(1,2929)	1:120:B:ILE:HG21	1:139:B:THR:HA	8	0.23
(1,2929)	1:120:B:ILE:HG22	1:139:B:THR:HA	8	0.23
(1,2929)	1:120:B:ILE:HG23	1:139:B:THR:HA	8	0.23
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	8	0.23
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	8	0.23
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	8	0.23
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG11	7	0.23
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG12	7	0.23
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG13	7	0.23
(1,2776)	1:113:B:THR:HG21	1:116:B:GLY:HA3	2	0.23
(1,2776)	1:113:B:THR:HG22	1:116:B:GLY:HA3	2	0.23
(1,2776)	1:113:B:THR:HG23	1:116:B:GLY:HA3	2	0.23
(1,2749)	1:112:B:LYS:HG2	1:121:B:THR:HB	8	0.23
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	5	0.23
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	5	0.23
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	5	0.23
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	6	0.23
(1,2627)	1:108:B:GLU:HG3	1:123:B:LYS:HG3	3	0.23
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	3	0.23
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	6	0.23
(1,2560)	1:102:B:ASN:HB3	1:161:B:GLY:HA2	10	0.23
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD21	9	0.23
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD22	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD23	9	0.23
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	8	0.23
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	8	0.23
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	8	0.23
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	8	0.23
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	8	0.23
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	8	0.23
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	8	0.23
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	8	0.23
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	8	0.23
(1,2484)	1:99:B:LEU:HA	1:100:B:ASP:HB3	10	0.23
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	5	0.23
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	8	0.23
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	8	0.23
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	8	0.23
(1,2352)	1:95:B:TRP:HB3	1:168:B:PRO:HB2	8	0.23
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	8	0.23
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	8	0.23
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	8	0.23
(1,2332)	1:95:B:TRP:HA	1:95:B:TRP:HB2	1	0.23
(1,2310)	1:94:B:ARG:HA	1:168:B:PRO:HA	7	0.23
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	10	0.23
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	10	0.23
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	10	0.23
(1,2215)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	8	0.23
(1,2198)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	3	0.23
(1,2198)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	3	0.23
(1,2198)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	3	0.23
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	10	0.23
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	10	0.23
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	10	0.23
(1,2083)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	8	0.23
(1,2066)	1:134:B:ILE:HG21	1:138:A:PHE:HB3	3	0.23
(1,2066)	1:134:B:ILE:HG22	1:138:A:PHE:HB3	3	0.23
(1,2066)	1:134:B:ILE:HG23	1:138:A:PHE:HB3	3	0.23
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	1	0.23
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	3	0.23
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	1	0.23
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	5	0.23
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	5	0.23
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	5	0.23
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD21	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD22	1	0.23
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD23	1	0.23
(1,1675)	1:137:A:CYS:H	1:136:A:ARG:HG2	4	0.23
(1,1655)	1:134:A:ILE:H	1:127:A:ARG:HG2	7	0.23
(1,1650)	1:132:A:GLY:H	1:133:A:TYR:HD1	4	0.23
(1,1650)	1:132:A:GLY:H	1:133:A:TYR:HD2	4	0.23
(1,1643)	1:132:A:GLY:H	1:130:A:GLU:HB2	8	0.23
(1,1626)	1:129:A:ASP:H	1:132:A:GLY:HA3	2	0.23
(1,1621)	1:129:A:ASP:H	1:129:A:ASP:HB2	2	0.23
(1,1621)	1:129:A:ASP:H	1:129:A:ASP:HB2	5	0.23
(1,1580)	1:125:A:GLU:H	1:108:A:GLU:HG2	5	0.23
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	10	0.23
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	8	0.23
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	8	0.23
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	8	0.23
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	5	0.23
(1,1383)	1:102:A:ASN:HD22	1:161:A:GLY:HA3	2	0.23
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD21	4	0.23
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD22	4	0.23
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD23	4	0.23
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD21	7	0.23
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD22	7	0.23
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD23	7	0.23
(1,1321)	1:94:A:ARG:H	1:93:A:ASP:HA	1	0.23
(1,1318)	1:171:A:LYS:HA	1:171:A:LYS:HD2	5	0.23
(1,1314)	1:170:A:PRO:HB3	1:170:A:PRO:HD2	7	0.23
(1,1289)	1:169:A:MET:HA	1:169:A:MET:HG3	8	0.23
(1,1193)	1:158:A:SER:HB3	1:160:A:GLU:HB3	10	0.23
(1,1173)	1:157:A:LEU:HD11	1:163:A:LEU:HB3	5	0.23
(1,1173)	1:157:A:LEU:HD12	1:163:A:LEU:HB3	5	0.23
(1,1173)	1:157:A:LEU:HD13	1:163:A:LEU:HB3	5	0.23
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	2	0.23
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	2	0.23
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	6	0.23
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	2	0.23
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG21	1	0.23
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG22	1	0.23
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG23	1	0.23
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG21	1	0.23
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG22	1	0.23
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG23	1	0.23
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:139:A:THR:HA	1:140:A:ARG:HG2	2	0.23
(1,773)	1:130:A:GLU:HA	1:130:A:GLU:HG3	9	0.23
(1,756)	1:128:A:GLN:HB3	1:133:A:TYR:HD1	1	0.23
(1,756)	1:128:A:GLN:HB3	1:133:A:TYR:HD2	1	0.23
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	9	0.23
(1,737)	1:127:A:ARG:HA	1:127:A:ARG:HD3	2	0.23
(1,664)	1:121:A:THR:HA	1:139:A:THR:HA	6	0.23
(1,648)	1:120:A:ILE:HG21	1:139:A:THR:HA	5	0.23
(1,648)	1:120:A:ILE:HG22	1:139:A:THR:HA	5	0.23
(1,648)	1:120:A:ILE:HG23	1:139:A:THR:HA	5	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	1	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	1	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	1	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	1	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	1	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	1	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	1	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	1	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	1	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	4	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	4	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	4	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	4	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	4	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	4	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	4	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	4	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	4	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	6	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	6	0.23
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	6	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	6	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	6	0.23
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	6	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	6	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	6	0.23
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	6	0.23
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	10	0.23
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	10	0.23
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	10	0.23
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	3	0.23
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	3	0.23
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	1	0.23
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	10	0.23
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	5	0.23
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	5	0.23
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	5	0.23
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	7	0.23
(1,338)	1:108:A:GLU:HA	1:123:A:LYS:HD2	10	0.23
(1,336)	1:108:A:GLU:HA	1:108:A:GLU:HG2	8	0.23
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	2	0.23
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	2	0.23
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	2	0.23
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	2	0.23
(1,255)	1:99:A:LEU:HD21	1:109:A:LEU:HG	9	0.23
(1,255)	1:99:A:LEU:HD22	1:109:A:LEU:HG	9	0.23
(1,255)	1:99:A:LEU:HD23	1:109:A:LEU:HG	9	0.23
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	3	0.23
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	3	0.23
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	3	0.23
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD21	6	0.23
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD22	6	0.23
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD23	6	0.23
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	1	0.23
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	1	0.23
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	1	0.23
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	6	0.23
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	6	0.23
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	6	0.23
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG21	9	0.23
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG22	9	0.23
(1,83)	1:96:A:ARG:HA	1:97:A:VAL:HG23	9	0.23
(1,80)	1:96:A:ARG:HA	1:96:A:ARG:HD2	2	0.23
(1,72)	1:95:A:TRP:HB3	1:168:A:PRO:HB3	9	0.23
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	6	0.23
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG21	8	0.22
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG22	8	0.22
(1,4273)	1:169:B:MET:H	1:148:B:VAL:HG23	8	0.22
(1,4263)	1:167:B:ALA:H	1:166:B:GLU:HB3	5	0.22
(1,4259)	1:167:B:ALA:H	1:96:B:ARG:HD2	3	0.22
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	5	0.22
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	4	0.22
(1,4052)	1:151:B:THR:H	1:149:B:ASP:HB3	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	1	0.22
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	1	0.22
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	1	0.22
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	2	0.22
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	2	0.22
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	2	0.22
(1,3955)	1:137:B:CYS:H	1:136:B:ARG:HB3	1	0.22
(1,3955)	1:137:B:CYS:H	1:136:B:ARG:HB3	6	0.22
(1,3908)	1:129:B:ASP:H	1:132:B:GLY:H	8	0.22
(1,3861)	1:125:B:GLU:H	1:108:B:GLU:HG2	1	0.22
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	5	0.22
(1,3795)	1:118:B:VAL:H	1:119:B:GLU:HG3	1	0.22
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	1	0.22
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	7	0.22
(1,3759)	1:114:B:LYS:H	1:112:B:LYS:HD3	8	0.22
(1,3680)	1:107:B:ASP:H	1:106:B:PRO:HB2	7	0.22
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD11	6	0.22
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD12	6	0.22
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD13	6	0.22
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG21	2	0.22
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG22	2	0.22
(1,3625)	1:97:B:VAL:H	1:165:B:VAL:HG23	2	0.22
(1,3604)	1:94:B:ARG:H	1:93:B:ASP:HB3	10	0.22
(1,3595)	1:170:B:PRO:HB3	1:170:B:PRO:HD2	4	0.22
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	8	0.22
(1,3473)	1:158:B:SER:HB2	1:162:B:THR:HB	3	0.22
(1,3436)	1:157:B:LEU:HB2	1:163:B:LEU:HA	6	0.22
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	6	0.22
(1,3319)	1:150:B:PRO:HB2	1:150:B:PRO:HD2	9	0.22
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	2	0.22
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	10	0.22
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	6	0.22
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	6	0.22
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	6	0.22
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	1	0.22
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	1	0.22
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	1	0.22
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	6	0.22
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	6	0.22
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	6	0.22
(1,3139)	1:141:B:LYS:HG3	1:141:B:LYS:HE2	4	0.22
(1,3137)	1:141:B:LYS:HG2	1:142:B:TYR:HB3	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	2	0.22
(1,3028)	1:128:B:GLN:HA	1:133:B:TYR:HB2	7	0.22
(1,3005)	1:126:B:GLU:HG2	1:135:B:SER:HB3	5	0.22
(1,2986)	1:126:B:GLU:HA	1:126:B:GLU:HG3	8	0.22
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	4	0.22
(1,2965)	1:123:B:LYS:HA	1:135:B:SER:HB3	1	0.22
(1,2945)	1:121:B:THR:HA	1:139:B:THR:HA	2	0.22
(1,2929)	1:120:B:ILE:HG21	1:139:B:THR:HA	9	0.22
(1,2929)	1:120:B:ILE:HG22	1:139:B:THR:HA	9	0.22
(1,2929)	1:120:B:ILE:HG23	1:139:B:THR:HA	9	0.22
(1,2924)	1:120:B:ILE:HG13	1:163:B:LEU:HD11	3	0.22
(1,2924)	1:120:B:ILE:HG13	1:163:B:LEU:HD12	3	0.22
(1,2924)	1:120:B:ILE:HG13	1:163:B:LEU:HD13	3	0.22
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG21	4	0.22
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG22	4	0.22
(1,2922)	1:120:B:ILE:HG13	1:120:B:ILE:HG23	4	0.22
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	5	0.22
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	5	0.22
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	5	0.22
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	5	0.22
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	5	0.22
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	5	0.22
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	5	0.22
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	5	0.22
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	5	0.22
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	9	0.22
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	9	0.22
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	9	0.22
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	9	0.22
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	9	0.22
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	9	0.22
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	9	0.22
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	9	0.22
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	9	0.22
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	5	0.22
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	5	0.22
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	5	0.22
(1,2790)	1:114:B:LYS:HA	1:114:B:LYS:HB2	6	0.22
(1,2783)	1:113:B:THR:HG21	1:150:B:PRO:HB3	5	0.22
(1,2783)	1:113:B:THR:HG22	1:150:B:PRO:HB3	5	0.22
(1,2783)	1:113:B:THR:HG23	1:150:B:PRO:HB3	5	0.22
(1,2783)	1:113:B:THR:HG21	1:150:B:PRO:HB3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2783)	1:113:B:THR:HG22	1:150:B:PRO:HB3	6	0.22
(1,2783)	1:113:B:THR:HG23	1:150:B:PRO:HB3	6	0.22
(1,2747)	1:112:B:LYS:HG3	1:119:B:GLU:HA	10	0.22
(1,2736)	1:112:B:LYS:HB2	1:112:B:LYS:HE3	1	0.22
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE3	8	0.22
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG21	5	0.22
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG22	5	0.22
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG23	5	0.22
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG21	5	0.22
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG22	5	0.22
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG23	5	0.22
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG21	5	0.22
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG22	5	0.22
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG23	5	0.22
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG21	6	0.22
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG22	6	0.22
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG23	6	0.22
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG21	6	0.22
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG22	6	0.22
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG23	6	0.22
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG21	6	0.22
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG22	6	0.22
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG23	6	0.22
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	2	0.22
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	2	0.22
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	2	0.22
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	10	0.22
(1,2578)	1:105:B:ALA:HB1	1:107:B:ASP:HB3	6	0.22
(1,2578)	1:105:B:ALA:HB2	1:107:B:ASP:HB3	6	0.22
(1,2578)	1:105:B:ALA:HB3	1:107:B:ASP:HB3	6	0.22
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	2	0.22
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	2	0.22
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	2	0.22
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	2	0.22
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	2	0.22
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	2	0.22
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	2	0.22
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	2	0.22
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	2	0.22
(1,2447)	1:97:B:VAL:HG21	1:118:B:VAL:HB	4	0.22
(1,2447)	1:97:B:VAL:HG22	1:118:B:VAL:HB	4	0.22
(1,2447)	1:97:B:VAL:HG23	1:118:B:VAL:HB	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD1	10	0.22
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD2	10	0.22
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD1	10	0.22
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD2	10	0.22
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD1	10	0.22
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD2	10	0.22
(1,2282)	1:88:B:ILE:HG21	1:90:B:HIS:HA	8	0.22
(1,2282)	1:88:B:ILE:HG22	1:90:B:HIS:HA	8	0.22
(1,2282)	1:88:B:ILE:HG23	1:90:B:HIS:HA	8	0.22
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	9	0.22
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	9	0.22
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	9	0.22
(1,2169)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	8	0.22
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	9	0.22
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	9	0.22
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	9	0.22
(1,2037)	1:132:A:GLY:HA3	1:140:B:ARG:HB3	8	0.22
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	6	0.22
(1,1902)	1:161:A:GLY:H	1:102:A:ASN:HB3	3	0.22
(1,1844)	1:154:A:SER:H	1:168:A:PRO:HD2	7	0.22
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	2	0.22
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	2	0.22
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	2	0.22
(1,1703)	1:142:A:TYR:H	1:141:A:LYS:HG3	2	0.22
(1,1615)	1:128:A:GLN:HE21	1:128:A:GLN:HB3	7	0.22
(1,1602)	1:128:A:GLN:H	1:128:A:GLN:HB3	7	0.22
(1,1598)	1:128:A:GLN:H	1:127:A:ARG:HG2	1	0.22
(1,1581)	1:125:A:GLU:H	1:108:A:GLU:HG3	8	0.22
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	8	0.22
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	9	0.22
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	4	0.22
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	1	0.22
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	6	0.22
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	9	0.22
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD11	7	0.22
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD12	7	0.22
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD13	7	0.22
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD22	4	0.22
(1,1327)	1:94:A:ARG:H	1:169:A:MET:HG2	9	0.22
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD21	7	0.22
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD22	7	0.22
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD23	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	8	0.22
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	7	0.22
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	7	0.22
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	7	0.22
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	10	0.22
(1,1114)	1:155:A:SER:HB2	1:163:A:LEU:HA	8	0.22
(1,1097)	1:154:A:SER:HB3	1:155:A:SER:HA	10	0.22
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	9	0.22
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	2	0.22
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	5	0.22
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	8	0.22
(1,1014)	1:148:A:VAL:HG11	1:170:A:PRO:HG3	9	0.22
(1,1014)	1:148:A:VAL:HG12	1:170:A:PRO:HG3	9	0.22
(1,1014)	1:148:A:VAL:HG13	1:170:A:PRO:HG3	9	0.22
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	1	0.22
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	1	0.22
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	1	0.22
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	3	0.22
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	3	0.22
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	3	0.22
(1,744)	1:127:A:ARG:HB3	1:127:A:ARG:HD3	4	0.22
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	4	0.22
(1,717)	1:126:A:GLU:HG2	1:127:A:ARG:HG3	5	0.22
(1,700)	1:125:A:GLU:HA	1:125:A:GLU:HG3	8	0.22
(1,655)	1:120:A:ILE:HD11	1:140:A:ARG:HD3	6	0.22
(1,655)	1:120:A:ILE:HD12	1:140:A:ARG:HD3	6	0.22
(1,655)	1:120:A:ILE:HD13	1:140:A:ARG:HD3	6	0.22
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	1	0.22
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	1	0.22
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	1	0.22
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	2	0.22
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	2	0.22
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	2	0.22
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	2	0.22
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	2	0.22
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	2	0.22
(1,558)	1:117:A:VAL:HG11	1:141:A:LYS:HE2	6	0.22
(1,558)	1:117:A:VAL:HG12	1:141:A:LYS:HE2	6	0.22
(1,558)	1:117:A:VAL:HG13	1:141:A:LYS:HE2	6	0.22
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	5	0.22
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	5	0.22
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:113:A:THR:HG21	1:150:A:PRO:HB3	3	0.22
(1,502)	1:113:A:THR:HG22	1:150:A:PRO:HB3	3	0.22
(1,502)	1:113:A:THR:HG23	1:150:A:PRO:HB3	3	0.22
(1,494)	1:113:A:THR:HG21	1:116:A:GLY:HA2	5	0.22
(1,494)	1:113:A:THR:HG22	1:116:A:GLY:HA2	5	0.22
(1,494)	1:113:A:THR:HG23	1:116:A:GLY:HA2	5	0.22
(1,457)	1:112:A:LYS:HB2	1:120:A:ILE:HA	8	0.22
(1,457)	1:112:A:LYS:HB2	1:120:A:ILE:HA	9	0.22
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	8	0.22
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	3	0.22
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	4	0.22
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	4	0.22
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	4	0.22
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	8	0.22
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	8	0.22
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	8	0.22
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	2	0.22
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	3	0.22
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	7	0.22
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	7	0.22
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	7	0.22
(1,279)	1:102:A:ASN:HB3	1:161:A:GLY:HA2	7	0.22
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	3	0.22
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	3	0.22
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	3	0.22
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	9	0.22
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	9	0.22
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	9	0.22
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	9	0.22
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	9	0.22
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	9	0.22
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	9	0.22
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	9	0.22
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	9	0.22
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	3	0.22
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	3	0.22
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	3	0.22
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	4	0.22
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	4	0.22
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	4	0.22
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG21	2	0.22
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG22	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG23	2	0.22
(1,72)	1:95:A:TRP:HB3	1:168:A:PRO:HB3	2	0.22
(1,72)	1:95:A:TRP:HB2	1:168:A:PRO:HB3	3	0.22
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	10	0.22
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	10	0.22
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	10	0.22
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG11	6	0.22
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG12	6	0.22
(1,62)	1:95:A:TRP:HB2	1:148:A:VAL:HG13	6	0.22
(1,61)	1:95:A:TRP:HB2	1:96:A:ARG:HA	4	0.22
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG3	5	0.21
(1,4182)	1:161:B:GLY:H	1:102:B:ASN:HB2	6	0.21
(1,4128)	1:155:B:SER:H	1:154:B:SER:HB2	8	0.21
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	9	0.21
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	9	0.21
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	9	0.21
(1,4034)	1:148:B:VAL:H	1:149:B:ASP:H	5	0.21
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	7	0.21
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	7	0.21
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	7	0.21
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD21	7	0.21
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD22	7	0.21
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD23	7	0.21
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	8	0.21
(1,3861)	1:125:B:GLU:H	1:108:B:GLU:HG2	2	0.21
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	9	0.21
(1,3795)	1:118:B:VAL:H	1:119:B:GLU:HG3	10	0.21
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD21	4	0.21
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD22	4	0.21
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD23	4	0.21
(1,3664)	1:102:B:ASN:HD22	1:161:B:GLY:HA3	8	0.21
(1,3663)	1:102:B:ASN:HD22	1:161:B:GLY:HA2	5	0.21
(1,3654)	1:102:B:ASN:HD21	1:161:B:GLY:HA2	3	0.21
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG21	3	0.21
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG22	3	0.21
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG23	3	0.21
(1,3599)	1:171:B:LYS:HA	1:171:B:LYS:HD2	8	0.21
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	9	0.21
(1,3481)	1:159:B:PRO:HA	1:159:B:PRO:HG3	7	0.21
(1,3458)	1:157:B:LEU:HD21	1:161:B:GLY:HA3	8	0.21
(1,3458)	1:157:B:LEU:HD22	1:161:B:GLY:HA3	8	0.21
(1,3458)	1:157:B:LEU:HD23	1:161:B:GLY:HA3	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	10	0.21
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	10	0.21
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	10	0.21
(1,3430)	1:157:B:LEU:HA	1:163:B:LEU:HB3	9	0.21
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	8	0.21
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD21	1	0.21
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD22	1	0.21
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD23	1	0.21
(1,3409)	1:155:B:SER:HB2	1:157:B:LEU:HB3	9	0.21
(1,3358)	1:153:B:VAL:HA	1:168:B:PRO:HD2	10	0.21
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG21	3	0.21
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG22	3	0.21
(1,3327)	1:150:B:PRO:HD2	1:151:B:THR:HG23	3	0.21
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	5	0.21
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	7	0.21
(1,3288)	1:148:B:VAL:HG11	1:153:B:VAL:HA	2	0.21
(1,3288)	1:148:B:VAL:HG12	1:153:B:VAL:HA	2	0.21
(1,3288)	1:148:B:VAL:HG13	1:153:B:VAL:HA	2	0.21
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	6	0.21
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	6	0.21
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	6	0.21
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	2	0.21
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	2	0.21
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	2	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	2	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	2	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	2	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	2	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	2	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	2	0.21
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	5	0.21
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	5	0.21
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	5	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	5	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	5	0.21
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	5	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	5	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	5	0.21
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	5	0.21
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	7	0.21
(1,3108)	1:139:B:THR:HA	1:140:B:ARG:HG2	9	0.21
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE1	2	0.21
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE2	2	0.21
(1,3015)	1:127:B:ARG:HA	1:127:B:ARG:HB3	7	0.21
(1,3010)	1:126:B:GLU:HG3	1:133:B:TYR:HB3	7	0.21
(1,2999)	1:126:B:GLU:HG2	1:133:B:TYR:HB3	1	0.21
(1,2984)	1:125:B:GLU:HA	1:135:B:SER:HB2	1	0.21
(1,2981)	1:125:B:GLU:HA	1:125:B:GLU:HG3	2	0.21
(1,2973)	1:123:B:LYS:HG3	1:137:B:CYS:HB2	10	0.21
(1,2945)	1:121:B:THR:HA	1:139:B:THR:HA	3	0.21
(1,2928)	1:120:B:ILE:HG21	1:122:B:GLY:HA3	9	0.21
(1,2928)	1:120:B:ILE:HG22	1:122:B:GLY:HA3	9	0.21
(1,2928)	1:120:B:ILE:HG23	1:122:B:GLY:HA3	9	0.21
(1,2894)	1:119:B:GLU:HB3	1:121:B:THR:HB	9	0.21
(1,2894)	1:119:B:GLU:HB3	1:121:B:THR:HB	10	0.21
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG11	3	0.21
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG12	3	0.21
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG13	3	0.21
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG21	9	0.21
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG22	9	0.21
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG23	9	0.21
(1,2738)	1:112:B:LYS:HB2	1:120:B:ILE:HA	9	0.21
(1,2687)	1:110:B:THR:HG21	1:112:B:LYS:HE3	2	0.21
(1,2687)	1:110:B:THR:HG22	1:112:B:LYS:HE3	2	0.21
(1,2687)	1:110:B:THR:HG23	1:112:B:LYS:HE3	2	0.21
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	2	0.21
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	2	0.21
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	2	0.21
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	2	0.21
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	2	0.21
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	2	0.21
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	2	0.21
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	2	0.21
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	2	0.21
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	4	0.21
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	4	0.21
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	4	0.21
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	8	0.21
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	8	0.21
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	8	0.21
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	2	0.21
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	8	0.21
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	8	0.21
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	8	0.21
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	8	0.21
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	2	0.21
(1,2560)	1:102:B:ASN:HB3	1:161:B:GLY:HA2	8	0.21
(1,2559)	1:102:B:ASN:HB2	1:161:B:GLY:HA3	5	0.21
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD21	3	0.21
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD22	3	0.21
(1,2558)	1:102:B:ASN:HB2	1:157:B:LEU:HD23	3	0.21
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD11	8	0.21
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD12	8	0.21
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD13	8	0.21
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	6	0.21
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	8	0.21
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	9	0.21
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	6	0.21
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	6	0.21
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	6	0.21
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG21	2	0.21
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG22	2	0.21
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG23	2	0.21
(1,2341)	1:95:B:TRP:HB2	1:95:B:TRP:HE3	10	0.21
(1,2306)	1:94:B:ARG:HA	1:94:B:ARG:HG3	7	0.21
(1,2215)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	1	0.21
(1,2212)	1:134:A:ILE:HA	1:140:B:ARG:HD2	3	0.21
(1,2150)	1:97:B:VAL:HG11	1:131:A:HIS:HB3	6	0.21
(1,2150)	1:97:B:VAL:HG12	1:131:A:HIS:HB3	6	0.21
(1,2150)	1:97:B:VAL:HG13	1:131:A:HIS:HB3	6	0.21
(1,2083)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	1	0.21
(1,2080)	1:134:A:ILE:HA	1:140:B:ARG:HD2	3	0.21
(1,2018)	1:97:B:VAL:HG11	1:131:A:HIS:HB3	6	0.21
(1,2018)	1:97:B:VAL:HG12	1:131:A:HIS:HB3	6	0.21
(1,2018)	1:97:B:VAL:HG13	1:131:A:HIS:HB3	6	0.21
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	2	0.21
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG11	2	0.21
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG12	2	0.21
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG13	2	0.21
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG21	1	0.21
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG22	1	0.21
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG23	1	0.21
(1,1816)	1:153:A:VAL:H	1:149:A:ASP:HB2	2	0.21
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	4	0.21
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	3	0.21
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	3	0.21
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	3	0.21
(1,1653)	1:132:A:GLY:H	1:134:A:ILE:HG21	6	0.21
(1,1653)	1:132:A:GLY:H	1:134:A:ILE:HG22	6	0.21
(1,1653)	1:132:A:GLY:H	1:134:A:ILE:HG23	6	0.21
(1,1647)	1:132:A:GLY:H	1:131:A:HIS:HB3	6	0.21
(1,1647)	1:132:A:GLY:H	1:131:A:HIS:HB3	9	0.21
(1,1626)	1:129:A:ASP:H	1:132:A:GLY:HA3	8	0.21
(1,1621)	1:129:A:ASP:H	1:129:A:ASP:HB2	4	0.21
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	3	0.21
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	4	0.21
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	8	0.21
(1,1611)	1:128:A:GLN:HE22	1:128:A:GLN:H	6	0.21
(1,1580)	1:125:A:GLU:H	1:108:A:GLU:HG2	1	0.21
(1,1545)	1:120:A:ILE:H	1:140:A:ARG:HG3	9	0.21
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD11	5	0.21
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD12	5	0.21
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD13	5	0.21
(1,1517)	1:118:A:VAL:H	1:142:A:TYR:HB2	6	0.21
(1,1514)	1:118:A:VAL:H	1:119:A:GLU:HG3	5	0.21
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	2	0.21
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	3	0.21
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	4	0.21
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	7	0.21
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD21	2	0.21
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD22	2	0.21
(1,1381)	1:102:A:ASN:HD22	1:157:A:LEU:HD23	2	0.21
(1,1369)	1:102:A:ASN:HD21	1:109:A:LEU:HD11	3	0.21
(1,1369)	1:102:A:ASN:HD21	1:109:A:LEU:HD12	3	0.21
(1,1369)	1:102:A:ASN:HD21	1:109:A:LEU:HD13	3	0.21
(1,1326)	1:94:A:ARG:H	1:168:A:PRO:HA	5	0.21
(1,1314)	1:170:A:PRO:HB3	1:170:A:PRO:HD3	9	0.21
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD21	1	0.21
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD22	1	0.21
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD23	1	0.21
(1,1210)	1:160:A:GLU:HB2	1:162:A:THR:HB	8	0.21
(1,1193)	1:158:A:SER:HB3	1:160:A:GLU:HB3	3	0.21
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	4	0.21
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	7	0.21
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:150:A:PRO:HB2	1:150:A:PRO:HD2	7	0.21
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	1	0.21
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	9	0.21
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	7	0.21
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	7	0.21
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	7	0.21
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	4	0.21
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	8	0.21
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	9	0.21
(1,827)	1:139:A:THR:HA	1:140:A:ARG:HG2	7	0.21
(1,737)	1:127:A:ARG:HA	1:127:A:ARG:HD3	6	0.21
(1,736)	1:127:A:ARG:HA	1:127:A:ARG:HG3	7	0.21
(1,710)	1:126:A:GLU:HA	1:135:A:SER:HB2	6	0.21
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	5	0.21
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	5	0.21
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	5	0.21
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG21	3	0.21
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG22	3	0.21
(1,641)	1:120:A:ILE:HG13	1:120:A:ILE:HG23	3	0.21
(1,612)	1:119:A:GLU:HA	1:141:A:LYS:HE3	6	0.21
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD21	9	0.21
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD22	9	0.21
(1,588)	1:118:A:VAL:HG11	1:144:A:LEU:HD23	9	0.21
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD21	9	0.21
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD22	9	0.21
(1,588)	1:118:A:VAL:HG12	1:144:A:LEU:HD23	9	0.21
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD21	9	0.21
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD22	9	0.21
(1,588)	1:118:A:VAL:HG13	1:144:A:LEU:HD23	9	0.21
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	9	0.21
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	9	0.21
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	9	0.21
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	9	0.21
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	9	0.21
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	9	0.21
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	3	0.21
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	3	0.21
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	3	0.21
(1,473)	1:112:A:LYS:HE2	1:114:A:LYS:HB2	8	0.21
(1,472)	1:112:A:LYS:HD2	1:120:A:ILE:HA	3	0.21
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	1	0.21
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG21	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG22	7	0.21
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG23	7	0.21
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG21	7	0.21
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG22	7	0.21
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG23	7	0.21
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG21	7	0.21
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG22	7	0.21
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG23	7	0.21
(1,404)	1:110:A:THR:HG21	1:112:A:LYS:HB2	9	0.21
(1,404)	1:110:A:THR:HG22	1:112:A:LYS:HB2	9	0.21
(1,404)	1:110:A:THR:HG23	1:112:A:LYS:HB2	9	0.21
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD11	5	0.21
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD12	5	0.21
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD13	5	0.21
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	5	0.21
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	9	0.21
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	3	0.21
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	3	0.21
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	3	0.21
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	3	0.21
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	10	0.21
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	1	0.21
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	2	0.21
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	6	0.21
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	8	0.21
(1,279)	1:102:A:ASN:HB3	1:161:A:GLY:HA2	9	0.21
(1,248)	1:99:A:LEU:HD21	1:140:A:ARG:HD2	6	0.21
(1,248)	1:99:A:LEU:HD22	1:140:A:ARG:HD2	6	0.21
(1,248)	1:99:A:LEU:HD23	1:140:A:ARG:HD2	6	0.21
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	4	0.21
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	4	0.21
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	4	0.21
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	4	0.21
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	4	0.21
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	4	0.21
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	4	0.21
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	4	0.21
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	4	0.21
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	5	0.21
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	5	0.21
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	5	0.21
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	10	0.21
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	10	0.21
(1,4205)	1:162:B:THR:H	1:160:B:GLU:HB2	8	0.2
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG21	1	0.2
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG22	1	0.2
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG23	1	0.2
(1,4183)	1:161:B:GLY:H	1:102:B:ASN:HB3	8	0.2
(1,4182)	1:161:B:GLY:H	1:102:B:ASN:HB2	2	0.2
(1,4141)	1:156:B:SER:H	1:157:B:LEU:HB3	3	0.2
(1,4115)	1:154:B:SER:H	1:155:B:SER:HB2	5	0.2
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	4	0.2
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	4	0.2
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	4	0.2
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD11	5	0.2
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD12	5	0.2
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD13	5	0.2
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	7	0.2
(1,3868)	1:126:B:GLU:H	1:125:B:GLU:HG2	4	0.2
(1,3847)	1:123:B:LYS:H	1:109:B:LEU:HB2	8	0.2
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	6	0.2
(1,3806)	1:119:B:GLU:H	1:114:B:LYS:HB3	7	0.2
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	7	0.2
(1,3795)	1:118:B:VAL:H	1:119:B:GLU:HG3	8	0.2
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	8	0.2
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	10	0.2
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	2	0.2
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	10	0.2
(1,3358)	1:153:B:VAL:HA	1:168:B:PRO:HD2	3	0.2
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	6	0.2
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	8	0.2
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG2	9	0.2
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	3	0.2
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	3	0.2
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	3	0.2
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	3	0.2
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	3	0.2
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	3	0.2
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	3	0.2
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	3	0.2
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	3	0.2
(1,3133)	1:141:B:LYS:HG2	1:141:B:LYS:HE2	5	0.2
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	8	0.2
(1,3093)	1:136:B:ARG:HA	1:136:B:ARG:HD2	8	0.2
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD11	8	0.2
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD12	8	0.2
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD13	8	0.2
(1,3018)	1:127:B:ARG:HA	1:127:B:ARG:HD3	3	0.2
(1,2981)	1:125:B:GLU:HA	1:125:B:GLU:HG3	1	0.2
(1,2891)	1:119:B:GLU:HA	1:141:B:LYS:HD3	10	0.2
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	7	0.2
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	7	0.2
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	7	0.2
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	4	0.2
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	4	0.2
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	4	0.2
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	4	0.2
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	4	0.2
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	4	0.2
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	4	0.2
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	4	0.2
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	4	0.2
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	5	0.2
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	7	0.2
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	8	0.2
(1,2628)	1:108:B:GLU:HG3	1:123:B:LYS:HD2	9	0.2
(1,2626)	1:108:B:GLU:HG2	1:123:B:LYS:HE2	1	0.2
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	1	0.2
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	2	0.2
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	5	0.2
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	6	0.2
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	7	0.2
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	9	0.2
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	9	0.2
(1,2561)	1:102:B:ASN:HB3	1:161:B:GLY:HA3	2	0.2
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	6	0.2
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	6	0.2
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	6	0.2
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	8	0.2
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	8	0.2
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	8	0.2
(1,2540)	1:100:B:ASP:HA	1:100:B:ASP:HB3	4	0.2
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	6	0.2
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	6	0.2
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	6	0.2
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	6	0.2
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	6	0.2
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	6	0.2
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	6	0.2
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	6	0.2
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD11	3	0.2
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD12	3	0.2
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD13	3	0.2
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	1	0.2
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	1	0.2
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	1	0.2
(1,2383)	1:96:B:ARG:HB3	1:166:B:GLU:HB3	5	0.2
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG21	3	0.2
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG22	3	0.2
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG23	3	0.2
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG21	8	0.2
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG22	8	0.2
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG23	8	0.2
(1,2297)	1:93:B:ASP:HA	1:94:B:ARG:HD2	6	0.2
(1,2281)	1:143:A:THR:H	1:132:B:GLY:HA2	7	0.2
(1,2148)	1:143:A:THR:H	1:132:B:GLY:HA2	7	0.2
(1,2006)	1:171:A:LYS:H	1:170:A:PRO:HG3	5	0.2
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD11	10	0.2
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD12	10	0.2
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD13	10	0.2
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG21	3	0.2
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG22	3	0.2
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG23	3	0.2
(1,1796)	1:152:A:GLN:HE21	1:149:A:ASP:HB2	2	0.2
(1,1733)	1:147:A:GLY:H	1:146:A:PRO:HG2	3	0.2
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	6	0.2
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	6	0.2
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	6	0.2
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD11	5	0.2
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD12	5	0.2
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD13	5	0.2
(1,1664)	1:135:A:SER:H	1:134:A:ILE:HG13	8	0.2
(1,1621)	1:129:A:ASP:H	1:129:A:ASP:HB2	10	0.2
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	2	0.2
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD1	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD2	9	0.2
(1,1576)	1:124:A:HIS:H	1:136:A:ARG:HA	3	0.2
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	10	0.2
(1,1545)	1:120:A:ILE:H	1:140:A:ARG:HG3	5	0.2
(1,1489)	1:114:A:LYS:H	1:119:A:GLU:H	6	0.2
(1,1391)	1:105:A:ALA:H	1:108:A:GLU:HB3	4	0.2
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD22	2	0.2
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG21	4	0.2
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG22	4	0.2
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG23	4	0.2
(1,1314)	1:170:A:PRO:HB3	1:170:A:PRO:HD2	2	0.2
(1,1210)	1:160:A:GLU:HB2	1:162:A:THR:HB	1	0.2
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	9	0.2
(1,1173)	1:157:A:LEU:HD11	1:163:A:LEU:HB3	1	0.2
(1,1173)	1:157:A:LEU:HD12	1:163:A:LEU:HB3	1	0.2
(1,1173)	1:157:A:LEU:HD13	1:163:A:LEU:HB3	1	0.2
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	1	0.2
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	4	0.2
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD21	6	0.2
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD22	6	0.2
(1,1140)	1:156:A:SER:HB3	1:157:A:LEU:HD23	6	0.2
(1,1077)	1:153:A:VAL:HA	1:168:A:PRO:HD2	4	0.2
(1,1014)	1:148:A:VAL:HG11	1:170:A:PRO:HG3	7	0.2
(1,1014)	1:148:A:VAL:HG12	1:170:A:PRO:HG3	7	0.2
(1,1014)	1:148:A:VAL:HG13	1:170:A:PRO:HG3	7	0.2
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	4	0.2
(1,967)	1:146:A:PRO:HB3	1:147:A:GLY:HA2	10	0.2
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	6	0.2
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	6	0.2
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	6	0.2
(1,858)	1:141:A:LYS:HG3	1:141:A:LYS:HE2	2	0.2
(1,857)	1:141:A:LYS:HG2	1:143:A:THR:HA	8	0.2
(1,849)	1:141:A:LYS:HB2	1:141:A:LYS:HE2	1	0.2
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	3	0.2
(1,815)	1:136:A:ARG:HG3	1:138:A:PHE:HA	6	0.2
(1,773)	1:130:A:GLU:HA	1:130:A:GLU:HG3	7	0.2
(1,749)	1:128:A:GLN:HA	1:133:A:TYR:HE1	6	0.2
(1,749)	1:128:A:GLN:HA	1:133:A:TYR:HE2	6	0.2
(1,746)	1:128:A:GLN:HA	1:128:A:GLN:HG3	9	0.2
(1,746)	1:128:A:GLN:HA	1:128:A:GLN:HG3	10	0.2
(1,705)	1:126:A:GLU:HA	1:126:A:GLU:HG3	10	0.2
(1,700)	1:125:A:GLU:HA	1:125:A:GLU:HG3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	2	0.2
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	2	0.2
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	2	0.2
(1,643)	1:120:A:ILE:HG13	1:163:A:LEU:HD11	2	0.2
(1,643)	1:120:A:ILE:HG13	1:163:A:LEU:HD12	2	0.2
(1,643)	1:120:A:ILE:HG13	1:163:A:LEU:HD13	2	0.2
(1,635)	1:120:A:ILE:HB	1:140:A:ARG:HD2	8	0.2
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	3	0.2
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	3	0.2
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	3	0.2
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG21	10	0.2
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG22	10	0.2
(1,514)	1:115:A:ASP:HB2	1:143:A:THR:HG23	10	0.2
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG21	6	0.2
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG22	6	0.2
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG23	6	0.2
(1,489)	1:113:A:THR:HB	1:150:A:PRO:HB2	4	0.2
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	6	0.2
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	6	0.2
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	6	0.2
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	6	0.2
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	6	0.2
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	6	0.2
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	6	0.2
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	6	0.2
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	6	0.2
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	9	0.2
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	9	0.2
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	9	0.2
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	9	0.2
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	9	0.2
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	9	0.2
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	9	0.2
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	9	0.2
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	9	0.2
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	3	0.2
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	3	0.2
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	3	0.2
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	6	0.2
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	1	0.2
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	2	0.2
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	5	0.2
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	6	0.2
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	9	0.2
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	9	0.2
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	9	0.2
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	9	0.2
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	6	0.2
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	6	0.2
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	6	0.2
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	6	0.2
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	6	0.2
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	6	0.2
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	6	0.2
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	6	0.2
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	6	0.2
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	1	0.2
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	1	0.2
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	1	0.2
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	1	0.2
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	1	0.2
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	1	0.2
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	1	0.2
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	1	0.2
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	1	0.2
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	1	0.2
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	1	0.2
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	1	0.2
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	8	0.2
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	8	0.2
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	8	0.2
(1,175)	1:98:A:SER:HA	1:142:A:TYR:HE1	3	0.2
(1,175)	1:98:A:SER:HA	1:142:A:TYR:HE2	3	0.2
(1,102)	1:96:A:ARG:HB3	1:166:A:GLU:HB3	10	0.2
(1,96)	1:96:A:ARG:HB2	1:166:A:GLU:HB2	8	0.2
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	9	0.2
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	9	0.2
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	9	0.2
(1,23)	1:94:A:ARG:HA	1:94:A:ARG:HB3	6	0.2
(1,4281)	1:169:B:MET:H	1:169:B:MET:HG3	5	0.19
(1,4263)	1:167:B:ALA:H	1:166:B:GLU:HB3	4	0.19
(1,4089)	1:152:B:GLN:HE22	1:152:B:GLN:HB2	1	0.19
(1,4089)	1:152:B:GLN:HE22	1:152:B:GLN:HB2	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4084)	1:152:B:GLN:HE21	1:168:B:PRO:HD2	5	0.19
(1,4082)	1:152:B:GLN:HE21	1:167:B:ALA:HB1	3	0.19
(1,4082)	1:152:B:GLN:HE21	1:167:B:ALA:HB2	3	0.19
(1,4082)	1:152:B:GLN:HE21	1:167:B:ALA:HB3	3	0.19
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	8	0.19
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	8	0.19
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	8	0.19
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD11	10	0.19
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD12	10	0.19
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD13	10	0.19
(1,3915)	1:131:B:HIS:H	1:129:B:ASP:HB3	8	0.19
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD11	1	0.19
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD12	1	0.19
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD13	1	0.19
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD11	10	0.19
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD12	10	0.19
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD13	10	0.19
(1,3806)	1:119:B:GLU:H	1:114:B:LYS:HB3	1	0.19
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	4	0.19
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	8	0.19
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	8	0.19
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	8	0.19
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	8	0.19
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD21	8	0.19
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD22	8	0.19
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD23	8	0.19
(1,3607)	1:94:B:ARG:H	1:168:B:PRO:HA	3	0.19
(1,3607)	1:94:B:ARG:H	1:168:B:PRO:HA	4	0.19
(1,3595)	1:170:B:PRO:HB3	1:170:B:PRO:HD2	6	0.19
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	1	0.19
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	10	0.19
(1,3470)	1:158:B:SER:HA	1:160:B:GLU:HB3	9	0.19
(1,3454)	1:157:B:LEU:HD11	1:163:B:LEU:HB3	1	0.19
(1,3454)	1:157:B:LEU:HD12	1:163:B:LEU:HB3	1	0.19
(1,3454)	1:157:B:LEU:HD13	1:163:B:LEU:HB3	1	0.19
(1,3430)	1:157:B:LEU:HA	1:163:B:LEU:HB3	4	0.19
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	4	0.19
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	5	0.19
(1,3424)	1:157:B:LEU:HA	1:157:B:LEU:HB2	7	0.19
(1,3391)	1:155:B:SER:HA	1:165:B:VAL:HA	9	0.19
(1,3358)	1:153:B:VAL:HA	1:168:B:PRO:HD2	1	0.19
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	2	0.19
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	2	0.19
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	2	0.19
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	2	0.19
(1,3143)	1:141:B:LYS:HG3	1:142:B:TYR:HB3	6	0.19
(1,3143)	1:141:B:LYS:HG3	1:142:B:TYR:HB3	7	0.19
(1,3138)	1:141:B:LYS:HG2	1:143:B:THR:HA	10	0.19
(1,3120)	1:140:B:ARG:HB2	1:140:B:ARG:HD2	3	0.19
(1,2971)	1:123:B:LYS:HB3	1:137:B:CYS:HB2	3	0.19
(1,2969)	1:123:B:LYS:HB2	1:137:B:CYS:HB3	3	0.19
(1,2928)	1:120:B:ILE:HG21	1:122:B:GLY:HA3	8	0.19
(1,2928)	1:120:B:ILE:HG22	1:122:B:GLY:HA3	8	0.19
(1,2928)	1:120:B:ILE:HG23	1:122:B:GLY:HA3	8	0.19
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD11	3	0.19
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD12	3	0.19
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD13	3	0.19
(1,2892)	1:119:B:GLU:HA	1:141:B:LYS:HE2	10	0.19
(1,2870)	1:118:B:VAL:HG11	1:148:B:VAL:HB	2	0.19
(1,2870)	1:118:B:VAL:HG12	1:148:B:VAL:HB	2	0.19
(1,2870)	1:118:B:VAL:HG13	1:148:B:VAL:HB	2	0.19
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG11	9	0.19
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG12	9	0.19
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG13	9	0.19
(1,2759)	1:112:B:LYS:HE3	1:121:B:THR:HB	4	0.19
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE3	9	0.19
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	1	0.19
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	9	0.19
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	10	0.19
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	10	0.19
(1,2560)	1:102:B:ASN:HB3	1:161:B:GLY:HA2	6	0.19
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG11	4	0.19
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG12	4	0.19
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG13	4	0.19
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG11	4	0.19
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG12	4	0.19
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG13	4	0.19
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG11	4	0.19
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG12	4	0.19
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG13	4	0.19
(1,2518)	1:99:B:LEU:HD21	1:101:B:VAL:HB	4	0.19
(1,2518)	1:99:B:LEU:HD22	1:101:B:VAL:HB	4	0.19
(1,2518)	1:99:B:LEU:HD23	1:101:B:VAL:HB	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	5	0.19
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	5	0.19
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	5	0.19
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	5	0.19
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	5	0.19
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	5	0.19
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	5	0.19
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	5	0.19
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	5	0.19
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG21	4	0.19
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG22	4	0.19
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG23	4	0.19
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG21	4	0.19
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG22	4	0.19
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG23	4	0.19
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG21	4	0.19
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG22	4	0.19
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG23	4	0.19
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD11	9	0.19
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD12	9	0.19
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD13	9	0.19
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG21	6	0.19
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG22	6	0.19
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG23	6	0.19
(1,2383)	1:96:B:ARG:HB3	1:166:B:GLU:HB3	7	0.19
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	10	0.19
(1,2329)	1:94:B:ARG:HD2	1:168:B:PRO:HA	10	0.19
(1,2215)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	2	0.19
(1,2209)	1:134:A:ILE:HA	1:140:B:ARG:HB3	4	0.19
(1,2205)	1:134:B:ILE:HD11	1:140:A:ARG:HD2	2	0.19
(1,2205)	1:134:B:ILE:HD12	1:140:A:ARG:HD2	2	0.19
(1,2205)	1:134:B:ILE:HD13	1:140:A:ARG:HD2	2	0.19
(1,2177)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	1	0.19
(1,2083)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	2	0.19
(1,2077)	1:134:A:ILE:HA	1:140:B:ARG:HB3	4	0.19
(1,2073)	1:134:B:ILE:HD11	1:140:A:ARG:HD2	2	0.19
(1,2073)	1:134:B:ILE:HD12	1:140:A:ARG:HD2	2	0.19
(1,2073)	1:134:B:ILE:HD13	1:140:A:ARG:HD2	2	0.19
(1,2045)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	1	0.19
(1,1958)	1:165:A:VAL:H	1:166:A:GLU:HB3	5	0.19
(1,1925)	1:162:A:THR:H	1:160:A:GLU:HG2	6	0.19
(1,1924)	1:162:A:THR:H	1:160:A:GLU:HB2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1913)	1:161:A:GLY:H	1:162:A:THR:HB	2	0.19
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	8	0.19
(1,1902)	1:161:A:GLY:H	1:102:A:ASN:HB3	4	0.19
(1,1901)	1:161:A:GLY:H	1:102:A:ASN:HB2	7	0.19
(1,1860)	1:156:A:SER:H	1:157:A:LEU:HB3	6	0.19
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	4	0.19
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	4	0.19
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	4	0.19
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG21	10	0.19
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG22	10	0.19
(1,1797)	1:152:A:GLN:HE21	1:151:A:THR:HG23	10	0.19
(1,1767)	1:149:A:ASP:H	1:170:A:PRO:HG3	2	0.19
(1,1738)	1:148:A:VAL:H	1:144:A:LEU:HB2	6	0.19
(1,1657)	1:134:A:ILE:H	1:133:A:TYR:HB3	6	0.19
(1,1647)	1:132:A:GLY:H	1:131:A:HIS:HB3	10	0.19
(1,1634)	1:131:A:HIS:H	1:129:A:ASP:HB3	10	0.19
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	9	0.19
(1,1608)	1:128:A:GLN:HE22	1:128:A:GLN:HB2	3	0.19
(1,1584)	1:125:A:GLU:H	1:126:A:GLU:H	9	0.19
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	7	0.19
(1,1514)	1:118:A:VAL:H	1:119:A:GLU:HG3	6	0.19
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	1	0.19
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	1	0.19
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	1	0.19
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	5	0.19
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	5	0.19
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	5	0.19
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD21	8	0.19
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD22	8	0.19
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD23	8	0.19
(1,1383)	1:102:A:ASN:HD22	1:161:A:GLY:HA3	4	0.19
(1,1373)	1:102:A:ASN:HD21	1:161:A:GLY:HA2	7	0.19
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD11	4	0.19
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD12	4	0.19
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD13	4	0.19
(1,1367)	1:102:A:ASN:H	1:102:A:ASN:HD22	7	0.19
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	1	0.19
(1,1282)	1:168:A:PRO:HB3	1:169:A:MET:HA	2	0.19
(1,1282)	1:168:A:PRO:HB3	1:169:A:MET:HA	4	0.19
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	4	0.19
(1,1173)	1:157:A:LEU:HD11	1:163:A:LEU:HB3	3	0.19
(1,1173)	1:157:A:LEU:HD12	1:163:A:LEU:HB3	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:157:A:LEU:HD13	1:163:A:LEU:HB3	3	0.19
(1,1173)	1:157:A:LEU:HD11	1:163:A:LEU:HB3	6	0.19
(1,1173)	1:157:A:LEU:HD12	1:163:A:LEU:HB3	6	0.19
(1,1173)	1:157:A:LEU:HD13	1:163:A:LEU:HB3	6	0.19
(1,1168)	1:157:A:LEU:HD11	1:161:A:GLY:HA3	8	0.19
(1,1168)	1:157:A:LEU:HD12	1:161:A:GLY:HA3	8	0.19
(1,1168)	1:157:A:LEU:HD13	1:161:A:GLY:HA3	8	0.19
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	1	0.19
(1,1143)	1:157:A:LEU:HA	1:157:A:LEU:HB2	8	0.19
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	1	0.19
(1,1104)	1:155:A:SER:HA	1:156:A:SER:HB3	3	0.19
(1,1097)	1:154:A:SER:HB3	1:155:A:SER:HA	8	0.19
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	6	0.19
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG11	5	0.19
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG12	5	0.19
(1,987)	1:148:A:VAL:HA	1:153:A:VAL:HG13	5	0.19
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	10	0.19
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	1	0.19
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	9	0.19
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	9	0.19
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	9	0.19
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	9	0.19
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	9	0.19
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	9	0.19
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG11	4	0.19
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG12	4	0.19
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG13	4	0.19
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG11	4	0.19
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG12	4	0.19
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG13	4	0.19
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	7	0.19
(1,782)	1:131:A:HIS:HB2	1:132:A:GLY:HA2	4	0.19
(1,766)	1:129:A:ASP:HA	1:130:A:GLU:HB3	6	0.19
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD11	3	0.19
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD12	3	0.19
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD13	3	0.19
(1,721)	1:126:A:GLU:HG2	1:134:A:ILE:HG21	7	0.19
(1,721)	1:126:A:GLU:HG2	1:134:A:ILE:HG22	7	0.19
(1,721)	1:126:A:GLU:HG2	1:134:A:ILE:HG23	7	0.19
(1,680)	1:123:A:LYS:HA	1:123:A:LYS:HG3	2	0.19
(1,618)	1:119:A:GLU:HG2	1:141:A:LYS:HG3	6	0.19
(1,610)	1:119:A:GLU:HA	1:141:A:LYS:HD3	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:117:A:VAL:HG11	1:142:A:TYR:HB3	1	0.19
(1,562)	1:117:A:VAL:HG12	1:142:A:TYR:HB3	1	0.19
(1,562)	1:117:A:VAL:HG13	1:142:A:TYR:HB3	1	0.19
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	8	0.19
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	8	0.19
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	8	0.19
(1,419)	1:111:A:VAL:HA	1:120:A:ILE:HG13	4	0.19
(1,419)	1:111:A:VAL:HA	1:120:A:ILE:HG13	9	0.19
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	8	0.19
(1,348)	1:108:A:GLU:HG3	1:123:A:LYS:HE3	2	0.19
(1,337)	1:108:A:GLU:HA	1:108:A:GLU:HG3	5	0.19
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	7	0.19
(1,306)	1:106:A:PRO:HA	1:106:A:PRO:HB3	8	0.19
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	7	0.19
(1,279)	1:102:A:ASN:HB3	1:161:A:GLY:HA2	4	0.19
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	10	0.19
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	10	0.19
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	10	0.19
(1,256)	1:99:A:LEU:HD11	1:111:A:VAL:HB	8	0.19
(1,256)	1:99:A:LEU:HD12	1:111:A:VAL:HB	8	0.19
(1,256)	1:99:A:LEU:HD13	1:111:A:VAL:HB	8	0.19
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	1	0.19
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	1	0.19
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	1	0.19
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	1	0.19
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	1	0.19
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	1	0.19
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	1	0.19
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	1	0.19
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	1	0.19
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	7	0.19
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	7	0.19
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	7	0.19
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	7	0.19
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	7	0.19
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	7	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	7	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	7	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	7	0.19
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	10	0.19
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	10	0.19
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	10	0.19
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	10	0.19
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	10	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	10	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	10	0.19
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	10	0.19
(1,112)	1:96:A:ARG:HD3	1:164:A:THR:HA	2	0.19
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG21	6	0.19
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG22	6	0.19
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG23	6	0.19
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG21	7	0.19
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG22	7	0.19
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG23	7	0.19
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	2	0.19
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	2	0.19
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	2	0.19
(1,48)	1:94:A:ARG:HD2	1:168:A:PRO:HA	7	0.19
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	9	0.19
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	10	0.19
(1,17)	1:93:A:ASP:HA	1:169:A:MET:HG2	4	0.19
(1,9)	1:90:A:HIS:HB3	1:91:A:THR:HA	9	0.19
(1,4286)	1:171:B:LYS:H	1:170:B:PRO:HB2	4	0.18
(1,4267)	1:167:B:ALA:H	1:169:B:MET:H	5	0.18
(1,4196)	1:162:B:THR:H	1:102:B:ASN:HB2	4	0.18
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG21	9	0.18
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG22	9	0.18
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG23	9	0.18
(1,4194)	1:161:B:GLY:H	1:162:B:THR:HB	9	0.18
(1,4149)	1:157:B:LEU:H	1:155:B:SER:HB2	10	0.18
(1,4125)	1:154:B:SER:H	1:168:B:PRO:HD2	7	0.18
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB1	10	0.18
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB2	10	0.18
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB3	10	0.18
(1,4086)	1:152:B:GLN:HE21	1:170:B:PRO:HD3	10	0.18
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	8	0.18
(1,4076)	1:152:B:GLN:H	1:170:B:PRO:HD3	7	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	4	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	4	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	4	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	5	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	5	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	6	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	6	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	6	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	10	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	10	0.18
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	10	0.18
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD21	2	0.18
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD22	2	0.18
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD23	2	0.18
(1,3952)	1:136:B:ARG:H	1:135:B:SER:HB3	4	0.18
(1,3936)	1:134:B:ILE:H	1:127:B:ARG:HG2	9	0.18
(1,3903)	1:129:B:ASP:H	1:129:B:ASP:HB3	10	0.18
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	5	0.18
(1,3887)	1:128:B:GLN:H	1:133:B:TYR:HD1	7	0.18
(1,3887)	1:128:B:GLN:H	1:133:B:TYR:HD2	7	0.18
(1,3868)	1:126:B:GLU:H	1:125:B:GLU:HG2	9	0.18
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD21	4	0.18
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD22	4	0.18
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD23	4	0.18
(1,3849)	1:123:B:LYS:H	1:109:B:LEU:HD11	6	0.18
(1,3849)	1:123:B:LYS:H	1:109:B:LEU:HD12	6	0.18
(1,3849)	1:123:B:LYS:H	1:109:B:LEU:HD13	6	0.18
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD11	7	0.18
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD12	7	0.18
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD13	7	0.18
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	3	0.18
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	7	0.18
(1,3748)	1:113:B:THR:H	1:112:B:LYS:HB2	6	0.18
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	1	0.18
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	1	0.18
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	1	0.18
(1,3681)	1:107:B:ASP:H	1:106:B:PRO:HB3	4	0.18
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD11	1	0.18
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD12	1	0.18
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD13	1	0.18
(1,3663)	1:102:B:ASN:HD22	1:161:B:GLY:HA2	4	0.18
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD11	8	0.18
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD12	8	0.18
(1,3652)	1:102:B:ASN:HD21	1:157:B:LEU:HD13	8	0.18
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG21	9	0.18
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG22	9	0.18
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG23	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	3	0.18
(1,3491)	1:160:B:GLU:HB2	1:162:B:THR:HB	3	0.18
(1,3309)	1:149:B:ASP:HA	1:150:B:PRO:HD3	3	0.18
(1,3304)	1:149:B:ASP:HA	1:149:B:ASP:HB3	3	0.18
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	8	0.18
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	8	0.18
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	8	0.18
(1,3252)	1:146:B:PRO:HG2	1:147:B:GLY:HA2	3	0.18
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG11	4	0.18
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG12	4	0.18
(1,3234)	1:145:B:PRO:HB3	1:148:B:VAL:HG13	4	0.18
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	10	0.18
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	10	0.18
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	10	0.18
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	10	0.18
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	10	0.18
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	10	0.18
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	10	0.18
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	10	0.18
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	10	0.18
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	8	0.18
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	8	0.18
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	8	0.18
(1,3112)	1:139:B:THR:HB	1:141:B:LYS:HE2	9	0.18
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD1	4	0.18
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD2	4	0.18
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD1	4	0.18
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD2	4	0.18
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD1	4	0.18
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD2	4	0.18
(1,3060)	1:131:B:HIS:HA	1:131:B:HIS:HE1	4	0.18
(1,3037)	1:128:B:GLN:HB3	1:133:B:TYR:HD1	7	0.18
(1,3037)	1:128:B:GLN:HB3	1:133:B:TYR:HD2	7	0.18
(1,3003)	1:126:B:GLU:HG2	1:135:B:SER:HA	7	0.18
(1,3000)	1:126:B:GLU:HG2	1:133:B:TYR:HD1	2	0.18
(1,3000)	1:126:B:GLU:HG2	1:133:B:TYR:HD2	2	0.18
(1,2996)	1:126:B:GLU:HB2	1:135:B:SER:HB3	10	0.18
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	1	0.18
(1,2957)	1:122:B:GLY:HA3	1:137:B:CYS:HA	6	0.18
(1,2892)	1:119:B:GLU:HA	1:141:B:LYS:HE2	1	0.18
(1,2891)	1:119:B:GLU:HA	1:141:B:LYS:HD3	7	0.18
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	1	0.18
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	1	0.18
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	1	0.18
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	1	0.18
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	1	0.18
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	1	0.18
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	1	0.18
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	1	0.18
(1,2852)	1:118:B:VAL:HB	1:142:B:TYR:HD1	2	0.18
(1,2852)	1:118:B:VAL:HB	1:142:B:TYR:HD2	2	0.18
(1,2783)	1:113:B:THR:HG21	1:150:B:PRO:HB3	9	0.18
(1,2783)	1:113:B:THR:HG22	1:150:B:PRO:HB3	9	0.18
(1,2783)	1:113:B:THR:HG23	1:150:B:PRO:HB3	9	0.18
(1,2734)	1:112:B:LYS:HA	1:114:B:LYS:HB3	3	0.18
(1,2687)	1:110:B:THR:HG21	1:112:B:LYS:HE3	4	0.18
(1,2687)	1:110:B:THR:HG22	1:112:B:LYS:HE3	4	0.18
(1,2687)	1:110:B:THR:HG23	1:112:B:LYS:HE3	4	0.18
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	3	0.18
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	3	0.18
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	3	0.18
(1,2618)	1:108:B:GLU:HA	1:108:B:GLU:HG3	2	0.18
(1,2596)	1:106:B:PRO:HA	1:157:B:LEU:HB2	2	0.18
(1,2587)	1:106:B:PRO:HA	1:106:B:PRO:HB3	4	0.18
(1,2578)	1:105:B:ALA:HB1	1:107:B:ASP:HB3	4	0.18
(1,2578)	1:105:B:ALA:HB2	1:107:B:ASP:HB3	4	0.18
(1,2578)	1:105:B:ALA:HB3	1:107:B:ASP:HB3	4	0.18
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	3	0.18
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	3	0.18
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	3	0.18
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD11	2	0.18
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD12	2	0.18
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD13	2	0.18
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD11	2	0.18
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD12	2	0.18
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD13	2	0.18
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD11	2	0.18
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD12	2	0.18
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD13	2	0.18
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	3	0.18
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	3	0.18
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	3	0.18
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	3	0.18
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	3	0.18
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	3	0.18
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	3	0.18
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	3	0.18
(1,2467)	1:98:B:SER:HB2	1:164:B:THR:HA	7	0.18
(1,2442)	1:97:B:VAL:HG21	1:166:B:GLU:HA	1	0.18
(1,2442)	1:97:B:VAL:HG22	1:166:B:GLU:HA	1	0.18
(1,2442)	1:97:B:VAL:HG23	1:166:B:GLU:HA	1	0.18
(1,2442)	1:97:B:VAL:HG21	1:166:B:GLU:HA	2	0.18
(1,2442)	1:97:B:VAL:HG22	1:166:B:GLU:HA	2	0.18
(1,2442)	1:97:B:VAL:HG23	1:166:B:GLU:HA	2	0.18
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG21	1	0.18
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG22	1	0.18
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG23	1	0.18
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG21	9	0.18
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG22	9	0.18
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG23	9	0.18
(1,2361)	1:96:B:ARG:HA	1:96:B:ARG:HD3	8	0.18
(1,2332)	1:95:B:TRP:HA	1:95:B:TRP:HB2	7	0.18
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	5	0.18
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	6	0.18
(1,2310)	1:94:B:ARG:HA	1:168:B:PRO:HA	5	0.18
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG21	9	0.18
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG22	9	0.18
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG23	9	0.18
(1,2152)	1:97:A:VAL:HG11	1:131:B:HIS:HB3	7	0.18
(1,2152)	1:97:A:VAL:HG12	1:131:B:HIS:HB3	7	0.18
(1,2152)	1:97:A:VAL:HG13	1:131:B:HIS:HB3	7	0.18
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG21	9	0.18
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG22	9	0.18
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG23	9	0.18
(1,2020)	1:97:A:VAL:HG11	1:131:B:HIS:HB3	7	0.18
(1,2020)	1:97:A:VAL:HG12	1:131:B:HIS:HB3	7	0.18
(1,2020)	1:97:A:VAL:HG13	1:131:B:HIS:HB3	7	0.18
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	8	0.18
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	9	0.18
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	5	0.18
(1,1920)	1:162:A:THR:H	1:158:A:SER:HB2	2	0.18
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	4	0.18
(1,1910)	1:161:A:GLY:H	1:160:A:GLU:HG3	8	0.18
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB1	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB2	3	0.18
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB3	3	0.18
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	5	0.18
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	7	0.18
(1,1655)	1:134:A:ILE:H	1:127:A:ARG:HG2	6	0.18
(1,1655)	1:134:A:ILE:H	1:127:A:ARG:HG2	10	0.18
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	5	0.18
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	10	0.18
(1,1597)	1:128:A:GLN:H	1:127:A:ARG:HB3	7	0.18
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	1	0.18
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	6	0.18
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	8	0.18
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	6	0.18
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	10	0.18
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	10	0.18
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	10	0.18
(1,1391)	1:105:A:ALA:H	1:108:A:GLU:HB3	1	0.18
(1,1391)	1:105:A:ALA:H	1:108:A:GLU:HB3	7	0.18
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD11	1	0.18
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD12	1	0.18
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD13	1	0.18
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD11	5	0.18
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD12	5	0.18
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD13	5	0.18
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG21	9	0.18
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG22	9	0.18
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG23	9	0.18
(1,1304)	1:169:A:MET:HG3	1:170:A:PRO:HD2	10	0.18
(1,1276)	1:168:A:PRO:HA	1:169:A:MET:HG2	6	0.18
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD21	6	0.18
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD22	6	0.18
(1,1218)	1:161:A:GLY:HA3	1:163:A:LEU:HD23	6	0.18
(1,1206)	1:159:A:PRO:HD2	1:160:A:GLU:HB3	7	0.18
(1,1197)	1:158:A:SER:HB3	1:159:A:PRO:HD3	7	0.18
(1,1168)	1:157:A:LEU:HD11	1:161:A:GLY:HA3	5	0.18
(1,1168)	1:157:A:LEU:HD12	1:161:A:GLY:HA3	5	0.18
(1,1168)	1:157:A:LEU:HD13	1:161:A:GLY:HA3	5	0.18
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG21	4	0.18
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG22	4	0.18
(1,1100)	1:154:A:SER:HB2	1:165:A:VAL:HG23	4	0.18
(1,1065)	1:152:A:GLN:HB2	1:169:A:MET:HA	6	0.18
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:148:A:VAL:HG11	1:170:A:PRO:HG3	6	0.18
(1,1014)	1:148:A:VAL:HG12	1:170:A:PRO:HG3	6	0.18
(1,1014)	1:148:A:VAL:HG13	1:170:A:PRO:HG3	6	0.18
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	2	0.18
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	4	0.18
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	7	0.18
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG21	6	0.18
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG22	6	0.18
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG23	6	0.18
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG21	6	0.18
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG22	6	0.18
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG23	6	0.18
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG21	6	0.18
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG22	6	0.18
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG23	6	0.18
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	4	0.18
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	4	0.18
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	4	0.18
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	8	0.18
(1,849)	1:141:A:LYS:HB2	1:141:A:LYS:HE2	6	0.18
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	2	0.18
(1,749)	1:128:A:GLN:HA	1:133:A:TYR:HE1	1	0.18
(1,749)	1:128:A:GLN:HA	1:133:A:TYR:HE2	1	0.18
(1,664)	1:121:A:THR:HA	1:139:A:THR:HA	2	0.18
(1,664)	1:121:A:THR:HA	1:139:A:THR:HA	9	0.18
(1,614)	1:119:A:GLU:HB3	1:139:A:THR:HA	1	0.18
(1,562)	1:117:A:VAL:HG11	1:142:A:TYR:HB3	8	0.18
(1,562)	1:117:A:VAL:HG12	1:142:A:TYR:HB3	8	0.18
(1,562)	1:117:A:VAL:HG13	1:142:A:TYR:HB3	8	0.18
(1,558)	1:117:A:VAL:HG11	1:141:A:LYS:HE2	1	0.18
(1,558)	1:117:A:VAL:HG12	1:141:A:LYS:HE2	1	0.18
(1,558)	1:117:A:VAL:HG13	1:141:A:LYS:HE2	1	0.18
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	9	0.18
(1,457)	1:112:A:LYS:HB2	1:120:A:ILE:HA	7	0.18
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	3	0.18
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD11	10	0.18
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD12	10	0.18
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD13	10	0.18
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD11	10	0.18
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD12	10	0.18
(1,358)	1:109:A:LEU:HB2	1:109:A:LEU:HD13	10	0.18
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:109:A:LEU:HA	1:109:A:LEU:HB2	10	0.18
(1,337)	1:108:A:GLU:HA	1:108:A:GLU:HG3	7	0.18
(1,315)	1:106:A:PRO:HA	1:157:A:LEU:HB2	4	0.18
(1,296)	1:105:A:ALA:HB1	1:107:A:ASP:HB2	7	0.18
(1,296)	1:105:A:ALA:HB2	1:107:A:ASP:HB2	7	0.18
(1,296)	1:105:A:ALA:HB3	1:107:A:ASP:HB2	7	0.18
(1,296)	1:105:A:ALA:HB1	1:107:A:ASP:HB2	9	0.18
(1,296)	1:105:A:ALA:HB2	1:107:A:ASP:HB2	9	0.18
(1,296)	1:105:A:ALA:HB3	1:107:A:ASP:HB2	9	0.18
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	5	0.18
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	9	0.18
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	9	0.18
(1,279)	1:102:A:ASN:HB3	1:161:A:GLY:HA2	2	0.18
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD11	2	0.18
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD12	2	0.18
(1,276)	1:102:A:ASN:HB2	1:157:A:LEU:HD13	2	0.18
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	3	0.18
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	3	0.18
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	3	0.18
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	3	0.18
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	3	0.18
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	3	0.18
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	3	0.18
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	3	0.18
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	3	0.18
(1,237)	1:99:A:LEU:HD21	1:101:A:VAL:HB	8	0.18
(1,237)	1:99:A:LEU:HD22	1:101:A:VAL:HB	8	0.18
(1,237)	1:99:A:LEU:HD23	1:101:A:VAL:HB	8	0.18
(1,166)	1:97:A:VAL:HG11	1:118:A:VAL:HB	6	0.18
(1,166)	1:97:A:VAL:HG12	1:118:A:VAL:HB	6	0.18
(1,166)	1:97:A:VAL:HG13	1:118:A:VAL:HB	6	0.18
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG11	8	0.18
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG12	8	0.18
(1,129)	1:97:A:VAL:HB	1:148:A:VAL:HG13	8	0.18
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	10	0.18
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	10	0.18
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	10	0.18
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	7	0.18
(1,9)	1:90:A:HIS:HB3	1:91:A:THR:HA	8	0.18
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG21	7	0.18
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG22	7	0.18
(1,6)	1:90:A:HIS:HA	1:91:A:THR:HG23	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4197)	1:162:B:THR:H	1:102:B:ASN:HB3	3	0.17
(1,4194)	1:161:B:GLY:H	1:162:B:THR:HB	1	0.17
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	4	0.17
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	10	0.17
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	3	0.17
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	3	0.17
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	3	0.17
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD11	4	0.17
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD12	4	0.17
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD13	4	0.17
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD21	8	0.17
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD22	8	0.17
(1,3971)	1:140:B:ARG:H	1:99:B:LEU:HD23	8	0.17
(1,3910)	1:129:B:ASP:H	1:133:B:TYR:HB2	6	0.17
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	2	0.17
(1,3878)	1:128:B:GLN:H	1:127:B:ARG:HB3	9	0.17
(1,3869)	1:126:B:GLU:H	1:125:B:GLU:HG3	7	0.17
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB1	9	0.17
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB2	9	0.17
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB3	9	0.17
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	6	0.17
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	3	0.17
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	7	0.17
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	7	0.17
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	7	0.17
(1,3663)	1:102:B:ASN:HD22	1:161:B:GLY:HA2	7	0.17
(1,3648)	1:102:B:ASN:H	1:102:B:ASN:HD21	10	0.17
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG21	10	0.17
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG22	10	0.17
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG23	10	0.17
(1,3569)	1:169:B:MET:HA	1:169:B:MET:HG2	7	0.17
(1,3460)	1:157:B:LEU:HD21	1:163:B:LEU:HB3	10	0.17
(1,3460)	1:157:B:LEU:HD22	1:163:B:LEU:HB3	10	0.17
(1,3460)	1:157:B:LEU:HD23	1:163:B:LEU:HB3	10	0.17
(1,3455)	1:157:B:LEU:HD11	1:163:B:LEU:HG	5	0.17
(1,3455)	1:157:B:LEU:HD12	1:163:B:LEU:HG	5	0.17
(1,3455)	1:157:B:LEU:HD13	1:163:B:LEU:HG	5	0.17
(1,3454)	1:157:B:LEU:HD11	1:163:B:LEU:HB3	2	0.17
(1,3454)	1:157:B:LEU:HD12	1:163:B:LEU:HB3	2	0.17
(1,3454)	1:157:B:LEU:HD13	1:163:B:LEU:HB3	2	0.17
(1,3454)	1:157:B:LEU:HD11	1:163:B:LEU:HB3	10	0.17
(1,3454)	1:157:B:LEU:HD12	1:163:B:LEU:HB3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3454)	1:157:B:LEU:HD13	1:163:B:LEU:HB3	10	0.17
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	6	0.17
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	6	0.17
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	6	0.17
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD21	5	0.17
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD22	5	0.17
(1,3422)	1:156:B:SER:HB3	1:163:B:LEU:HD23	5	0.17
(1,3391)	1:155:B:SER:HA	1:165:B:VAL:HA	1	0.17
(1,3358)	1:153:B:VAL:HA	1:168:B:PRO:HD2	9	0.17
(1,3336)	1:151:B:THR:HB	1:153:B:VAL:HG21	5	0.17
(1,3336)	1:151:B:THR:HB	1:153:B:VAL:HG22	5	0.17
(1,3336)	1:151:B:THR:HB	1:153:B:VAL:HG23	5	0.17
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	4	0.17
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	8	0.17
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	10	0.17
(1,3302)	1:148:B:VAL:HG21	1:169:B:MET:HB3	2	0.17
(1,3302)	1:148:B:VAL:HG22	1:169:B:MET:HB3	2	0.17
(1,3302)	1:148:B:VAL:HG23	1:169:B:MET:HB3	2	0.17
(1,3295)	1:148:B:VAL:HG11	1:170:B:PRO:HG3	6	0.17
(1,3295)	1:148:B:VAL:HG12	1:170:B:PRO:HG3	6	0.17
(1,3295)	1:148:B:VAL:HG13	1:170:B:PRO:HG3	6	0.17
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	2	0.17
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	2	0.17
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	2	0.17
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG11	4	0.17
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG12	4	0.17
(1,3268)	1:148:B:VAL:HA	1:153:B:VAL:HG13	4	0.17
(1,3252)	1:146:B:PRO:HG2	1:147:B:GLY:HA2	10	0.17
(1,3249)	1:146:B:PRO:HB3	1:147:B:GLY:HA3	3	0.17
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	6	0.17
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	7	0.17
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	7	0.17
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	7	0.17
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	7	0.17
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	7	0.17
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	7	0.17
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	7	0.17
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	7	0.17
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	7	0.17
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG21	8	0.17
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG22	8	0.17
(1,3219)	1:144:B:LEU:HD21	1:148:B:VAL:HG23	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG21	8	0.17
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG22	8	0.17
(1,3219)	1:144:B:LEU:HD22	1:148:B:VAL:HG23	8	0.17
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG21	8	0.17
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG22	8	0.17
(1,3219)	1:144:B:LEU:HD23	1:148:B:VAL:HG23	8	0.17
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	1	0.17
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	1	0.17
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	1	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	2	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	2	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	2	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	9	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	9	0.17
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	9	0.17
(1,3138)	1:141:B:LYS:HG2	1:143:B:THR:HA	8	0.17
(1,3133)	1:141:B:LYS:HG2	1:141:B:LYS:HE2	7	0.17
(1,3130)	1:141:B:LYS:HB2	1:141:B:LYS:HE2	9	0.17
(1,3027)	1:128:B:GLN:HA	1:128:B:GLN:HG3	8	0.17
(1,3014)	1:126:B:GLU:HG3	1:135:B:SER:HB3	2	0.17
(1,3000)	1:126:B:GLU:HG2	1:133:B:TYR:HD1	3	0.17
(1,3000)	1:126:B:GLU:HG2	1:133:B:TYR:HD2	3	0.17
(1,2945)	1:121:B:THR:HA	1:139:B:THR:HA	8	0.17
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	6	0.17
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	6	0.17
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	6	0.17
(1,2831)	1:117:B:VAL:HA	1:148:B:VAL:HB	8	0.17
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG21	4	0.17
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG22	4	0.17
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG23	4	0.17
(1,2790)	1:114:B:LYS:HA	1:114:B:LYS:HB2	1	0.17
(1,2716)	1:111:B:VAL:HG21	1:120:B:ILE:HG13	1	0.17
(1,2716)	1:111:B:VAL:HG22	1:120:B:ILE:HG13	1	0.17
(1,2716)	1:111:B:VAL:HG23	1:120:B:ILE:HG13	1	0.17
(1,2700)	1:111:B:VAL:HA	1:120:B:ILE:HG13	2	0.17
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	7	0.17
(1,2664)	1:109:B:LEU:HD21	1:122:B:GLY:HA3	1	0.17
(1,2664)	1:109:B:LEU:HD22	1:122:B:GLY:HA3	1	0.17
(1,2664)	1:109:B:LEU:HD23	1:122:B:GLY:HA3	1	0.17
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	5	0.17
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	5	0.17
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	5	0.17
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	5	0.17
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	5	0.17
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	5	0.17
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	5	0.17
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	5	0.17
(1,2619)	1:108:B:GLU:HA	1:123:B:LYS:HD2	4	0.17
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	7	0.17
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	7	0.17
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	7	0.17
(1,2561)	1:102:B:ASN:HB3	1:161:B:GLY:HA3	6	0.17
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD11	7	0.17
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD12	7	0.17
(1,2550)	1:101:B:VAL:HB	1:157:B:LEU:HD13	7	0.17
(1,2546)	1:100:B:ASP:HB3	1:162:B:THR:HA	2	0.17
(1,2518)	1:99:B:LEU:HD21	1:101:B:VAL:HB	3	0.17
(1,2518)	1:99:B:LEU:HD22	1:101:B:VAL:HB	3	0.17
(1,2518)	1:99:B:LEU:HD23	1:101:B:VAL:HB	3	0.17
(1,2518)	1:99:B:LEU:HD21	1:101:B:VAL:HB	5	0.17
(1,2518)	1:99:B:LEU:HD22	1:101:B:VAL:HB	5	0.17
(1,2518)	1:99:B:LEU:HD23	1:101:B:VAL:HB	5	0.17
(1,2447)	1:97:B:VAL:HG21	1:118:B:VAL:HB	3	0.17
(1,2447)	1:97:B:VAL:HG22	1:118:B:VAL:HB	3	0.17
(1,2447)	1:97:B:VAL:HG23	1:118:B:VAL:HB	3	0.17
(1,2397)	1:96:B:ARG:HD2	1:166:B:GLU:HB3	10	0.17
(1,2394)	1:96:B:ARG:HD2	1:164:B:THR:HB	1	0.17
(1,2301)	1:93:B:ASP:HB3	1:94:B:ARG:HA	4	0.17
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG21	7	0.17
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG22	7	0.17
(1,2289)	1:90:B:HIS:HB2	1:91:B:THR:HG23	7	0.17
(1,2177)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	4	0.17
(1,2045)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	4	0.17
(1,2013)	1:172:A:LEU:H	1:172:A:LEU:HB2	3	0.17
(1,1998)	1:169:A:MET:H	1:169:A:MET:HB2	6	0.17
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	7	0.17
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG21	3	0.17
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG22	3	0.17
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG23	3	0.17
(1,1901)	1:161:A:GLY:H	1:102:A:ASN:HB2	9	0.17
(1,1799)	1:152:A:GLN:HE21	1:152:A:GLN:HB3	5	0.17
(1,1756)	1:148:A:VAL:H	1:170:A:PRO:HG3	6	0.17
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	8	0.17
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	8	0.17
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	8	0.17
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	8	0.17
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	8	0.17
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	8	0.17
(1,1634)	1:131:A:HIS:H	1:129:A:ASP:HB3	5	0.17
(1,1634)	1:131:A:HIS:H	1:129:A:ASP:HB3	6	0.17
(1,1588)	1:126:A:GLU:H	1:125:A:GLU:HG3	6	0.17
(1,1525)	1:119:A:GLU:H	1:114:A:LYS:HB3	6	0.17
(1,1525)	1:119:A:GLU:H	1:114:A:LYS:HB3	9	0.17
(1,1489)	1:114:A:LYS:H	1:119:A:GLU:H	3	0.17
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	5	0.17
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	2	0.17
(1,1391)	1:105:A:ALA:H	1:108:A:GLU:HB3	6	0.17
(1,1389)	1:105:A:ALA:H	1:106:A:PRO:HD3	3	0.17
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD21	10	0.17
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD22	10	0.17
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD23	10	0.17
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD11	1	0.17
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD12	1	0.17
(1,1380)	1:102:A:ASN:HD22	1:157:A:LEU:HD13	1	0.17
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	2	0.17
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	5	0.17
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	3	0.17
(1,1168)	1:157:A:LEU:HD11	1:161:A:GLY:HA3	9	0.17
(1,1168)	1:157:A:LEU:HD12	1:161:A:GLY:HA3	9	0.17
(1,1168)	1:157:A:LEU:HD13	1:161:A:GLY:HA3	9	0.17
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	6	0.17
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	1	0.17
(1,1104)	1:155:A:SER:HA	1:156:A:SER:HB3	6	0.17
(1,1064)	1:152:A:GLN:HB2	1:168:A:PRO:HD3	4	0.17
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG21	7	0.17
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG22	7	0.17
(1,1046)	1:150:A:PRO:HD2	1:151:A:THR:HG23	7	0.17
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	1	0.17
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	5	0.17
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	4	0.17
(1,992)	1:148:A:VAL:HA	1:170:A:PRO:HB3	7	0.17
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	7	0.17
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	8	0.17
(1,858)	1:141:A:LYS:HG3	1:141:A:LYS:HE2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	7	0.17
(1,747)	1:128:A:GLN:HA	1:133:A:TYR:HB2	10	0.17
(1,726)	1:126:A:GLU:HG3	1:127:A:ARG:HG2	7	0.17
(1,680)	1:123:A:LYS:HA	1:123:A:LYS:HG3	4	0.17
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD11	9	0.17
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD12	9	0.17
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD13	9	0.17
(1,611)	1:119:A:GLU:HA	1:141:A:LYS:HE2	5	0.17
(1,605)	1:119:A:GLU:HA	1:120:A:ILE:HG13	8	0.17
(1,602)	1:119:A:GLU:HA	1:119:A:GLU:HG3	5	0.17
(1,602)	1:119:A:GLU:HA	1:119:A:GLU:HG3	6	0.17
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	3	0.17
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	3	0.17
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	3	0.17
(1,478)	1:112:A:LYS:HE2	1:121:A:THR:HB	1	0.17
(1,436)	1:111:A:VAL:HG21	1:120:A:ILE:HD11	4	0.17
(1,436)	1:111:A:VAL:HG21	1:120:A:ILE:HD12	4	0.17
(1,436)	1:111:A:VAL:HG21	1:120:A:ILE:HD13	4	0.17
(1,436)	1:111:A:VAL:HG22	1:120:A:ILE:HD11	4	0.17
(1,436)	1:111:A:VAL:HG22	1:120:A:ILE:HD12	4	0.17
(1,436)	1:111:A:VAL:HG22	1:120:A:ILE:HD13	4	0.17
(1,436)	1:111:A:VAL:HG23	1:120:A:ILE:HD11	4	0.17
(1,436)	1:111:A:VAL:HG23	1:120:A:ILE:HD12	4	0.17
(1,436)	1:111:A:VAL:HG23	1:120:A:ILE:HD13	4	0.17
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG21	6	0.17
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG22	6	0.17
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG23	6	0.17
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG21	6	0.17
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG22	6	0.17
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG23	6	0.17
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG21	6	0.17
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG22	6	0.17
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG23	6	0.17
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	10	0.17
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	10	0.17
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	10	0.17
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	10	0.17
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	10	0.17
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	10	0.17
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	10	0.17
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	10	0.17
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD21	2	0.17
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD22	2	0.17
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD23	2	0.17
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	7	0.17
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	4	0.17
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	4	0.17
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	4	0.17
(1,331)	1:107:A:ASP:HA	1:108:A:GLU:HG2	6	0.17
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD11	3	0.17
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD12	3	0.17
(1,327)	1:106:A:PRO:HG3	1:157:A:LEU:HD13	3	0.17
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	4	0.17
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	4	0.17
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	4	0.17
(1,279)	1:102:A:ASN:HB3	1:161:A:GLY:HA2	6	0.17
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	2	0.17
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	2	0.17
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	2	0.17
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	2	0.17
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	2	0.17
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	2	0.17
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	2	0.17
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	2	0.17
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	2	0.17
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	10	0.17
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	10	0.17
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	10	0.17
(1,101)	1:96:A:ARG:HB3	1:166:A:GLU:HA	8	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	1	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	1	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	1	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	3	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	3	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	3	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	6	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	6	0.17
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	6	0.17
(1,37)	1:94:A:ARG:HB2	1:96:A:ARG:HA	5	0.17
(1,29)	1:94:A:ARG:HA	1:168:A:PRO:HA	6	0.17
(1,23)	1:94:A:ARG:HA	1:94:A:ARG:HB3	8	0.17
(1,4278)	1:169:B:MET:H	1:169:B:MET:HA	5	0.16
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG21	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG22	5	0.16
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG23	5	0.16
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG21	10	0.16
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG22	10	0.16
(1,4195)	1:161:B:GLY:H	1:162:B:THR:HG23	10	0.16
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	8	0.16
(1,4191)	1:161:B:GLY:H	1:160:B:GLU:HG2	3	0.16
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	9	0.16
(1,4182)	1:161:B:GLY:H	1:102:B:ASN:HB2	1	0.16
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG21	9	0.16
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG22	9	0.16
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG23	9	0.16
(1,4125)	1:154:B:SER:H	1:168:B:PRO:HD2	3	0.16
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	10	0.16
(1,4036)	1:148:B:VAL:H	1:170:B:PRO:HB2	3	0.16
(1,3984)	1:142:B:TYR:H	1:141:B:LYS:HG2	6	0.16
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG3	9	0.16
(1,3907)	1:129:B:ASP:H	1:132:B:GLY:HA3	2	0.16
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD21	10	0.16
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD22	10	0.16
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD23	10	0.16
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB1	5	0.16
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB2	5	0.16
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB3	5	0.16
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD11	2	0.16
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD12	2	0.16
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD13	2	0.16
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD11	9	0.16
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD12	9	0.16
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD13	9	0.16
(1,3770)	1:114:B:LYS:H	1:119:B:GLU:H	3	0.16
(1,3770)	1:114:B:LYS:H	1:119:B:GLU:H	10	0.16
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	4	0.16
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	4	0.16
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	4	0.16
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD21	6	0.16
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD22	6	0.16
(1,3662)	1:102:B:ASN:HD22	1:157:B:LEU:HD23	6	0.16
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG21	8	0.16
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG22	8	0.16
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG23	8	0.16
(1,3569)	1:169:B:MET:HA	1:169:B:MET:HG2	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	4	0.16
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	2	0.16
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	2	0.16
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	2	0.16
(1,3430)	1:157:B:LEU:HA	1:163:B:LEU:HB3	5	0.16
(1,3360)	1:153:B:VAL:HB	1:154:B:SER:HA	9	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG21	7	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG22	7	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG23	7	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG21	8	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG22	8	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG23	8	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG21	10	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG22	10	0.16
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG23	10	0.16
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	2	0.16
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	6	0.16
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	9	0.16
(1,3292)	1:148:B:VAL:HG11	1:169:B:MET:HA	1	0.16
(1,3292)	1:148:B:VAL:HG12	1:169:B:MET:HA	1	0.16
(1,3292)	1:148:B:VAL:HG13	1:169:B:MET:HA	1	0.16
(1,3292)	1:148:B:VAL:HG11	1:169:B:MET:HA	2	0.16
(1,3292)	1:148:B:VAL:HG12	1:169:B:MET:HA	2	0.16
(1,3292)	1:148:B:VAL:HG13	1:169:B:MET:HA	2	0.16
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	3	0.16
(1,3243)	1:145:B:PRO:HD2	1:146:B:PRO:HG3	10	0.16
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	4	0.16
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	5	0.16
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	5	0.16
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	5	0.16
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	5	0.16
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	6	0.16
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	2	0.16
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	8	0.16
(1,3005)	1:126:B:GLU:HG2	1:135:B:SER:HB3	9	0.16
(1,2993)	1:126:B:GLU:HB3	1:133:B:TYR:HB2	3	0.16
(1,2980)	1:125:B:GLU:HA	1:125:B:GLU:HG2	2	0.16
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	8	0.16
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	9	0.16
(1,2928)	1:120:B:ILE:HG21	1:122:B:GLY:HA3	4	0.16
(1,2928)	1:120:B:ILE:HG22	1:122:B:GLY:HA3	4	0.16
(1,2928)	1:120:B:ILE:HG23	1:122:B:GLY:HA3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2886)	1:119:B:GLU:HA	1:120:B:ILE:HG13	9	0.16
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	3	0.16
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	3	0.16
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	3	0.16
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	3	0.16
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	3	0.16
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	3	0.16
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	3	0.16
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	3	0.16
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	3	0.16
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD21	4	0.16
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD22	4	0.16
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD23	4	0.16
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	9	0.16
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	9	0.16
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	9	0.16
(1,2831)	1:117:B:VAL:HA	1:148:B:VAL:HB	3	0.16
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	1	0.16
(1,2630)	1:109:B:LEU:HA	1:109:B:LEU:HB2	4	0.16
(1,2577)	1:105:B:ALA:HB1	1:107:B:ASP:HB2	2	0.16
(1,2577)	1:105:B:ALA:HB2	1:107:B:ASP:HB2	2	0.16
(1,2577)	1:105:B:ALA:HB3	1:107:B:ASP:HB2	2	0.16
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG11	2	0.16
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG12	2	0.16
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG13	2	0.16
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG11	2	0.16
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG12	2	0.16
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG13	2	0.16
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG11	2	0.16
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG12	2	0.16
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG13	2	0.16
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	4	0.16
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	4	0.16
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	4	0.16
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	4	0.16
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	4	0.16
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	4	0.16
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	4	0.16
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	4	0.16
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	4	0.16
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	7	0.16
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	7	0.16
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	7	0.16
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	7	0.16
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	7	0.16
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	7	0.16
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	7	0.16
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	7	0.16
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG21	9	0.16
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG22	9	0.16
(1,2507)	1:99:B:LEU:HD11	1:101:B:VAL:HG23	9	0.16
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG21	9	0.16
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG22	9	0.16
(1,2507)	1:99:B:LEU:HD12	1:101:B:VAL:HG23	9	0.16
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG21	9	0.16
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG22	9	0.16
(1,2507)	1:99:B:LEU:HD13	1:101:B:VAL:HG23	9	0.16
(1,2474)	1:98:B:SER:HB3	1:162:B:THR:HA	3	0.16
(1,2447)	1:97:B:VAL:HG21	1:118:B:VAL:HB	7	0.16
(1,2447)	1:97:B:VAL:HG22	1:118:B:VAL:HB	7	0.16
(1,2447)	1:97:B:VAL:HG23	1:118:B:VAL:HB	7	0.16
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD1	7	0.16
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD2	7	0.16
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD1	7	0.16
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD2	7	0.16
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD1	7	0.16
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD2	7	0.16
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG21	5	0.16
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG22	5	0.16
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG23	5	0.16
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG21	3	0.16
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG22	3	0.16
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG23	3	0.16
(1,2383)	1:96:B:ARG:HB3	1:166:B:GLU:HB3	10	0.16
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG21	5	0.16
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG22	5	0.16
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG23	5	0.16
(1,2353)	1:95:B:TRP:HB2	1:168:B:PRO:HB3	4	0.16
(1,2227)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	5	0.16
(1,2227)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	5	0.16
(1,2227)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	5	0.16
(1,2194)	1:134:B:ILE:HA	1:140:A:ARG:HD3	8	0.16
(1,2177)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2160)	1:132:B:GLY:HA2	1:142:A:TYR:HB3	6	0.16
(1,2160)	1:132:B:GLY:HA2	1:142:A:TYR:HB3	9	0.16
(1,2095)	1:134:A:ILE:HD11	1:140:B:ARG:HG2	5	0.16
(1,2095)	1:134:A:ILE:HD12	1:140:B:ARG:HG2	5	0.16
(1,2095)	1:134:A:ILE:HD13	1:140:B:ARG:HG2	5	0.16
(1,2062)	1:134:B:ILE:HA	1:140:A:ARG:HD3	8	0.16
(1,2045)	1:133:B:TYR:HB3	1:141:A:LYS:HD2	8	0.16
(1,2028)	1:132:B:GLY:HA2	1:142:A:TYR:HB3	6	0.16
(1,2028)	1:132:B:GLY:HA2	1:142:A:TYR:HB3	9	0.16
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	4	0.16
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	8	0.16
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	2	0.16
(1,1901)	1:161:A:GLY:H	1:102:A:ASN:HB2	5	0.16
(1,1806)	1:152:A:GLN:HE22	1:149:A:ASP:HB2	10	0.16
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	3	0.16
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	3	0.16
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	3	0.16
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	3	0.16
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD11	6	0.16
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD12	6	0.16
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD13	6	0.16
(1,1668)	1:135:A:SER:H	1:135:A:SER:HB3	3	0.16
(1,1654)	1:134:A:ILE:H	1:127:A:ARG:HB2	5	0.16
(1,1647)	1:132:A:GLY:H	1:131:A:HIS:HB3	3	0.16
(1,1618)	1:128:A:GLN:HE21	1:129:A:ASP:H	1	0.16
(1,1606)	1:128:A:GLN:H	1:133:A:TYR:HD1	8	0.16
(1,1606)	1:128:A:GLN:H	1:133:A:TYR:HD2	8	0.16
(1,1588)	1:126:A:GLU:H	1:125:A:GLU:HG3	10	0.16
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	2	0.16
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG21	10	0.16
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG22	10	0.16
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG23	10	0.16
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	9	0.16
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	8	0.16
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD21	2	0.16
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD22	2	0.16
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD23	2	0.16
(1,1382)	1:102:A:ASN:HD22	1:161:A:GLY:HA2	8	0.16
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG21	3	0.16
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG22	3	0.16
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG23	3	0.16
(1,1333)	1:95:A:TRP:H	1:166:A:GLU:HG3	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	7	0.16
(1,1277)	1:168:A:PRO:HA	1:169:A:MET:HG3	7	0.16
(1,1197)	1:158:A:SER:HB3	1:159:A:PRO:HD3	10	0.16
(1,1191)	1:158:A:SER:HB2	1:160:A:GLU:HG2	1	0.16
(1,1181)	1:158:A:SER:HA	1:158:A:SER:HB2	2	0.16
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	2	0.16
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	2	0.16
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	2	0.16
(1,1172)	1:157:A:LEU:HD11	1:163:A:LEU:HB2	8	0.16
(1,1172)	1:157:A:LEU:HD12	1:163:A:LEU:HB2	8	0.16
(1,1172)	1:157:A:LEU:HD13	1:163:A:LEU:HB2	8	0.16
(1,1149)	1:157:A:LEU:HA	1:163:A:LEU:HB3	8	0.16
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD21	2	0.16
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD22	2	0.16
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD23	2	0.16
(1,1085)	1:153:A:VAL:HG11	1:155:A:SER:HB3	2	0.16
(1,1085)	1:153:A:VAL:HG12	1:155:A:SER:HB3	2	0.16
(1,1085)	1:153:A:VAL:HG13	1:155:A:SER:HB3	2	0.16
(1,1079)	1:153:A:VAL:HB	1:154:A:SER:HA	2	0.16
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	2	0.16
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	3	0.16
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	4	0.16
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	7	0.16
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	8	0.16
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	9	0.16
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	10	0.16
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	1	0.16
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	3	0.16
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	8	0.16
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	9	0.16
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	1	0.16
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	1	0.16
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	1	0.16
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD11	8	0.16
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD12	8	0.16
(1,896)	1:143:A:THR:HB	1:144:A:LEU:HD13	8	0.16
(1,858)	1:141:A:LYS:HG3	1:141:A:LYS:HE2	3	0.16
(1,856)	1:141:A:LYS:HG2	1:142:A:TYR:HB3	3	0.16
(1,831)	1:139:A:THR:HB	1:141:A:LYS:HE2	3	0.16
(1,779)	1:131:A:HIS:HA	1:131:A:HIS:HE1	2	0.16
(1,773)	1:130:A:GLU:HA	1:130:A:GLU:HG3	2	0.16
(1,764)	1:129:A:ASP:HA	1:129:A:ASP:HB3	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:128:A:GLN:HB3	1:133:A:TYR:HD1	8	0.16
(1,756)	1:128:A:GLN:HB3	1:133:A:TYR:HD2	8	0.16
(1,723)	1:126:A:GLU:HG2	1:135:A:SER:HB2	6	0.16
(1,703)	1:125:A:GLU:HA	1:135:A:SER:HB2	5	0.16
(1,680)	1:123:A:LYS:HA	1:123:A:LYS:HG3	9	0.16
(1,680)	1:123:A:LYS:HA	1:123:A:LYS:HG3	10	0.16
(1,654)	1:120:A:ILE:HD11	1:140:A:ARG:HD2	10	0.16
(1,654)	1:120:A:ILE:HD12	1:140:A:ARG:HD2	10	0.16
(1,654)	1:120:A:ILE:HD13	1:140:A:ARG:HD2	10	0.16
(1,648)	1:120:A:ILE:HG21	1:139:A:THR:HA	10	0.16
(1,648)	1:120:A:ILE:HG22	1:139:A:THR:HA	10	0.16
(1,648)	1:120:A:ILE:HG23	1:139:A:THR:HA	10	0.16
(1,605)	1:119:A:GLU:HA	1:120:A:ILE:HG13	1	0.16
(1,605)	1:119:A:GLU:HA	1:120:A:ILE:HG13	10	0.16
(1,559)	1:117:A:VAL:HG11	1:141:A:LYS:HE3	4	0.16
(1,559)	1:117:A:VAL:HG12	1:141:A:LYS:HE3	4	0.16
(1,559)	1:117:A:VAL:HG13	1:141:A:LYS:HE3	4	0.16
(1,558)	1:117:A:VAL:HG11	1:141:A:LYS:HE2	4	0.16
(1,558)	1:117:A:VAL:HG12	1:141:A:LYS:HE2	4	0.16
(1,558)	1:117:A:VAL:HG13	1:141:A:LYS:HE2	4	0.16
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	7	0.16
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	7	0.16
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	7	0.16
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	9	0.16
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	9	0.16
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	9	0.16
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG21	4	0.16
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG22	4	0.16
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG23	4	0.16
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG21	6	0.16
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG22	6	0.16
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG23	6	0.16
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	2	0.16
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	2	0.16
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	2	0.16
(1,502)	1:113:A:THR:HG21	1:150:A:PRO:HB3	1	0.16
(1,502)	1:113:A:THR:HG22	1:150:A:PRO:HB3	1	0.16
(1,502)	1:113:A:THR:HG23	1:150:A:PRO:HB3	1	0.16
(1,502)	1:113:A:THR:HG21	1:150:A:PRO:HB3	8	0.16
(1,502)	1:113:A:THR:HG22	1:150:A:PRO:HB3	8	0.16
(1,502)	1:113:A:THR:HG23	1:150:A:PRO:HB3	8	0.16
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG21	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG22	3	0.16
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG23	3	0.16
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG21	3	0.16
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG22	3	0.16
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG23	3	0.16
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG21	3	0.16
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG22	3	0.16
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG23	3	0.16
(1,347)	1:108:A:GLU:HG3	1:123:A:LYS:HD2	2	0.16
(1,337)	1:108:A:GLU:HA	1:108:A:GLU:HG3	1	0.16
(1,331)	1:107:A:ASP:HA	1:108:A:GLU:HG2	1	0.16
(1,298)	1:105:A:ALA:HB1	1:108:A:GLU:HB2	1	0.16
(1,298)	1:105:A:ALA:HB2	1:108:A:GLU:HB2	1	0.16
(1,298)	1:105:A:ALA:HB3	1:108:A:GLU:HB2	1	0.16
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	6	0.16
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	6	0.16
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	6	0.16
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	8	0.16
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	8	0.16
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	8	0.16
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	4	0.16
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	4	0.16
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	4	0.16
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	4	0.16
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	4	0.16
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	4	0.16
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	4	0.16
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	4	0.16
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	4	0.16
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	4	0.16
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	4	0.16
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	4	0.16
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	4	0.16
(1,155)	1:97:A:VAL:HG21	1:144:A:LEU:HB2	8	0.16
(1,155)	1:97:A:VAL:HG22	1:144:A:LEU:HB2	8	0.16
(1,155)	1:97:A:VAL:HG23	1:144:A:LEU:HB2	8	0.16
(1,154)	1:97:A:VAL:HG21	1:142:A:TYR:HE1	8	0.16
(1,154)	1:97:A:VAL:HG21	1:142:A:TYR:HE2	8	0.16
(1,154)	1:97:A:VAL:HG22	1:142:A:TYR:HE1	8	0.16
(1,154)	1:97:A:VAL:HG22	1:142:A:TYR:HE2	8	0.16
(1,154)	1:97:A:VAL:HG23	1:142:A:TYR:HE1	8	0.16
(1,154)	1:97:A:VAL:HG23	1:142:A:TYR:HE2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG21	5	0.16
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG22	5	0.16
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG23	5	0.16
(1,101)	1:96:A:ARG:HB3	1:166:A:GLU:HA	2	0.16
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG21	5	0.16
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG22	5	0.16
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG23	5	0.16
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	4	0.16
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	4	0.16
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	4	0.16
(1,72)	1:95:A:TRP:HB2	1:168:A:PRO:HB3	5	0.16
(1,60)	1:95:A:TRP:HB2	1:95:A:TRP:HE3	3	0.16
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	2	0.15
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	7	0.15
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	1	0.15
(1,4128)	1:155:B:SER:H	1:154:B:SER:HB2	5	0.15
(1,4115)	1:154:B:SER:H	1:155:B:SER:HB2	6	0.15
(1,4077)	1:152:B:GLN:HE21	1:149:B:ASP:HB2	6	0.15
(1,4034)	1:148:B:VAL:H	1:149:B:ASP:H	6	0.15
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD11	9	0.15
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD12	9	0.15
(1,4007)	1:144:B:LEU:H	1:144:B:LEU:HD13	9	0.15
(1,3955)	1:137:B:CYS:H	1:136:B:ARG:HB3	7	0.15
(1,3936)	1:134:B:ILE:H	1:127:B:ARG:HG2	4	0.15
(1,3936)	1:134:B:ILE:H	1:127:B:ARG:HG2	5	0.15
(1,3918)	1:131:B:HIS:H	1:130:B:GLU:HG2	2	0.15
(1,3907)	1:129:B:ASP:H	1:132:B:GLY:HA3	5	0.15
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	9	0.15
(1,3889)	1:128:B:GLN:HE22	1:128:B:GLN:HB2	3	0.15
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD1	9	0.15
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD2	9	0.15
(1,3826)	1:120:B:ILE:H	1:140:B:ARG:HG3	8	0.15
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG21	10	0.15
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG22	10	0.15
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG23	10	0.15
(1,3781)	1:117:B:VAL:H	1:115:B:ASP:HB2	6	0.15
(1,3739)	1:112:B:LYS:H	1:112:B:LYS:HB3	2	0.15
(1,3737)	1:112:B:LYS:H	1:111:B:VAL:HG11	5	0.15
(1,3737)	1:112:B:LYS:H	1:111:B:VAL:HG12	5	0.15
(1,3737)	1:112:B:LYS:H	1:111:B:VAL:HG13	5	0.15
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	10	0.15
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	10	0.15
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	4	0.15
(1,3672)	1:105:B:ALA:H	1:108:B:GLU:HB3	4	0.15
(1,3664)	1:102:B:ASN:HD22	1:161:B:GLY:HA3	6	0.15
(1,3608)	1:94:B:ARG:H	1:169:B:MET:HG2	10	0.15
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG21	8	0.15
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG22	8	0.15
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG23	8	0.15
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	9	0.15
(1,3557)	1:168:B:PRO:HA	1:169:B:MET:HG2	6	0.15
(1,3498)	1:161:B:GLY:HA3	1:163:B:LEU:HA	7	0.15
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	6	0.15
(1,3479)	1:159:B:PRO:HA	1:159:B:PRO:HB3	4	0.15
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	6	0.15
(1,3453)	1:157:B:LEU:HD11	1:163:B:LEU:HB2	5	0.15
(1,3453)	1:157:B:LEU:HD12	1:163:B:LEU:HB2	5	0.15
(1,3453)	1:157:B:LEU:HD13	1:163:B:LEU:HB2	5	0.15
(1,3444)	1:157:B:LEU:HG	1:161:B:GLY:HA3	3	0.15
(1,3438)	1:157:B:LEU:HB3	1:157:B:LEU:HG	9	0.15
(1,3430)	1:157:B:LEU:HA	1:163:B:LEU:HB3	2	0.15
(1,3430)	1:157:B:LEU:HA	1:163:B:LEU:HB3	3	0.15
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD21	3	0.15
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD22	3	0.15
(1,3421)	1:156:B:SER:HB3	1:157:B:LEU:HD23	3	0.15
(1,3391)	1:155:B:SER:HA	1:165:B:VAL:HA	6	0.15
(1,3358)	1:153:B:VAL:HA	1:168:B:PRO:HD2	4	0.15
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	5	0.15
(1,3270)	1:148:B:VAL:HA	1:169:B:MET:HA	5	0.15
(1,3266)	1:148:B:VAL:HA	1:149:B:ASP:HB3	1	0.15
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	8	0.15
(1,3143)	1:141:B:LYS:HG3	1:142:B:TYR:HB3	9	0.15
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	9	0.15
(1,3063)	1:131:B:HIS:HB2	1:132:B:GLY:HA2	10	0.15
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE1	1	0.15
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE2	1	0.15
(1,3018)	1:127:B:ARG:HA	1:127:B:ARG:HD3	4	0.15
(1,3018)	1:127:B:ARG:HA	1:127:B:ARG:HD3	6	0.15
(1,3005)	1:126:B:GLU:HG2	1:135:B:SER:HB3	1	0.15
(1,2993)	1:126:B:GLU:HB3	1:133:B:TYR:HB2	7	0.15
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	4	0.15
(1,2945)	1:121:B:THR:HA	1:139:B:THR:HA	9	0.15
(1,2929)	1:120:B:ILE:HG21	1:139:B:THR:HA	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:120:B:ILE:HG22	1:139:B:THR:HA	4	0.15
(1,2929)	1:120:B:ILE:HG23	1:139:B:THR:HA	4	0.15
(1,2929)	1:120:B:ILE:HG21	1:139:B:THR:HA	7	0.15
(1,2929)	1:120:B:ILE:HG22	1:139:B:THR:HA	7	0.15
(1,2929)	1:120:B:ILE:HG23	1:139:B:THR:HA	7	0.15
(1,2928)	1:120:B:ILE:HG21	1:122:B:GLY:HA3	10	0.15
(1,2928)	1:120:B:ILE:HG22	1:122:B:GLY:HA3	10	0.15
(1,2928)	1:120:B:ILE:HG23	1:122:B:GLY:HA3	10	0.15
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD11	2	0.15
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD12	2	0.15
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD13	2	0.15
(1,2918)	1:120:B:ILE:HB	1:142:B:TYR:HE1	10	0.15
(1,2918)	1:120:B:ILE:HB	1:142:B:TYR:HE2	10	0.15
(1,2900)	1:119:B:GLU:HG2	1:141:B:LYS:HE3	2	0.15
(1,2889)	1:119:B:GLU:HA	1:141:B:LYS:HA	3	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	2	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	2	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	2	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	2	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	2	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	2	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	2	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	2	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	2	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	6	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	6	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	6	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	6	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	6	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	6	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	6	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	6	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	6	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	10	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	10	0.15
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	10	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	10	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	10	0.15
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	10	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	10	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	10	0.15
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG11	4	0.15
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG12	4	0.15
(1,2832)	1:117:B:VAL:HA	1:148:B:VAL:HG13	4	0.15
(1,2831)	1:117:B:VAL:HA	1:148:B:VAL:HB	10	0.15
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG11	1	0.15
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG12	1	0.15
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG13	1	0.15
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG11	8	0.15
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG12	8	0.15
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG13	8	0.15
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG21	3	0.15
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG22	3	0.15
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG23	3	0.15
(1,2738)	1:112:B:LYS:HB2	1:120:B:ILE:HA	7	0.15
(1,2736)	1:112:B:LYS:HB2	1:112:B:LYS:HE3	9	0.15
(1,2708)	1:111:B:VAL:HG11	1:112:B:LYS:HE3	4	0.15
(1,2708)	1:111:B:VAL:HG12	1:112:B:LYS:HE3	4	0.15
(1,2708)	1:111:B:VAL:HG13	1:112:B:LYS:HE3	4	0.15
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	9	0.15
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	4	0.15
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	4	0.15
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	4	0.15
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	4	0.15
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	4	0.15
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	4	0.15
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	4	0.15
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	4	0.15
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	4	0.15
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	7	0.15
(1,2592)	1:106:B:PRO:HA	1:109:B:LEU:HB2	1	0.15
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	4	0.15
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	4	0.15
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	4	0.15
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD11	6	0.15
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD12	6	0.15
(1,2570)	1:105:B:ALA:HA	1:157:B:LEU:HD13	6	0.15
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD11	6	0.15
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD12	6	0.15
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD13	6	0.15
(1,2540)	1:100:B:ASP:HA	1:100:B:ASP:HB3	9	0.15
(1,2436)	1:97:B:VAL:HG21	1:144:B:LEU:HB2	8	0.15
(1,2436)	1:97:B:VAL:HG22	1:144:B:LEU:HB2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2436)	1:97:B:VAL:HG23	1:144:B:LEU:HB2	8	0.15
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG21	4	0.15
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG22	4	0.15
(1,2389)	1:96:B:ARG:HG2	1:97:B:VAL:HG23	4	0.15
(1,2361)	1:96:B:ARG:HA	1:96:B:ARG:HD3	7	0.15
(1,2361)	1:96:B:ARG:HA	1:96:B:ARG:HD3	10	0.15
(1,2355)	1:95:B:TRP:HB3	1:169:B:MET:HB3	1	0.15
(1,2342)	1:95:B:TRP:HB2	1:96:B:ARG:HA	8	0.15
(1,2318)	1:94:B:ARG:HB2	1:96:B:ARG:HA	6	0.15
(1,2304)	1:94:B:ARG:HA	1:94:B:ARG:HB3	10	0.15
(1,2225)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	2	0.15
(1,2225)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	2	0.15
(1,2225)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	2	0.15
(1,2225)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	8	0.15
(1,2225)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	8	0.15
(1,2225)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	8	0.15
(1,2160)	1:132:B:GLY:HA2	1:142:A:TYR:HB3	1	0.15
(1,2093)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	2	0.15
(1,2093)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	2	0.15
(1,2093)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	2	0.15
(1,2093)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	8	0.15
(1,2093)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	8	0.15
(1,2093)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	8	0.15
(1,2028)	1:132:B:GLY:HA2	1:142:A:TYR:HB3	1	0.15
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	10	0.15
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG11	9	0.15
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG12	9	0.15
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG13	9	0.15
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG21	6	0.15
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG22	6	0.15
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG23	6	0.15
(1,1901)	1:161:A:GLY:H	1:102:A:ASN:HB2	4	0.15
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG21	10	0.15
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG22	10	0.15
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG23	10	0.15
(1,1816)	1:153:A:VAL:H	1:149:A:ASP:HB2	4	0.15
(1,1766)	1:149:A:ASP:H	1:169:A:MET:HG3	4	0.15
(1,1743)	1:148:A:VAL:H	1:146:A:PRO:HB3	5	0.15
(1,1733)	1:147:A:GLY:H	1:146:A:PRO:HG2	8	0.15
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	5	0.15
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	5	0.15
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	10	0.15
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	10	0.15
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	10	0.15
(1,1703)	1:142:A:TYR:H	1:141:A:LYS:HG2	9	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD21	2	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD22	2	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD23	2	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD21	10	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD22	10	0.15
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD23	10	0.15
(1,1667)	1:135:A:SER:H	1:135:A:SER:HB2	9	0.15
(1,1647)	1:132:A:GLY:H	1:131:A:HIS:HB3	7	0.15
(1,1642)	1:132:A:GLY:H	1:129:A:ASP:HB2	4	0.15
(1,1626)	1:129:A:ASP:H	1:132:A:GLY:HA3	3	0.15
(1,1622)	1:129:A:ASP:H	1:129:A:ASP:HB3	9	0.15
(1,1611)	1:128:A:GLN:HE22	1:128:A:GLN:H	2	0.15
(1,1600)	1:128:A:GLN:H	1:127:A:ARG:HD2	1	0.15
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB1	7	0.15
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB2	7	0.15
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB3	7	0.15
(1,1546)	1:120:A:ILE:H	1:142:A:TYR:H	4	0.15
(1,1517)	1:118:A:VAL:H	1:142:A:TYR:HB2	5	0.15
(1,1509)	1:117:A:VAL:H	1:144:A:LEU:H	5	0.15
(1,1489)	1:114:A:LYS:H	1:119:A:GLU:H	2	0.15
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD11	3	0.15
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD12	3	0.15
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD13	3	0.15
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD11	5	0.15
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD12	5	0.15
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD13	5	0.15
(1,1389)	1:105:A:ALA:H	1:106:A:PRO:HD3	10	0.15
(1,1373)	1:102:A:ASN:HD21	1:161:A:GLY:HA2	2	0.15
(1,1345)	1:97:A:VAL:H	1:165:A:VAL:H	7	0.15
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	6	0.15
(1,1210)	1:160:A:GLU:HB2	1:162:A:THR:HB	6	0.15
(1,1197)	1:158:A:SER:HB3	1:159:A:PRO:HD3	3	0.15
(1,1189)	1:158:A:SER:HA	1:160:A:GLU:HB3	5	0.15
(1,1177)	1:157:A:LEU:HD21	1:161:A:GLY:HA3	4	0.15
(1,1177)	1:157:A:LEU:HD22	1:161:A:GLY:HA3	4	0.15
(1,1177)	1:157:A:LEU:HD23	1:161:A:GLY:HA3	4	0.15
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	3	0.15
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1149)	1:157:A:LEU:HA	1:163:A:LEU:HB3	4	0.15
(1,1148)	1:157:A:LEU:HA	1:162:A:THR:HB	2	0.15
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	4	0.15
(1,1119)	1:155:A:SER:HB2	1:165:A:VAL:HA	6	0.15
(1,1110)	1:155:A:SER:HA	1:165:A:VAL:HA	10	0.15
(1,1035)	1:150:A:PRO:HA	1:150:A:PRO:HB3	6	0.15
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	5	0.15
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	10	0.15
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	3	0.15
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	5	0.15
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	5	0.15
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	5	0.15
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG11	9	0.15
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG12	9	0.15
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG13	9	0.15
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG11	9	0.15
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG12	9	0.15
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG13	9	0.15
(1,862)	1:141:A:LYS:HG3	1:142:A:TYR:HB3	6	0.15
(1,845)	1:141:A:LYS:HA	1:141:A:LYS:HD3	1	0.15
(1,816)	1:137:A:CYS:HA	1:138:A:PHE:HD1	8	0.15
(1,816)	1:137:A:CYS:HA	1:138:A:PHE:HD2	8	0.15
(1,779)	1:131:A:HIS:HA	1:131:A:HIS:HE1	3	0.15
(1,772)	1:130:A:GLU:HA	1:130:A:GLU:HG2	4	0.15
(1,734)	1:127:A:ARG:HA	1:127:A:ARG:HB3	2	0.15
(1,717)	1:126:A:GLU:HG2	1:127:A:ARG:HG3	9	0.15
(1,700)	1:125:A:GLU:HA	1:125:A:GLU:HG3	5	0.15
(1,699)	1:125:A:GLU:HA	1:125:A:GLU:HG2	8	0.15
(1,680)	1:123:A:LYS:HA	1:123:A:LYS:HG3	6	0.15
(1,664)	1:121:A:THR:HA	1:139:A:THR:HA	5	0.15
(1,664)	1:121:A:THR:HA	1:139:A:THR:HA	7	0.15
(1,652)	1:120:A:ILE:HD11	1:140:A:ARG:HB2	6	0.15
(1,652)	1:120:A:ILE:HD12	1:140:A:ARG:HB2	6	0.15
(1,652)	1:120:A:ILE:HD13	1:140:A:ARG:HB2	6	0.15
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD11	4	0.15
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD12	4	0.15
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD13	4	0.15
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	9	0.15
(1,637)	1:120:A:ILE:HB	1:142:A:TYR:HE1	10	0.15
(1,637)	1:120:A:ILE:HB	1:142:A:TYR:HE2	10	0.15
(1,610)	1:119:A:GLU:HA	1:141:A:LYS:HD3	9	0.15
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	7	0.15
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	7	0.15
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	7	0.15
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	7	0.15
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	7	0.15
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD21	6	0.15
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD22	6	0.15
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD23	6	0.15
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG21	9	0.15
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG22	9	0.15
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG23	9	0.15
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	6	0.15
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	6	0.15
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	6	0.15
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG21	1	0.15
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG22	1	0.15
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG23	1	0.15
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	6	0.15
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	6	0.15
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	6	0.15
(1,383)	1:109:A:LEU:HD21	1:122:A:GLY:HA3	10	0.15
(1,383)	1:109:A:LEU:HD22	1:122:A:GLY:HA3	10	0.15
(1,383)	1:109:A:LEU:HD23	1:122:A:GLY:HA3	10	0.15
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	7	0.15
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	7	0.15
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	7	0.15
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	7	0.15
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	7	0.15
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	7	0.15
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	7	0.15
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	7	0.15
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	7	0.15
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD11	8	0.15
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD12	8	0.15
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD13	8	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD21	4	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD22	4	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD23	4	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD21	6	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD22	6	0.15
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD23	6	0.15
(1,298)	1:105:A:ALA:HB1	1:108:A:GLU:HB2	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:105:A:ALA:HB2	1:108:A:GLU:HB2	6	0.15
(1,298)	1:105:A:ALA:HB3	1:108:A:GLU:HB2	6	0.15
(1,206)	1:99:A:LEU:HA	1:120:A:ILE:HD11	2	0.15
(1,206)	1:99:A:LEU:HA	1:120:A:ILE:HD12	2	0.15
(1,206)	1:99:A:LEU:HA	1:120:A:ILE:HD13	2	0.15
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG21	2	0.15
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG22	2	0.15
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG23	2	0.15
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	7	0.15
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	7	0.15
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	7	0.15
(1,80)	1:96:A:ARG:HA	1:96:A:ARG:HD3	9	0.15
(1,76)	1:95:A:TRP:HE3	1:166:A:GLU:HA	10	0.15
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	1	0.15
(1,4280)	1:169:B:MET:H	1:169:B:MET:HB3	6	0.14
(1,4278)	1:169:B:MET:H	1:169:B:MET:HA	4	0.14
(1,4262)	1:167:B:ALA:H	1:166:B:GLU:HB2	1	0.14
(1,4239)	1:165:B:VAL:H	1:166:B:GLU:HB3	10	0.14
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD11	9	0.14
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD12	9	0.14
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD13	9	0.14
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	6	0.14
(1,4183)	1:161:B:GLY:H	1:102:B:ASN:HB3	9	0.14
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG21	3	0.14
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG22	3	0.14
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG23	3	0.14
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG21	5	0.14
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG22	5	0.14
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG23	5	0.14
(1,4089)	1:152:B:GLN:HE22	1:152:B:GLN:HB2	4	0.14
(1,4085)	1:152:B:GLN:HE21	1:169:B:MET:HA	10	0.14
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	5	0.14
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	5	0.14
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	5	0.14
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	6	0.14
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	6	0.14
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	6	0.14
(1,4075)	1:152:B:GLN:H	1:168:B:PRO:HD3	5	0.14
(1,4033)	1:148:B:VAL:H	1:149:B:ASP:HB2	1	0.14
(1,4014)	1:147:B:GLY:H	1:146:B:PRO:HG2	9	0.14
(1,3936)	1:134:B:ILE:H	1:127:B:ARG:HG2	1	0.14
(1,3915)	1:131:B:HIS:H	1:129:B:ASP:HB3	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3910)	1:129:B:ASP:H	1:133:B:TYR:HB2	2	0.14
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	3	0.14
(1,3879)	1:128:B:GLN:H	1:127:B:ARG:HG2	3	0.14
(1,3869)	1:126:B:GLU:H	1:125:B:GLU:HG3	8	0.14
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG21	1	0.14
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG22	1	0.14
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG23	1	0.14
(1,3759)	1:114:B:LYS:H	1:112:B:LYS:HD3	1	0.14
(1,3733)	1:112:B:LYS:H	1:99:B:LEU:HD21	2	0.14
(1,3733)	1:112:B:LYS:H	1:99:B:LEU:HD22	2	0.14
(1,3733)	1:112:B:LYS:H	1:99:B:LEU:HD23	2	0.14
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD11	9	0.14
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD12	9	0.14
(1,3730)	1:111:B:VAL:H	1:120:B:ILE:HD13	9	0.14
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD11	2	0.14
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD12	2	0.14
(1,3666)	1:103:B:HIS:H	1:157:B:LEU:HD13	2	0.14
(1,3654)	1:102:B:ASN:HD21	1:161:B:GLY:HA2	8	0.14
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG21	4	0.14
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG22	4	0.14
(1,3638)	1:99:B:LEU:H	1:101:B:VAL:HG23	4	0.14
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	5	0.14
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	8	0.14
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	2	0.14
(1,3453)	1:157:B:LEU:HD11	1:163:B:LEU:HB2	8	0.14
(1,3453)	1:157:B:LEU:HD12	1:163:B:LEU:HB2	8	0.14
(1,3453)	1:157:B:LEU:HD13	1:163:B:LEU:HB2	8	0.14
(1,3449)	1:157:B:LEU:HD11	1:161:B:GLY:HA3	9	0.14
(1,3449)	1:157:B:LEU:HD12	1:161:B:GLY:HA3	9	0.14
(1,3449)	1:157:B:LEU:HD13	1:161:B:GLY:HA3	9	0.14
(1,3438)	1:157:B:LEU:HB3	1:157:B:LEU:HG	6	0.14
(1,3360)	1:153:B:VAL:HB	1:154:B:SER:HA	10	0.14
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG21	2	0.14
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG22	2	0.14
(1,3317)	1:150:B:PRO:HA	1:151:B:THR:HG23	2	0.14
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	1	0.14
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	3	0.14
(1,3316)	1:150:B:PRO:HA	1:150:B:PRO:HB3	7	0.14
(1,3301)	1:148:B:VAL:HG21	1:169:B:MET:HB2	2	0.14
(1,3301)	1:148:B:VAL:HG22	1:169:B:MET:HB2	2	0.14
(1,3301)	1:148:B:VAL:HG23	1:169:B:MET:HB2	2	0.14
(1,3278)	1:148:B:VAL:HB	1:150:B:PRO:HA	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3274)	1:148:B:VAL:HA	1:170:B:PRO:HG2	7	0.14
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	7	0.14
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	7	0.14
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	7	0.14
(1,3123)	1:141:B:LYS:HA	1:141:B:LYS:HB2	10	0.14
(1,3024)	1:127:B:ARG:HB3	1:127:B:ARG:HD2	9	0.14
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD11	3	0.14
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD12	3	0.14
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD13	3	0.14
(1,2989)	1:126:B:GLU:HA	1:134:B:ILE:HG21	7	0.14
(1,2989)	1:126:B:GLU:HA	1:134:B:ILE:HG22	7	0.14
(1,2989)	1:126:B:GLU:HA	1:134:B:ILE:HG23	7	0.14
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD11	6	0.14
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD12	6	0.14
(1,2921)	1:120:B:ILE:HG12	1:163:B:LEU:HD13	6	0.14
(1,2918)	1:120:B:ILE:HB	1:142:B:TYR:HE1	1	0.14
(1,2918)	1:120:B:ILE:HB	1:142:B:TYR:HE2	1	0.14
(1,2883)	1:119:B:GLU:HA	1:119:B:GLU:HG3	8	0.14
(1,2883)	1:119:B:GLU:HA	1:119:B:GLU:HG3	10	0.14
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG21	2	0.14
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG22	2	0.14
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG23	2	0.14
(1,2799)	1:115:B:ASP:HB3	1:150:B:PRO:HG3	2	0.14
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG21	3	0.14
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG22	3	0.14
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG23	3	0.14
(1,2753)	1:112:B:LYS:HD2	1:120:B:ILE:HA	10	0.14
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE3	2	0.14
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE3	4	0.14
(1,2716)	1:111:B:VAL:HG11	1:120:B:ILE:HG13	4	0.14
(1,2716)	1:111:B:VAL:HG12	1:120:B:ILE:HG13	4	0.14
(1,2716)	1:111:B:VAL:HG13	1:120:B:ILE:HG13	4	0.14
(1,2704)	1:111:B:VAL:HB	1:112:B:LYS:HA	5	0.14
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	8	0.14
(1,2685)	1:110:B:THR:HG21	1:112:B:LYS:HB2	1	0.14
(1,2685)	1:110:B:THR:HG22	1:112:B:LYS:HB2	1	0.14
(1,2685)	1:110:B:THR:HG23	1:112:B:LYS:HB2	1	0.14
(1,2654)	1:109:B:LEU:HD11	1:161:B:GLY:HA3	4	0.14
(1,2654)	1:109:B:LEU:HD12	1:161:B:GLY:HA3	4	0.14
(1,2654)	1:109:B:LEU:HD13	1:161:B:GLY:HA3	4	0.14
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	3	0.14
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	3	0.14
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	3	0.14
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	3	0.14
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	3	0.14
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	3	0.14
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	3	0.14
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	3	0.14
(1,2561)	1:102:B:ASN:HB3	1:161:B:GLY:HA3	8	0.14
(1,2561)	1:102:B:ASN:HB3	1:161:B:GLY:HA3	10	0.14
(1,2560)	1:102:B:ASN:HB3	1:161:B:GLY:HA2	2	0.14
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD11	8	0.14
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD12	8	0.14
(1,2553)	1:101:B:VAL:HG21	1:120:B:ILE:HD13	8	0.14
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD11	8	0.14
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD12	8	0.14
(1,2553)	1:101:B:VAL:HG22	1:120:B:ILE:HD13	8	0.14
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD11	8	0.14
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD12	8	0.14
(1,2553)	1:101:B:VAL:HG23	1:120:B:ILE:HD13	8	0.14
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG11	1	0.14
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG12	1	0.14
(1,2510)	1:99:B:LEU:HD11	1:111:B:VAL:HG13	1	0.14
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG11	1	0.14
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG12	1	0.14
(1,2510)	1:99:B:LEU:HD12	1:111:B:VAL:HG13	1	0.14
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG11	1	0.14
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG12	1	0.14
(1,2510)	1:99:B:LEU:HD13	1:111:B:VAL:HG13	1	0.14
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD11	4	0.14
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD12	4	0.14
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD13	4	0.14
(1,2432)	1:97:B:VAL:HG21	1:142:B:TYR:HB2	5	0.14
(1,2432)	1:97:B:VAL:HG22	1:142:B:TYR:HB2	5	0.14
(1,2432)	1:97:B:VAL:HG23	1:142:B:TYR:HB2	5	0.14
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD1	9	0.14
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD2	9	0.14
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD1	9	0.14
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD2	9	0.14
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD1	9	0.14
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD2	9	0.14
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	4	0.14
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	4	0.14
(1,2380)	1:96:B:ARG:HB3	1:164:B:THR:HB	1	0.14
(1,2357)	1:95:B:TRP:HE3	1:166:B:GLU:HA	7	0.14
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	1	0.14
(1,2310)	1:94:B:ARG:HA	1:168:B:PRO:HA	1	0.14
(1,2284)	1:89:B:ARG:HB2	1:90:B:HIS:HB2	4	0.14
(1,2170)	1:132:A:GLY:HA3	1:142:B:TYR:HA	5	0.14
(1,2038)	1:132:A:GLY:HA3	1:142:B:TYR:HA	5	0.14
(1,1925)	1:162:A:THR:H	1:160:A:GLU:HG3	5	0.14
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	7	0.14
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	10	0.14
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG21	4	0.14
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG22	4	0.14
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG23	4	0.14
(1,1877)	1:158:A:SER:H	1:109:A:LEU:HD11	2	0.14
(1,1877)	1:158:A:SER:H	1:109:A:LEU:HD12	2	0.14
(1,1877)	1:158:A:SER:H	1:109:A:LEU:HD13	2	0.14
(1,1870)	1:157:A:LEU:H	1:157:A:LEU:HB3	5	0.14
(1,1847)	1:155:A:SER:H	1:154:A:SER:HB2	3	0.14
(1,1834)	1:154:A:SER:H	1:155:A:SER:HB2	6	0.14
(1,1771)	1:151:A:THR:H	1:149:A:ASP:HB3	6	0.14
(1,1762)	1:149:A:ASP:H	1:152:A:GLN:HB2	6	0.14
(1,1743)	1:148:A:VAL:H	1:146:A:PRO:HB3	9	0.14
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	9	0.14
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	9	0.14
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	9	0.14
(1,1703)	1:142:A:TYR:H	1:141:A:LYS:HG3	6	0.14
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG21	1	0.14
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG22	1	0.14
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG23	1	0.14
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG21	7	0.14
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG22	7	0.14
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG23	7	0.14
(1,1657)	1:134:A:ILE:H	1:133:A:TYR:HB3	1	0.14
(1,1657)	1:134:A:ILE:H	1:133:A:TYR:HB3	2	0.14
(1,1657)	1:134:A:ILE:H	1:133:A:TYR:HB3	3	0.14
(1,1657)	1:134:A:ILE:H	1:133:A:TYR:HB3	5	0.14
(1,1651)	1:132:A:GLY:H	1:133:A:TYR:HE1	9	0.14
(1,1651)	1:132:A:GLY:H	1:133:A:TYR:HE2	9	0.14
(1,1606)	1:128:A:GLN:H	1:133:A:TYR:HD1	3	0.14
(1,1606)	1:128:A:GLN:H	1:133:A:TYR:HD2	3	0.14
(1,1581)	1:125:A:GLU:H	1:108:A:GLU:HG3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD11	3	0.14
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD12	3	0.14
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD13	3	0.14
(1,1566)	1:123:A:LYS:H	1:109:A:LEU:HB2	1	0.14
(1,1525)	1:119:A:GLU:H	1:114:A:LYS:HB3	1	0.14
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG21	3	0.14
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG22	3	0.14
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG23	3	0.14
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG21	8	0.14
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG22	8	0.14
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG23	8	0.14
(1,1428)	1:109:A:LEU:H	1:109:A:LEU:HB3	7	0.14
(1,1400)	1:107:A:ASP:H	1:106:A:PRO:HB3	7	0.14
(1,1391)	1:105:A:ALA:H	1:108:A:GLU:HB3	3	0.14
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD11	6	0.14
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD12	6	0.14
(1,1385)	1:103:A:HIS:H	1:157:A:LEU:HD13	6	0.14
(1,1383)	1:102:A:ASN:HD22	1:161:A:GLY:HA3	7	0.14
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD11	2	0.14
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD12	2	0.14
(1,1371)	1:102:A:ASN:HD21	1:157:A:LEU:HD13	2	0.14
(1,1318)	1:171:A:LYS:HA	1:171:A:LYS:HD2	6	0.14
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	8	0.14
(1,1282)	1:168:A:PRO:HB3	1:169:A:MET:HA	3	0.14
(1,1174)	1:157:A:LEU:HD11	1:163:A:LEU:HG	10	0.14
(1,1174)	1:157:A:LEU:HD12	1:163:A:LEU:HG	10	0.14
(1,1174)	1:157:A:LEU:HD13	1:163:A:LEU:HG	10	0.14
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	1	0.14
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	2	0.14
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD11	10	0.14
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD12	10	0.14
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD13	10	0.14
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD21	8	0.14
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD22	8	0.14
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD23	8	0.14
(1,1110)	1:155:A:SER:HA	1:165:A:VAL:HA	7	0.14
(1,1110)	1:155:A:SER:HA	1:165:A:VAL:HA	9	0.14
(1,1098)	1:154:A:SER:HB3	1:166:A:GLU:HG3	8	0.14
(1,1079)	1:153:A:VAL:HB	1:154:A:SER:HA	3	0.14
(1,1065)	1:152:A:GLN:HB2	1:169:A:MET:HA	2	0.14
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	3	0.14
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:148:A:VAL:HA	1:170:A:PRO:HB3	1	0.14
(1,977)	1:147:A:GLY:HA3	1:148:A:VAL:HB	5	0.14
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	2	0.14
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG2	5	0.14
(1,962)	1:145:A:PRO:HD2	1:146:A:PRO:HG3	10	0.14
(1,917)	1:144:A:LEU:HB3	1:147:A:GLY:HA2	9	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	1	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	1	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	1	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	2	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	2	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	2	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	3	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	3	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	3	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	10	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	10	0.14
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	10	0.14
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG21	9	0.14
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG22	9	0.14
(1,883)	1:142:A:TYR:HD1	1:165:A:VAL:HG23	9	0.14
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG21	9	0.14
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG22	9	0.14
(1,883)	1:142:A:TYR:HD2	1:165:A:VAL:HG23	9	0.14
(1,857)	1:141:A:LYS:HG2	1:143:A:THR:HA	4	0.14
(1,857)	1:141:A:LYS:HG2	1:143:A:THR:HA	6	0.14
(1,853)	1:141:A:LYS:HG2	1:141:A:LYS:HE3	5	0.14
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	10	0.14
(1,831)	1:139:A:THR:HB	1:141:A:LYS:HE2	7	0.14
(1,766)	1:129:A:ASP:HA	1:130:A:GLU:HB2	1	0.14
(1,759)	1:128:A:GLN:HG2	1:133:A:TYR:HA	5	0.14
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD11	4	0.14
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD12	4	0.14
(1,751)	1:128:A:GLN:HA	1:134:A:ILE:HD13	4	0.14
(1,690)	1:123:A:LYS:HB3	1:137:A:CYS:HB2	1	0.14
(1,684)	1:123:A:LYS:HA	1:135:A:SER:HB3	1	0.14
(1,652)	1:120:A:ILE:HD11	1:140:A:ARG:HB2	8	0.14
(1,652)	1:120:A:ILE:HD12	1:140:A:ARG:HB2	8	0.14
(1,652)	1:120:A:ILE:HD13	1:140:A:ARG:HB2	8	0.14
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD1	1	0.14
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD2	1	0.14
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD1	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD2	1	0.14
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD1	1	0.14
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD2	1	0.14
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD11	6	0.14
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD12	6	0.14
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD13	6	0.14
(1,605)	1:119:A:GLU:HA	1:120:A:ILE:HG13	3	0.14
(1,604)	1:119:A:GLU:HA	1:120:A:ILE:HG12	6	0.14
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG11	2	0.14
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG12	2	0.14
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG13	2	0.14
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG11	2	0.14
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG12	2	0.14
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG13	2	0.14
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG11	2	0.14
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG12	2	0.14
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG13	2	0.14
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	3	0.14
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	3	0.14
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	3	0.14
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	3	0.14
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	3	0.14
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	3	0.14
(1,571)	1:118:A:VAL:HB	1:142:A:TYR:HD1	10	0.14
(1,571)	1:118:A:VAL:HB	1:142:A:TYR:HD2	10	0.14
(1,562)	1:117:A:VAL:HG11	1:142:A:TYR:HB3	4	0.14
(1,562)	1:117:A:VAL:HG12	1:142:A:TYR:HB3	4	0.14
(1,562)	1:117:A:VAL:HG13	1:142:A:TYR:HB3	4	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	5	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	5	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	5	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	8	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	8	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	8	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	10	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	10	0.14
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	10	0.14
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG11	10	0.14
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG12	10	0.14
(1,529)	1:116:A:GLY:HA2	1:148:A:VAL:HG13	10	0.14
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	7	0.14
(1,463)	1:112:A:LYS:HG2	1:112:A:LYS:HE3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	10	0.14
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	5	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	1	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	1	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	1	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	1	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	1	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	1	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	1	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	1	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	1	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	4	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	4	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	4	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	4	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	4	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	4	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	4	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	4	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	4	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	5	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	5	0.14
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	5	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	5	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	5	0.14
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	5	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	5	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	5	0.14
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	5	0.14
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD21	9	0.14
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD22	9	0.14
(1,335)	1:107:A:ASP:HA	1:157:A:LEU:HD23	9	0.14
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	9	0.14
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	9	0.14
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	9	0.14
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	10	0.14
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	10	0.14
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	10	0.14
(1,265)	1:100:A:ASP:HB3	1:162:A:THR:HA	9	0.14
(1,264)	1:100:A:ASP:HB2	1:162:A:THR:HB	4	0.14
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG11	5	0.14
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG12	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:99:A:LEU:HD21	1:111:A:VAL:HG13	5	0.14
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG11	5	0.14
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG12	5	0.14
(1,240)	1:99:A:LEU:HD22	1:111:A:VAL:HG13	5	0.14
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG11	5	0.14
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG12	5	0.14
(1,240)	1:99:A:LEU:HD23	1:111:A:VAL:HG13	5	0.14
(1,236)	1:99:A:LEU:HD11	1:164:A:THR:HA	8	0.14
(1,236)	1:99:A:LEU:HD12	1:164:A:THR:HA	8	0.14
(1,236)	1:99:A:LEU:HD13	1:164:A:THR:HA	8	0.14
(1,203)	1:99:A:LEU:HA	1:100:A:ASP:HB3	7	0.14
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD21	9	0.14
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD22	9	0.14
(1,201)	1:99:A:LEU:HA	1:99:A:LEU:HD23	9	0.14
(1,161)	1:97:A:VAL:HG21	1:166:A:GLU:HA	5	0.14
(1,161)	1:97:A:VAL:HG22	1:166:A:GLU:HA	5	0.14
(1,161)	1:97:A:VAL:HG23	1:166:A:GLU:HA	5	0.14
(1,143)	1:97:A:VAL:HG11	1:142:A:TYR:HE1	7	0.14
(1,143)	1:97:A:VAL:HG11	1:142:A:TYR:HE2	7	0.14
(1,143)	1:97:A:VAL:HG12	1:142:A:TYR:HE1	7	0.14
(1,143)	1:97:A:VAL:HG12	1:142:A:TYR:HE2	7	0.14
(1,143)	1:97:A:VAL:HG13	1:142:A:TYR:HE1	7	0.14
(1,143)	1:97:A:VAL:HG13	1:142:A:TYR:HE2	7	0.14
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG21	6	0.14
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG22	6	0.14
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG23	6	0.14
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG21	10	0.14
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG22	10	0.14
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG23	10	0.14
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	3	0.14
(1,23)	1:94:A:ARG:HA	1:94:A:ARG:HB3	7	0.14
(1,4220)	1:164:B:THR:H	1:162:B:THR:HA	9	0.13
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD11	5	0.13
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD12	5	0.13
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD13	5	0.13
(1,4196)	1:162:B:THR:H	1:102:B:ASN:HB2	5	0.13
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG21	2	0.13
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG22	2	0.13
(1,4168)	1:158:B:SER:H	1:162:B:THR:HG23	2	0.13
(1,4160)	1:158:B:SER:H	1:157:B:LEU:HG	5	0.13
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD11	9	0.13
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD12	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD13	9	0.13
(1,4096)	1:153:B:VAL:H	1:113:B:THR:HG21	2	0.13
(1,4096)	1:153:B:VAL:H	1:113:B:THR:HG22	2	0.13
(1,4096)	1:153:B:VAL:H	1:113:B:THR:HG23	2	0.13
(1,4089)	1:152:B:GLN:HE22	1:152:B:GLN:HB2	8	0.13
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	2	0.13
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	2	0.13
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	2	0.13
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG21	8	0.13
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG22	8	0.13
(1,4078)	1:152:B:GLN:HE21	1:151:B:THR:HG23	8	0.13
(1,4043)	1:149:B:ASP:H	1:152:B:GLN:HB2	4	0.13
(1,4043)	1:149:B:ASP:H	1:152:B:GLN:HB2	10	0.13
(1,4034)	1:148:B:VAL:H	1:149:B:ASP:H	1	0.13
(1,3935)	1:134:B:ILE:H	1:127:B:ARG:HB2	9	0.13
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE1	4	0.13
(1,3932)	1:132:B:GLY:H	1:133:B:TYR:HE2	4	0.13
(1,3928)	1:132:B:GLY:H	1:131:B:HIS:HB3	7	0.13
(1,3928)	1:132:B:GLY:H	1:131:B:HIS:HB3	8	0.13
(1,3881)	1:128:B:GLN:H	1:127:B:ARG:HD2	8	0.13
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD1	5	0.13
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD2	5	0.13
(1,3848)	1:123:B:LYS:H	1:109:B:LEU:HG	3	0.13
(1,3834)	1:121:B:THR:H	1:120:B:ILE:HG13	9	0.13
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD11	8	0.13
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD12	8	0.13
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD13	8	0.13
(1,3806)	1:119:B:GLU:H	1:114:B:LYS:HB3	2	0.13
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	4	0.13
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	2	0.13
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	8	0.13
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG21	5	0.13
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG22	5	0.13
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG23	5	0.13
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG21	2	0.13
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG22	2	0.13
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG23	2	0.13
(1,3770)	1:114:B:LYS:H	1:119:B:GLU:H	6	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD21	2	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD22	2	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD23	2	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD11	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD12	9	0.13
(1,3702)	1:108:B:GLU:H	1:109:B:LEU:HD13	9	0.13
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	5	0.13
(1,3614)	1:95:B:TRP:H	1:166:B:GLU:HG3	7	0.13
(1,3608)	1:94:B:ARG:H	1:169:B:MET:HG2	9	0.13
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	10	0.13
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	7	0.13
(1,3479)	1:159:B:PRO:HA	1:159:B:PRO:HB3	7	0.13
(1,3478)	1:158:B:SER:HB3	1:159:B:PRO:HD3	2	0.13
(1,3474)	1:158:B:SER:HB3	1:160:B:GLU:HB3	4	0.13
(1,3474)	1:158:B:SER:HB3	1:160:B:GLU:HB3	10	0.13
(1,3454)	1:157:B:LEU:HD11	1:163:B:LEU:HB3	6	0.13
(1,3454)	1:157:B:LEU:HD12	1:163:B:LEU:HB3	6	0.13
(1,3454)	1:157:B:LEU:HD13	1:163:B:LEU:HB3	6	0.13
(1,3438)	1:157:B:LEU:HB3	1:157:B:LEU:HG	1	0.13
(1,3385)	1:155:B:SER:HA	1:156:B:SER:HB3	3	0.13
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG21	9	0.13
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG22	9	0.13
(1,3381)	1:154:B:SER:HB2	1:165:B:VAL:HG23	9	0.13
(1,3360)	1:153:B:VAL:HB	1:154:B:SER:HA	5	0.13
(1,3358)	1:153:B:VAL:HA	1:168:B:PRO:HD2	7	0.13
(1,3288)	1:148:B:VAL:HG11	1:153:B:VAL:HA	7	0.13
(1,3288)	1:148:B:VAL:HG12	1:153:B:VAL:HA	7	0.13
(1,3288)	1:148:B:VAL:HG13	1:153:B:VAL:HA	7	0.13
(1,3288)	1:148:B:VAL:HG11	1:153:B:VAL:HA	10	0.13
(1,3288)	1:148:B:VAL:HG12	1:153:B:VAL:HA	10	0.13
(1,3288)	1:148:B:VAL:HG13	1:153:B:VAL:HA	10	0.13
(1,3258)	1:147:B:GLY:HA3	1:148:B:VAL:HB	9	0.13
(1,3249)	1:146:B:PRO:HB3	1:147:B:GLY:HA3	7	0.13
(1,3239)	1:145:B:PRO:HG3	1:146:B:PRO:HD2	5	0.13
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	10	0.13
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	10	0.13
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	10	0.13
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	3	0.13
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	3	0.13
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	3	0.13
(1,3163)	1:142:B:TYR:HD1	1:165:B:VAL:HG11	2	0.13
(1,3163)	1:142:B:TYR:HD1	1:165:B:VAL:HG12	2	0.13
(1,3163)	1:142:B:TYR:HD1	1:165:B:VAL:HG13	2	0.13
(1,3163)	1:142:B:TYR:HD2	1:165:B:VAL:HG11	2	0.13
(1,3163)	1:142:B:TYR:HD2	1:165:B:VAL:HG12	2	0.13
(1,3163)	1:142:B:TYR:HD2	1:165:B:VAL:HG13	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3153)	1:142:B:TYR:HB2	1:143:B:THR:HB	5	0.13
(1,3143)	1:141:B:LYS:HG3	1:142:B:TYR:HB3	5	0.13
(1,3133)	1:141:B:LYS:HG2	1:141:B:LYS:HE2	2	0.13
(1,3093)	1:136:B:ARG:HA	1:136:B:ARG:HD2	10	0.13
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD1	3	0.13
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD2	3	0.13
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD1	3	0.13
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD2	3	0.13
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD1	3	0.13
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD2	3	0.13
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD1	10	0.13
(1,3078)	1:134:B:ILE:HG21	1:133:B:TYR:HD2	10	0.13
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD1	10	0.13
(1,3078)	1:134:B:ILE:HG22	1:133:B:TYR:HD2	10	0.13
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD1	10	0.13
(1,3078)	1:134:B:ILE:HG23	1:133:B:TYR:HD2	10	0.13
(1,3048)	1:129:B:ASP:HA	1:133:B:TYR:HA	4	0.13
(1,3037)	1:128:B:GLN:HB3	1:133:B:TYR:HD1	9	0.13
(1,3037)	1:128:B:GLN:HB3	1:133:B:TYR:HD2	9	0.13
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE1	5	0.13
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE2	5	0.13
(1,3015)	1:127:B:ARG:HA	1:127:B:ARG:HB3	1	0.13
(1,3015)	1:127:B:ARG:HA	1:127:B:ARG:HB3	9	0.13
(1,2985)	1:125:B:GLU:HA	1:135:B:SER:HB3	2	0.13
(1,2963)	1:123:B:LYS:HA	1:123:B:LYS:HE2	7	0.13
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	10	0.13
(1,2933)	1:120:B:ILE:HD11	1:140:B:ARG:HB2	4	0.13
(1,2933)	1:120:B:ILE:HD12	1:140:B:ARG:HB2	4	0.13
(1,2933)	1:120:B:ILE:HD13	1:140:B:ARG:HB2	4	0.13
(1,2928)	1:120:B:ILE:HG21	1:122:B:GLY:HA3	7	0.13
(1,2928)	1:120:B:ILE:HG22	1:122:B:GLY:HA3	7	0.13
(1,2928)	1:120:B:ILE:HG23	1:122:B:GLY:HA3	7	0.13
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	5	0.13
(1,2885)	1:119:B:GLU:HA	1:120:B:ILE:HG12	5	0.13
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	7	0.13
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	7	0.13
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	7	0.13
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	7	0.13
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	7	0.13
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	7	0.13
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	7	0.13
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	7	0.13
(1,2866)	1:118:B:VAL:HG11	1:142:B:TYR:HD1	9	0.13
(1,2866)	1:118:B:VAL:HG11	1:142:B:TYR:HD2	9	0.13
(1,2866)	1:118:B:VAL:HG12	1:142:B:TYR:HD1	9	0.13
(1,2866)	1:118:B:VAL:HG12	1:142:B:TYR:HD2	9	0.13
(1,2866)	1:118:B:VAL:HG13	1:142:B:TYR:HD1	9	0.13
(1,2866)	1:118:B:VAL:HG13	1:142:B:TYR:HD2	9	0.13
(1,2858)	1:118:B:VAL:HB	1:153:B:VAL:HG21	5	0.13
(1,2858)	1:118:B:VAL:HB	1:153:B:VAL:HG22	5	0.13
(1,2858)	1:118:B:VAL:HB	1:153:B:VAL:HG23	5	0.13
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD21	9	0.13
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD22	9	0.13
(1,2847)	1:118:B:VAL:HA	1:144:B:LEU:HD23	9	0.13
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG21	6	0.13
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG22	6	0.13
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG23	6	0.13
(1,2798)	1:115:B:ASP:HB3	1:150:B:PRO:HG2	2	0.13
(1,2754)	1:112:B:LYS:HE2	1:114:B:LYS:HB2	10	0.13
(1,2753)	1:112:B:LYS:HD2	1:120:B:ILE:HA	9	0.13
(1,2740)	1:112:B:LYS:HB3	1:112:B:LYS:HE2	6	0.13
(1,2738)	1:112:B:LYS:HB2	1:120:B:ILE:HA	4	0.13
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG21	1	0.13
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG22	1	0.13
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG23	1	0.13
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG21	1	0.13
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG22	1	0.13
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG23	1	0.13
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG21	1	0.13
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG22	1	0.13
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG23	1	0.13
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	1	0.13
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	10	0.13
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD21	8	0.13
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD22	8	0.13
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD23	8	0.13
(1,2640)	1:109:B:LEU:HB2	1:122:B:GLY:HA2	4	0.13
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD11	7	0.13
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD12	7	0.13
(1,2639)	1:109:B:LEU:HB2	1:109:B:LEU:HD13	7	0.13
(1,2613)	1:107:B:ASP:HA	1:108:B:GLU:HG3	1	0.13
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD11	7	0.13
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD12	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD13	7	0.13
(1,2564)	1:105:B:ALA:HA	1:106:B:PRO:HB3	7	0.13
(1,2559)	1:102:B:ASN:HB2	1:161:B:GLY:HA3	4	0.13
(1,2446)	1:97:B:VAL:HG11	1:99:B:LEU:HD21	8	0.13
(1,2446)	1:97:B:VAL:HG11	1:99:B:LEU:HD22	8	0.13
(1,2446)	1:97:B:VAL:HG11	1:99:B:LEU:HD23	8	0.13
(1,2446)	1:97:B:VAL:HG12	1:99:B:LEU:HD21	8	0.13
(1,2446)	1:97:B:VAL:HG12	1:99:B:LEU:HD22	8	0.13
(1,2446)	1:97:B:VAL:HG12	1:99:B:LEU:HD23	8	0.13
(1,2446)	1:97:B:VAL:HG13	1:99:B:LEU:HD21	8	0.13
(1,2446)	1:97:B:VAL:HG13	1:99:B:LEU:HD22	8	0.13
(1,2446)	1:97:B:VAL:HG13	1:99:B:LEU:HD23	8	0.13
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD1	8	0.13
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD2	8	0.13
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD1	8	0.13
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD2	8	0.13
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD1	8	0.13
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD2	8	0.13
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG21	10	0.13
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG22	10	0.13
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG23	10	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	2	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	2	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	2	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	3	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	3	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	3	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG11	10	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG12	10	0.13
(1,2410)	1:97:B:VAL:HB	1:148:B:VAL:HG13	10	0.13
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG11	10	0.13
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG12	10	0.13
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG13	10	0.13
(1,2382)	1:96:B:ARG:HB3	1:166:B:GLU:HA	6	0.13
(1,2357)	1:95:B:TRP:HE3	1:166:B:GLU:HA	8	0.13
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG21	2	0.13
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG22	2	0.13
(1,2349)	1:95:B:TRP:HB3	1:148:B:VAL:HG23	2	0.13
(1,2329)	1:94:B:ARG:HD2	1:168:B:PRO:HA	4	0.13
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	2	0.13
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	3	0.13
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2326)	1:94:B:ARG:HG2	1:168:B:PRO:HB2	10	0.13
(1,2315)	1:94:B:ARG:HB2	1:94:B:ARG:HG2	9	0.13
(1,2304)	1:94:B:ARG:HA	1:94:B:ARG:HB3	8	0.13
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB1	8	0.13
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB2	8	0.13
(1,2292)	1:91:B:THR:HB	1:92:B:ALA:HB3	8	0.13
(1,2225)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	5	0.13
(1,2225)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	5	0.13
(1,2225)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	5	0.13
(1,2093)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	5	0.13
(1,2093)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	5	0.13
(1,2093)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	5	0.13
(1,2016)	1:174:A:THR:H	1:171:A:LYS:HG3	5	0.13
(1,2000)	1:169:A:MET:H	1:169:A:MET:HG3	5	0.13
(1,1981)	1:167:A:ALA:H	1:166:A:GLU:HB2	3	0.13
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD11	5	0.13
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD12	5	0.13
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD13	5	0.13
(1,1935)	1:163:A:LEU:H	1:164:A:THR:H	2	0.13
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	3	0.13
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	9	0.13
(1,1902)	1:161:A:GLY:H	1:102:A:ASN:HB3	8	0.13
(1,1901)	1:161:A:GLY:H	1:102:A:ASN:HB2	1	0.13
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG21	7	0.13
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG22	7	0.13
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG23	7	0.13
(1,1849)	1:155:A:SER:H	1:156:A:SER:HA	7	0.13
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	2	0.13
(1,1796)	1:152:A:GLN:HE21	1:149:A:ASP:HB2	7	0.13
(1,1766)	1:149:A:ASP:H	1:169:A:MET:HG3	3	0.13
(1,1751)	1:148:A:VAL:H	1:149:A:ASP:HA	6	0.13
(1,1744)	1:148:A:VAL:H	1:146:A:PRO:HG2	9	0.13
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	10	0.13
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	10	0.13
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	10	0.13
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD11	9	0.13
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD12	9	0.13
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD13	9	0.13
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG21	2	0.13
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG22	2	0.13
(1,1669)	1:136:A:ARG:H	1:134:A:ILE:HG23	2	0.13
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG21	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG22	6	0.13
(1,1665)	1:135:A:SER:H	1:134:A:ILE:HG23	6	0.13
(1,1654)	1:134:A:ILE:H	1:127:A:ARG:HB2	8	0.13
(1,1637)	1:131:A:HIS:H	1:130:A:GLU:HG3	4	0.13
(1,1627)	1:129:A:ASP:H	1:132:A:GLY:H	3	0.13
(1,1617)	1:128:A:GLN:HE21	1:128:A:GLN:HG3	6	0.13
(1,1588)	1:126:A:GLU:H	1:125:A:GLU:HG3	1	0.13
(1,1588)	1:126:A:GLU:H	1:125:A:GLU:HG3	9	0.13
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD11	8	0.13
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD12	8	0.13
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD13	8	0.13
(1,1525)	1:119:A:GLU:H	1:114:A:LYS:HB3	7	0.13
(1,1467)	1:113:A:THR:H	1:112:A:LYS:HB2	3	0.13
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD11	2	0.13
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD12	2	0.13
(1,1449)	1:111:A:VAL:H	1:120:A:ILE:HD13	2	0.13
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD21	5	0.13
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD22	5	0.13
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD23	5	0.13
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD21	3	0.13
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD22	3	0.13
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD23	3	0.13
(1,1373)	1:102:A:ASN:HD21	1:161:A:GLY:HA2	4	0.13
(1,1362)	1:101:A:VAL:H	1:120:A:ILE:HG21	1	0.13
(1,1362)	1:101:A:VAL:H	1:120:A:ILE:HG22	1	0.13
(1,1362)	1:101:A:VAL:H	1:120:A:ILE:HG23	1	0.13
(1,1345)	1:97:A:VAL:H	1:165:A:VAL:H	3	0.13
(1,1328)	1:94:A:ARG:H	1:169:A:MET:HG3	8	0.13
(1,1311)	1:170:A:PRO:HB2	1:170:A:PRO:HG2	9	0.13
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	9	0.13
(1,1285)	1:168:A:PRO:HD2	1:169:A:MET:HA	5	0.13
(1,1217)	1:161:A:GLY:HA3	1:163:A:LEU:HA	5	0.13
(1,1174)	1:157:A:LEU:HD11	1:163:A:LEU:HG	8	0.13
(1,1174)	1:157:A:LEU:HD12	1:163:A:LEU:HG	8	0.13
(1,1174)	1:157:A:LEU:HD13	1:163:A:LEU:HG	8	0.13
(1,1172)	1:157:A:LEU:HD11	1:163:A:LEU:HB2	7	0.13
(1,1172)	1:157:A:LEU:HD12	1:163:A:LEU:HB2	7	0.13
(1,1172)	1:157:A:LEU:HD13	1:163:A:LEU:HB2	7	0.13
(1,1168)	1:157:A:LEU:HD11	1:161:A:GLY:HA3	6	0.13
(1,1168)	1:157:A:LEU:HD12	1:161:A:GLY:HA3	6	0.13
(1,1168)	1:157:A:LEU:HD13	1:161:A:GLY:HA3	6	0.13
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	7	0.13
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	9	0.13
(1,1149)	1:157:A:LEU:HA	1:163:A:LEU:HB3	3	0.13
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD21	5	0.13
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD22	5	0.13
(1,1141)	1:156:A:SER:HB3	1:163:A:LEU:HD23	5	0.13
(1,1128)	1:155:A:SER:HB2	1:157:A:LEU:HB3	6	0.13
(1,1110)	1:155:A:SER:HA	1:165:A:VAL:HA	2	0.13
(1,1110)	1:155:A:SER:HA	1:165:A:VAL:HA	8	0.13
(1,1079)	1:153:A:VAL:HB	1:154:A:SER:HA	6	0.13
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	7	0.13
(1,1028)	1:149:A:ASP:HA	1:150:A:PRO:HD3	8	0.13
(1,1020)	1:148:A:VAL:HG21	1:169:A:MET:HB2	4	0.13
(1,1020)	1:148:A:VAL:HG22	1:169:A:MET:HB2	4	0.13
(1,1020)	1:148:A:VAL:HG23	1:169:A:MET:HB2	4	0.13
(1,857)	1:141:A:LYS:HG2	1:143:A:THR:HA	10	0.13
(1,852)	1:141:A:LYS:HG2	1:141:A:LYS:HE2	2	0.13
(1,852)	1:141:A:LYS:HG2	1:141:A:LYS:HE2	9	0.13
(1,812)	1:136:A:ARG:HA	1:136:A:ARG:HD2	3	0.13
(1,812)	1:136:A:ARG:HA	1:136:A:ARG:HD2	4	0.13
(1,782)	1:131:A:HIS:HB2	1:132:A:GLY:HA2	2	0.13
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	1	0.13
(1,704)	1:125:A:GLU:HA	1:135:A:SER:HB3	4	0.13
(1,684)	1:123:A:LYS:HA	1:135:A:SER:HB3	8	0.13
(1,682)	1:123:A:LYS:HA	1:123:A:LYS:HE3	10	0.13
(1,680)	1:123:A:LYS:HA	1:123:A:LYS:HG3	1	0.13
(1,658)	1:120:A:ILE:HD11	1:163:A:LEU:HA	1	0.13
(1,658)	1:120:A:ILE:HD12	1:163:A:LEU:HA	1	0.13
(1,658)	1:120:A:ILE:HD13	1:163:A:LEU:HA	1	0.13
(1,654)	1:120:A:ILE:HD11	1:140:A:ARG:HD2	1	0.13
(1,654)	1:120:A:ILE:HD12	1:140:A:ARG:HD2	1	0.13
(1,654)	1:120:A:ILE:HD13	1:140:A:ARG:HD2	1	0.13
(1,654)	1:120:A:ILE:HD11	1:140:A:ARG:HD2	4	0.13
(1,654)	1:120:A:ILE:HD12	1:140:A:ARG:HD2	4	0.13
(1,654)	1:120:A:ILE:HD13	1:140:A:ARG:HD2	4	0.13
(1,652)	1:120:A:ILE:HD11	1:140:A:ARG:HB2	1	0.13
(1,652)	1:120:A:ILE:HD12	1:140:A:ARG:HB2	1	0.13
(1,652)	1:120:A:ILE:HD13	1:140:A:ARG:HB2	1	0.13
(1,652)	1:120:A:ILE:HD11	1:140:A:ARG:HB2	5	0.13
(1,652)	1:120:A:ILE:HD12	1:140:A:ARG:HB2	5	0.13
(1,652)	1:120:A:ILE:HD13	1:140:A:ARG:HB2	5	0.13
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	4	0.13
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	4	0.13
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD11	2	0.13
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD12	2	0.13
(1,640)	1:120:A:ILE:HG12	1:163:A:LEU:HD13	2	0.13
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	4	0.13
(1,608)	1:119:A:GLU:HA	1:141:A:LYS:HA	4	0.13
(1,605)	1:119:A:GLU:HA	1:120:A:ILE:HG13	5	0.13
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG11	4	0.13
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG12	4	0.13
(1,590)	1:118:A:VAL:HG11	1:148:A:VAL:HG13	4	0.13
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG11	4	0.13
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG12	4	0.13
(1,590)	1:118:A:VAL:HG12	1:148:A:VAL:HG13	4	0.13
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG11	4	0.13
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG12	4	0.13
(1,590)	1:118:A:VAL:HG13	1:148:A:VAL:HG13	4	0.13
(1,571)	1:118:A:VAL:HB	1:142:A:TYR:HD1	1	0.13
(1,571)	1:118:A:VAL:HB	1:142:A:TYR:HD2	1	0.13
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD21	5	0.13
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD22	5	0.13
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD23	5	0.13
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG21	10	0.13
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG22	10	0.13
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG23	10	0.13
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG21	4	0.13
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG22	4	0.13
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG23	4	0.13
(1,449)	1:112:A:LYS:HA	1:112:A:LYS:HE3	6	0.13
(1,419)	1:111:A:VAL:HA	1:120:A:ILE:HG13	7	0.13
(1,418)	1:111:A:VAL:HA	1:120:A:ILE:HG12	1	0.13
(1,415)	1:111:A:VAL:HA	1:112:A:LYS:HE3	1	0.13
(1,405)	1:110:A:THR:HG21	1:112:A:LYS:HD3	5	0.13
(1,405)	1:110:A:THR:HG22	1:112:A:LYS:HD3	5	0.13
(1,405)	1:110:A:THR:HG23	1:112:A:LYS:HD3	5	0.13
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD21	9	0.13
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD22	9	0.13
(1,361)	1:109:A:LEU:HB3	1:109:A:LEU:HD23	9	0.13
(1,348)	1:108:A:GLU:HG3	1:123:A:LYS:HE2	10	0.13
(1,331)	1:107:A:ASP:HA	1:108:A:GLU:HG2	7	0.13
(1,279)	1:102:A:ASN:HB3	1:161:A:GLY:HA2	3	0.13
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	1	0.13
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	1	0.13
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD11	3	0.13
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD12	3	0.13
(1,269)	1:101:A:VAL:HB	1:157:A:LEU:HD13	3	0.13
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG21	3	0.13
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG22	3	0.13
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG23	3	0.13
(1,259)	1:100:A:ASP:HA	1:100:A:ASP:HB3	2	0.13
(1,236)	1:99:A:LEU:HD11	1:164:A:THR:HA	4	0.13
(1,236)	1:99:A:LEU:HD12	1:164:A:THR:HA	4	0.13
(1,236)	1:99:A:LEU:HD13	1:164:A:THR:HA	4	0.13
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	3	0.13
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	3	0.13
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	3	0.13
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	3	0.13
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	3	0.13
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	3	0.13
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	3	0.13
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	3	0.13
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	3	0.13
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG21	7	0.13
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG22	7	0.13
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG23	7	0.13
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG21	7	0.13
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG22	7	0.13
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG23	7	0.13
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG21	7	0.13
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG22	7	0.13
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG23	7	0.13
(1,187)	1:98:A:SER:HB2	1:164:A:THR:HB	3	0.13
(1,176)	1:98:A:SER:HA	1:162:A:THR:HG21	3	0.13
(1,176)	1:98:A:SER:HA	1:162:A:THR:HG22	3	0.13
(1,176)	1:98:A:SER:HA	1:162:A:THR:HG23	3	0.13
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD1	6	0.13
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD2	6	0.13
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD1	6	0.13
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD2	6	0.13
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD1	6	0.13
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD2	6	0.13
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG21	4	0.13
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG22	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:96:A:ARG:HG2	1:97:A:VAL:HG23	4	0.13
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG21	5	0.13
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG22	5	0.13
(1,88)	1:96:A:ARG:HA	1:165:A:VAL:HG23	5	0.13
(1,80)	1:96:A:ARG:HA	1:96:A:ARG:HD3	3	0.13
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG21	6	0.13
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG22	6	0.13
(1,68)	1:95:A:TRP:HB3	1:148:A:VAL:HG23	6	0.13
(1,33)	1:94:A:ARG:HA	1:169:A:MET:HB2	9	0.13
(1,32)	1:94:A:ARG:HA	1:168:A:PRO:HD3	2	0.13
(1,23)	1:94:A:ARG:HA	1:94:A:ARG:HB3	3	0.13
(1,23)	1:94:A:ARG:HA	1:94:A:ARG:HB3	4	0.13
(1,23)	1:94:A:ARG:HA	1:94:A:ARG:HB3	10	0.13
(1,4297)	1:174:B:THR:H	1:171:B:LYS:HG3	9	0.12
(1,4263)	1:167:B:ALA:H	1:166:B:GLU:HB3	3	0.12
(1,4263)	1:167:B:ALA:H	1:166:B:GLU:HB3	9	0.12
(1,4262)	1:167:B:ALA:H	1:166:B:GLU:HB2	7	0.12
(1,4239)	1:165:B:VAL:H	1:166:B:GLU:HB3	7	0.12
(1,4234)	1:165:B:VAL:H	1:153:B:VAL:HG11	9	0.12
(1,4234)	1:165:B:VAL:H	1:153:B:VAL:HG12	9	0.12
(1,4234)	1:165:B:VAL:H	1:153:B:VAL:HG13	9	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD11	4	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD12	4	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD13	4	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD11	7	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD12	7	0.12
(1,4219)	1:164:B:THR:H	1:157:B:LEU:HD13	7	0.12
(1,4216)	1:163:B:LEU:H	1:164:B:THR:H	9	0.12
(1,4190)	1:161:B:GLY:H	1:160:B:GLU:HB3	5	0.12
(1,4183)	1:161:B:GLY:H	1:102:B:ASN:HB3	6	0.12
(1,4175)	1:160:B:GLU:H	1:159:B:PRO:HG2	9	0.12
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD11	1	0.12
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD12	1	0.12
(1,4158)	1:158:B:SER:H	1:109:B:LEU:HD13	1	0.12
(1,4047)	1:149:B:ASP:H	1:169:B:MET:HG3	6	0.12
(1,4032)	1:148:B:VAL:H	1:149:B:ASP:HA	5	0.12
(1,3955)	1:137:B:CYS:H	1:136:B:ARG:HB3	5	0.12
(1,3948)	1:135:B:SER:H	1:135:B:SER:HB2	4	0.12
(1,3946)	1:135:B:SER:H	1:134:B:ILE:HG21	9	0.12
(1,3946)	1:135:B:SER:H	1:134:B:ILE:HG22	9	0.12
(1,3946)	1:135:B:SER:H	1:134:B:ILE:HG23	9	0.12
(1,3928)	1:132:B:GLY:H	1:131:B:HIS:HB3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3923)	1:132:B:GLY:H	1:129:B:ASP:HB2	6	0.12
(1,3903)	1:129:B:ASP:H	1:129:B:ASP:HB3	5	0.12
(1,3860)	1:124:B:HIS:H	1:138:B:PHE:HD1	2	0.12
(1,3860)	1:124:B:HIS:H	1:138:B:PHE:HD2	2	0.12
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD21	1	0.12
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD22	1	0.12
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD23	1	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG21	7	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG22	7	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG23	7	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG21	8	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG22	8	0.12
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG23	8	0.12
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	2	0.12
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	6	0.12
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG21	6	0.12
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG22	6	0.12
(1,3786)	1:117:B:VAL:H	1:117:B:VAL:HG23	6	0.12
(1,3723)	1:110:B:THR:H	1:122:B:GLY:H	9	0.12
(1,3720)	1:110:B:THR:H	1:120:B:ILE:HD11	9	0.12
(1,3720)	1:110:B:THR:H	1:120:B:ILE:HD12	9	0.12
(1,3720)	1:110:B:THR:H	1:120:B:ILE:HD13	9	0.12
(1,3692)	1:108:B:GLU:H	1:105:B:ALA:HA	2	0.12
(1,3670)	1:105:B:ALA:H	1:106:B:PRO:HD3	7	0.12
(1,3670)	1:105:B:ALA:H	1:106:B:PRO:HD3	10	0.12
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD21	5	0.12
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD22	5	0.12
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD23	5	0.12
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD21	6	0.12
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD22	6	0.12
(1,3665)	1:103:B:HIS:H	1:109:B:LEU:HD23	6	0.12
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD11	9	0.12
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD12	9	0.12
(1,3661)	1:102:B:ASN:HD22	1:157:B:LEU:HD13	9	0.12
(1,3655)	1:102:B:ASN:HD21	1:161:B:GLY:HA3	10	0.12
(1,3651)	1:102:B:ASN:HD21	1:109:B:LEU:HD21	10	0.12
(1,3651)	1:102:B:ASN:HD21	1:109:B:LEU:HD22	10	0.12
(1,3651)	1:102:B:ASN:HD21	1:109:B:LEU:HD23	10	0.12
(1,3592)	1:170:B:PRO:HB2	1:170:B:PRO:HG2	3	0.12
(1,3592)	1:170:B:PRO:HB2	1:170:B:PRO:HG2	9	0.12
(1,3498)	1:161:B:GLY:HA3	1:163:B:LEU:HA	5	0.12
(1,3487)	1:159:B:PRO:HD2	1:160:B:GLU:HB3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3455)	1:157:B:LEU:HD11	1:163:B:LEU:HG	4	0.12
(1,3455)	1:157:B:LEU:HD12	1:163:B:LEU:HG	4	0.12
(1,3455)	1:157:B:LEU:HD13	1:163:B:LEU:HG	4	0.12
(1,3438)	1:157:B:LEU:HB3	1:157:B:LEU:HG	10	0.12
(1,3436)	1:157:B:LEU:HB2	1:163:B:LEU:HA	3	0.12
(1,3423)	1:156:B:SER:HB3	1:164:B:THR:HG21	3	0.12
(1,3423)	1:156:B:SER:HB3	1:164:B:THR:HG22	3	0.12
(1,3423)	1:156:B:SER:HB3	1:164:B:THR:HG23	3	0.12
(1,3378)	1:154:B:SER:HB3	1:155:B:SER:HA	3	0.12
(1,3360)	1:153:B:VAL:HB	1:154:B:SER:HA	6	0.12
(1,3288)	1:148:B:VAL:HG11	1:153:B:VAL:HA	3	0.12
(1,3288)	1:148:B:VAL:HG12	1:153:B:VAL:HA	3	0.12
(1,3288)	1:148:B:VAL:HG13	1:153:B:VAL:HA	3	0.12
(1,3288)	1:148:B:VAL:HG11	1:153:B:VAL:HA	8	0.12
(1,3288)	1:148:B:VAL:HG12	1:153:B:VAL:HA	8	0.12
(1,3288)	1:148:B:VAL:HG13	1:153:B:VAL:HA	8	0.12
(1,3249)	1:146:B:PRO:HB3	1:147:B:GLY:HA3	10	0.12
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	7	0.12
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	7	0.12
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	7	0.12
(1,3186)	1:144:B:LEU:HA	1:145:B:PRO:HG3	3	0.12
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD11	8	0.12
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD12	8	0.12
(1,3177)	1:143:B:THR:HB	1:144:B:LEU:HD13	8	0.12
(1,3056)	1:130:B:GLU:HG2	1:131:B:HIS:HD2	3	0.12
(1,3037)	1:128:B:GLN:HB3	1:133:B:TYR:HD1	4	0.12
(1,3037)	1:128:B:GLN:HB3	1:133:B:TYR:HD2	4	0.12
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE1	4	0.12
(1,3035)	1:128:B:GLN:HB2	1:133:B:TYR:HE2	4	0.12
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE1	4	0.12
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE2	4	0.12
(1,2997)	1:126:B:GLU:HG2	1:127:B:ARG:HG2	6	0.12
(1,2996)	1:126:B:GLU:HB2	1:135:B:SER:HB3	3	0.12
(1,2996)	1:126:B:GLU:HB2	1:135:B:SER:HB3	9	0.12
(1,2993)	1:126:B:GLU:HB3	1:133:B:TYR:HB2	10	0.12
(1,2957)	1:122:B:GLY:HA3	1:137:B:CYS:HA	2	0.12
(1,2952)	1:121:B:THR:HG21	1:137:B:CYS:HB3	3	0.12
(1,2952)	1:121:B:THR:HG22	1:137:B:CYS:HB3	3	0.12
(1,2952)	1:121:B:THR:HG23	1:137:B:CYS:HB3	3	0.12
(1,2935)	1:120:B:ILE:HD11	1:140:B:ARG:HD2	8	0.12
(1,2935)	1:120:B:ILE:HD12	1:140:B:ARG:HD2	8	0.12
(1,2935)	1:120:B:ILE:HD13	1:140:B:ARG:HD2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2892)	1:119:B:GLU:HA	1:141:B:LYS:HE2	2	0.12
(1,2892)	1:119:B:GLU:HA	1:141:B:LYS:HE2	8	0.12
(1,2886)	1:119:B:GLU:HA	1:120:B:ILE:HG13	7	0.12
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD21	8	0.12
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD22	8	0.12
(1,2869)	1:118:B:VAL:HG11	1:144:B:LEU:HD23	8	0.12
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD21	8	0.12
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD22	8	0.12
(1,2869)	1:118:B:VAL:HG12	1:144:B:LEU:HD23	8	0.12
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD21	8	0.12
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD22	8	0.12
(1,2869)	1:118:B:VAL:HG13	1:144:B:LEU:HD23	8	0.12
(1,2866)	1:118:B:VAL:HG11	1:142:B:TYR:HD1	2	0.12
(1,2866)	1:118:B:VAL:HG11	1:142:B:TYR:HD2	2	0.12
(1,2866)	1:118:B:VAL:HG12	1:142:B:TYR:HD1	2	0.12
(1,2866)	1:118:B:VAL:HG12	1:142:B:TYR:HD2	2	0.12
(1,2866)	1:118:B:VAL:HG13	1:142:B:TYR:HD1	2	0.12
(1,2866)	1:118:B:VAL:HG13	1:142:B:TYR:HD2	2	0.12
(1,2844)	1:118:B:VAL:HA	1:118:B:VAL:HG11	2	0.12
(1,2844)	1:118:B:VAL:HA	1:118:B:VAL:HG12	2	0.12
(1,2844)	1:118:B:VAL:HA	1:118:B:VAL:HG13	2	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG21	1	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG22	1	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG23	1	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG21	5	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG22	5	0.12
(1,2827)	1:117:B:VAL:HA	1:143:B:THR:HG23	5	0.12
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG11	5	0.12
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG12	5	0.12
(1,2810)	1:116:B:GLY:HA2	1:148:B:VAL:HG13	5	0.12
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG21	7	0.12
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG22	7	0.12
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG23	7	0.12
(1,2798)	1:115:B:ASP:HB3	1:150:B:PRO:HG2	7	0.12
(1,2798)	1:115:B:ASP:HB3	1:150:B:PRO:HG2	10	0.12
(1,2759)	1:112:B:LYS:HE3	1:121:B:THR:HB	8	0.12
(1,2730)	1:112:B:LYS:HA	1:112:B:LYS:HE3	7	0.12
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG21	9	0.12
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG22	9	0.12
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG23	9	0.12
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG21	9	0.12
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG22	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG23	9	0.12
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG21	9	0.12
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG22	9	0.12
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG23	9	0.12
(1,2699)	1:111:B:VAL:HA	1:120:B:ILE:HG12	4	0.12
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	1	0.12
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	1	0.12
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	1	0.12
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	1	0.12
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	1	0.12
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	1	0.12
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	1	0.12
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	1	0.12
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	1	0.12
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	7	0.12
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	7	0.12
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	7	0.12
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	7	0.12
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	7	0.12
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	7	0.12
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	7	0.12
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	7	0.12
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	7	0.12
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD21	10	0.12
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD22	10	0.12
(1,2642)	1:109:B:LEU:HB3	1:109:B:LEU:HD23	10	0.12
(1,2582)	1:105:B:ALA:HB1	1:109:B:LEU:HD21	10	0.12
(1,2582)	1:105:B:ALA:HB1	1:109:B:LEU:HD22	10	0.12
(1,2582)	1:105:B:ALA:HB1	1:109:B:LEU:HD23	10	0.12
(1,2582)	1:105:B:ALA:HB2	1:109:B:LEU:HD21	10	0.12
(1,2582)	1:105:B:ALA:HB2	1:109:B:LEU:HD22	10	0.12
(1,2582)	1:105:B:ALA:HB2	1:109:B:LEU:HD23	10	0.12
(1,2582)	1:105:B:ALA:HB3	1:109:B:LEU:HD21	10	0.12
(1,2582)	1:105:B:ALA:HB3	1:109:B:LEU:HD22	10	0.12
(1,2582)	1:105:B:ALA:HB3	1:109:B:LEU:HD23	10	0.12
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD11	6	0.12
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD12	6	0.12
(1,2569)	1:105:B:ALA:HA	1:109:B:LEU:HD13	6	0.12
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD11	10	0.12
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD12	10	0.12
(1,2557)	1:102:B:ASN:HB2	1:157:B:LEU:HD13	10	0.12
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG21	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG22	2	0.12
(1,2543)	1:100:B:ASP:HA	1:162:B:THR:HG23	2	0.12
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	9	0.12
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	9	0.12
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	9	0.12
(1,2537)	1:99:B:LEU:HD11	1:111:B:VAL:HB	10	0.12
(1,2537)	1:99:B:LEU:HD12	1:111:B:VAL:HB	10	0.12
(1,2537)	1:99:B:LEU:HD13	1:111:B:VAL:HB	10	0.12
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG11	8	0.12
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG12	8	0.12
(1,2521)	1:99:B:LEU:HD21	1:111:B:VAL:HG13	8	0.12
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG11	8	0.12
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG12	8	0.12
(1,2521)	1:99:B:LEU:HD22	1:111:B:VAL:HG13	8	0.12
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG11	8	0.12
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG12	8	0.12
(1,2521)	1:99:B:LEU:HD23	1:111:B:VAL:HG13	8	0.12
(1,2493)	1:99:B:LEU:HB2	1:109:B:LEU:HD21	6	0.12
(1,2493)	1:99:B:LEU:HB2	1:109:B:LEU:HD22	6	0.12
(1,2493)	1:99:B:LEU:HB2	1:109:B:LEU:HD23	6	0.12
(1,2442)	1:97:B:VAL:HG21	1:166:B:GLU:HA	7	0.12
(1,2442)	1:97:B:VAL:HG22	1:166:B:GLU:HA	7	0.12
(1,2442)	1:97:B:VAL:HG23	1:166:B:GLU:HA	7	0.12
(1,2381)	1:96:B:ARG:HB3	1:164:B:THR:HG21	3	0.12
(1,2381)	1:96:B:ARG:HB3	1:164:B:THR:HG22	3	0.12
(1,2381)	1:96:B:ARG:HB3	1:164:B:THR:HG23	3	0.12
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG21	6	0.12
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG22	6	0.12
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG23	6	0.12
(1,2360)	1:96:B:ARG:HA	1:96:B:ARG:HG3	8	0.12
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG11	5	0.12
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG12	5	0.12
(1,2343)	1:95:B:TRP:HB2	1:148:B:VAL:HG13	5	0.12
(1,2330)	1:94:B:ARG:HD3	1:168:B:PRO:HA	7	0.12
(1,2323)	1:94:B:ARG:HB3	1:168:B:PRO:HA	2	0.12
(1,2291)	1:91:B:THR:HA	1:91:B:THR:HB	2	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG21	2	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG22	2	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG23	2	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG21	6	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG22	6	0.12
(1,2230)	1:135:B:SER:HB2	1:139:A:THR:HG23	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2225)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	9	0.12
(1,2225)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	9	0.12
(1,2225)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	9	0.12
(1,2159)	1:132:B:GLY:HA2	1:142:A:TYR:HB2	2	0.12
(1,2157)	1:132:B:GLY:HA2	1:140:A:ARG:HA	1	0.12
(1,2155)	1:131:A:HIS:HB2	1:142:B:TYR:HD1	1	0.12
(1,2155)	1:131:A:HIS:HB2	1:142:B:TYR:HD2	1	0.12
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG21	2	0.12
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG22	2	0.12
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG23	2	0.12
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG21	6	0.12
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG22	6	0.12
(1,2098)	1:135:B:SER:HB2	1:139:A:THR:HG23	6	0.12
(1,2093)	1:134:A:ILE:HD11	1:140:B:ARG:HD2	9	0.12
(1,2093)	1:134:A:ILE:HD12	1:140:B:ARG:HD2	9	0.12
(1,2093)	1:134:A:ILE:HD13	1:140:B:ARG:HD2	9	0.12
(1,2027)	1:132:B:GLY:HA2	1:142:A:TYR:HB2	2	0.12
(1,2025)	1:132:B:GLY:HA2	1:140:A:ARG:HA	1	0.12
(1,2023)	1:131:A:HIS:HB2	1:142:B:TYR:HD1	1	0.12
(1,2023)	1:131:A:HIS:HB2	1:142:B:TYR:HD2	1	0.12
(1,2010)	1:171:A:LYS:H	1:172:A:LEU:HA	5	0.12
(1,2000)	1:169:A:MET:H	1:169:A:MET:HG3	3	0.12
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG11	10	0.12
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG12	10	0.12
(1,1953)	1:165:A:VAL:H	1:153:A:VAL:HG13	10	0.12
(1,1925)	1:162:A:THR:H	1:160:A:GLU:HG3	1	0.12
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG21	10	0.12
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG22	10	0.12
(1,1914)	1:161:A:GLY:H	1:162:A:THR:HG23	10	0.12
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	1	0.12
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	5	0.12
(1,1911)	1:161:A:GLY:H	1:161:A:GLY:HA2	6	0.12
(1,1900)	1:160:A:GLU:H	1:162:A:THR:HB	4	0.12
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG21	5	0.12
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG22	5	0.12
(1,1887)	1:158:A:SER:H	1:162:A:THR:HG23	5	0.12
(1,1870)	1:157:A:LEU:H	1:157:A:LEU:HB3	10	0.12
(1,1849)	1:155:A:SER:H	1:156:A:SER:HA	4	0.12
(1,1844)	1:154:A:SER:H	1:168:A:PRO:HD2	10	0.12
(1,1804)	1:152:A:GLN:HE21	1:169:A:MET:HA	6	0.12
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB1	6	0.12
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1801)	1:152:A:GLN:HE21	1:167:A:ALA:HB3	6	0.12
(1,1766)	1:149:A:ASP:H	1:169:A:MET:HG3	9	0.12
(1,1743)	1:148:A:VAL:H	1:146:A:PRO:HB3	4	0.12
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	7	0.12
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	7	0.12
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	7	0.12
(1,1656)	1:134:A:ILE:H	1:127:A:ARG:HG3	7	0.12
(1,1655)	1:134:A:ILE:H	1:127:A:ARG:HG2	9	0.12
(1,1647)	1:132:A:GLY:H	1:131:A:HIS:HB3	8	0.12
(1,1642)	1:132:A:GLY:H	1:129:A:ASP:HB2	1	0.12
(1,1627)	1:129:A:ASP:H	1:132:A:GLY:H	2	0.12
(1,1627)	1:129:A:ASP:H	1:132:A:GLY:H	8	0.12
(1,1624)	1:129:A:ASP:H	1:131:A:HIS:HA	5	0.12
(1,1598)	1:128:A:GLN:H	1:127:A:ARG:HG2	9	0.12
(1,1588)	1:126:A:GLU:H	1:125:A:GLU:HG3	3	0.12
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD21	2	0.12
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD22	2	0.12
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD23	2	0.12
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	6	0.12
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG21	1	0.12
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG22	1	0.12
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG23	1	0.12
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG21	2	0.12
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG22	2	0.12
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG23	2	0.12
(1,1545)	1:120:A:ILE:H	1:140:A:ARG:HG3	1	0.12
(1,1517)	1:118:A:VAL:H	1:142:A:TYR:HB2	3	0.12
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG21	2	0.12
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG22	2	0.12
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG23	2	0.12
(1,1478)	1:114:A:LYS:H	1:112:A:LYS:HD3	5	0.12
(1,1445)	1:111:A:VAL:H	1:110:A:THR:HB	9	0.12
(1,1432)	1:109:A:LEU:H	1:157:A:LEU:HD11	2	0.12
(1,1432)	1:109:A:LEU:H	1:157:A:LEU:HD12	2	0.12
(1,1432)	1:109:A:LEU:H	1:157:A:LEU:HD13	2	0.12
(1,1428)	1:109:A:LEU:H	1:109:A:LEU:HB3	4	0.12
(1,1382)	1:102:A:ASN:HD22	1:161:A:GLY:HA2	10	0.12
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG21	2	0.12
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG22	2	0.12
(1,1357)	1:99:A:LEU:H	1:101:A:VAL:HG23	2	0.12
(1,1345)	1:97:A:VAL:H	1:165:A:VAL:H	1	0.12
(1,1327)	1:94:A:ARG:H	1:169:A:MET:HG2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1311)	1:170:A:PRO:HB2	1:170:A:PRO:HG2	7	0.12
(1,1287)	1:169:A:MET:HA	1:169:A:MET:HB3	10	0.12
(1,1280)	1:168:A:PRO:HB2	1:170:A:PRO:HD3	9	0.12
(1,1277)	1:168:A:PRO:HA	1:169:A:MET:HG3	8	0.12
(1,1193)	1:158:A:SER:HB3	1:160:A:GLU:HB3	7	0.12
(1,1173)	1:157:A:LEU:HD11	1:163:A:LEU:HB3	2	0.12
(1,1173)	1:157:A:LEU:HD12	1:163:A:LEU:HB3	2	0.12
(1,1173)	1:157:A:LEU:HD13	1:163:A:LEU:HB3	2	0.12
(1,1172)	1:157:A:LEU:HD11	1:163:A:LEU:HB2	4	0.12
(1,1172)	1:157:A:LEU:HD12	1:163:A:LEU:HB2	4	0.12
(1,1172)	1:157:A:LEU:HD13	1:163:A:LEU:HB2	4	0.12
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	4	0.12
(1,1149)	1:157:A:LEU:HA	1:163:A:LEU:HB3	9	0.12
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD11	3	0.12
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD12	3	0.12
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD13	3	0.12
(1,1139)	1:156:A:SER:HB3	1:157:A:LEU:HB3	3	0.12
(1,1079)	1:153:A:VAL:HB	1:154:A:SER:HA	5	0.12
(1,1079)	1:153:A:VAL:HB	1:154:A:SER:HA	8	0.12
(1,1036)	1:150:A:PRO:HA	1:151:A:THR:HG21	4	0.12
(1,1036)	1:150:A:PRO:HA	1:151:A:THR:HG22	4	0.12
(1,1036)	1:150:A:PRO:HA	1:151:A:THR:HG23	4	0.12
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	4	0.12
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	4	0.12
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	4	0.12
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG11	4	0.12
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG12	4	0.12
(1,912)	1:144:A:LEU:HB2	1:148:A:VAL:HG13	4	0.12
(1,849)	1:141:A:LYS:HB2	1:141:A:LYS:HE2	7	0.12
(1,782)	1:131:A:HIS:HB2	1:132:A:GLY:HA2	10	0.12
(1,766)	1:129:A:ASP:HA	1:130:A:GLU:HB2	10	0.12
(1,764)	1:129:A:ASP:HA	1:129:A:ASP:HB3	4	0.12
(1,719)	1:126:A:GLU:HG2	1:133:A:TYR:HD1	10	0.12
(1,719)	1:126:A:GLU:HG2	1:133:A:TYR:HD2	10	0.12
(1,718)	1:126:A:GLU:HG2	1:133:A:TYR:HB3	9	0.12
(1,712)	1:126:A:GLU:HB3	1:133:A:TYR:HB2	10	0.12
(1,695)	1:123:A:LYS:HD3	1:137:A:CYS:HB2	4	0.12
(1,680)	1:123:A:LYS:HA	1:123:A:LYS:HG3	5	0.12
(1,652)	1:120:A:ILE:HD11	1:140:A:ARG:HB2	2	0.12
(1,652)	1:120:A:ILE:HD12	1:140:A:ARG:HB2	2	0.12
(1,652)	1:120:A:ILE:HD13	1:140:A:ARG:HB2	2	0.12
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	7	0.12
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	7	0.12
(1,608)	1:119:A:GLU:HA	1:141:A:LYS:HA	5	0.12
(1,577)	1:118:A:VAL:HB	1:153:A:VAL:HG21	4	0.12
(1,577)	1:118:A:VAL:HB	1:153:A:VAL:HG22	4	0.12
(1,577)	1:118:A:VAL:HB	1:153:A:VAL:HG23	4	0.12
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD21	3	0.12
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD22	3	0.12
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD23	3	0.12
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	2	0.12
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	2	0.12
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	2	0.12
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG21	1	0.12
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG22	1	0.12
(1,546)	1:117:A:VAL:HA	1:143:A:THR:HG23	1	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	1	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	1	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	1	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	4	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	4	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	4	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG21	7	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG22	7	0.12
(1,521)	1:116:A:GLY:HA2	1:118:A:VAL:HG23	7	0.12
(1,517)	1:115:A:ASP:HB3	1:150:A:PRO:HG2	9	0.12
(1,509)	1:114:A:LYS:HA	1:114:A:LYS:HB2	6	0.12
(1,502)	1:113:A:THR:HG21	1:150:A:PRO:HB3	2	0.12
(1,502)	1:113:A:THR:HG22	1:150:A:PRO:HB3	2	0.12
(1,502)	1:113:A:THR:HG23	1:150:A:PRO:HB3	2	0.12
(1,502)	1:113:A:THR:HG21	1:150:A:PRO:HB3	9	0.12
(1,502)	1:113:A:THR:HG22	1:150:A:PRO:HB3	9	0.12
(1,502)	1:113:A:THR:HG23	1:150:A:PRO:HB3	9	0.12
(1,419)	1:111:A:VAL:HA	1:120:A:ILE:HG13	6	0.12
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD11	3	0.12
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD12	3	0.12
(1,364)	1:109:A:LEU:HG	1:120:A:ILE:HD13	3	0.12
(1,359)	1:109:A:LEU:HB2	1:122:A:GLY:HA2	8	0.12
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	7	0.12
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	7	0.12
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	7	0.12
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	3	0.12
(1,283)	1:105:A:ALA:HA	1:106:A:PRO:HB3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	4	0.12
(1,280)	1:102:A:ASN:HB3	1:161:A:GLY:HA3	6	0.12
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG21	4	0.12
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG22	4	0.12
(1,262)	1:100:A:ASP:HA	1:162:A:THR:HG23	4	0.12
(1,253)	1:99:A:LEU:HD21	1:142:A:TYR:HD1	10	0.12
(1,253)	1:99:A:LEU:HD21	1:142:A:TYR:HD2	10	0.12
(1,253)	1:99:A:LEU:HD22	1:142:A:TYR:HD1	10	0.12
(1,253)	1:99:A:LEU:HD22	1:142:A:TYR:HD2	10	0.12
(1,253)	1:99:A:LEU:HD23	1:142:A:TYR:HD1	10	0.12
(1,253)	1:99:A:LEU:HD23	1:142:A:TYR:HD2	10	0.12
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG11	5	0.12
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG12	5	0.12
(1,229)	1:99:A:LEU:HD11	1:111:A:VAL:HG13	5	0.12
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG11	5	0.12
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG12	5	0.12
(1,229)	1:99:A:LEU:HD12	1:111:A:VAL:HG13	5	0.12
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG11	5	0.12
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG12	5	0.12
(1,229)	1:99:A:LEU:HD13	1:111:A:VAL:HG13	5	0.12
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG21	10	0.12
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG22	10	0.12
(1,226)	1:99:A:LEU:HD11	1:101:A:VAL:HG23	10	0.12
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG21	10	0.12
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG22	10	0.12
(1,226)	1:99:A:LEU:HD12	1:101:A:VAL:HG23	10	0.12
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG21	10	0.12
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG22	10	0.12
(1,226)	1:99:A:LEU:HD13	1:101:A:VAL:HG23	10	0.12
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	2	0.12
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	2	0.12
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	2	0.12
(1,161)	1:97:A:VAL:HG21	1:166:A:GLU:HA	10	0.12
(1,161)	1:97:A:VAL:HG22	1:166:A:GLU:HA	10	0.12
(1,161)	1:97:A:VAL:HG23	1:166:A:GLU:HA	10	0.12
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD1	7	0.12
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD2	7	0.12
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD1	7	0.12
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD2	7	0.12
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD1	7	0.12
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD2	7	0.12
(1,69)	1:95:A:TRP:HB3	1:166:A:GLU:HB2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	4	0.12
(1,35)	1:94:A:ARG:HB2	1:94:A:ARG:HG3	8	0.12
(1,29)	1:94:A:ARG:HA	1:168:A:PRO:HA	10	0.12
(1,23)	1:94:A:ARG:HA	1:94:A:ARG:HB3	9	0.12
(1,4263)	1:167:B:ALA:H	1:166:B:GLU:HB3	1	0.11
(1,4197)	1:162:B:THR:H	1:102:B:ASN:HB3	1	0.11
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	1	0.11
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	3	0.11
(1,4192)	1:161:B:GLY:H	1:161:B:GLY:HA2	9	0.11
(1,4182)	1:161:B:GLY:H	1:102:B:ASN:HB2	8	0.11
(1,4128)	1:155:B:SER:H	1:154:B:SER:HB2	2	0.11
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB1	6	0.11
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB2	6	0.11
(1,4124)	1:154:B:SER:H	1:167:B:ALA:HB3	6	0.11
(1,4044)	1:149:B:ASP:H	1:152:B:GLN:HB3	7	0.11
(1,4043)	1:149:B:ASP:H	1:152:B:GLN:HB2	5	0.11
(1,4034)	1:148:B:VAL:H	1:149:B:ASP:H	3	0.11
(1,4034)	1:148:B:VAL:H	1:149:B:ASP:H	10	0.11
(1,3963)	1:137:B:CYS:H	1:138:B:PHE:HE1	4	0.11
(1,3963)	1:137:B:CYS:H	1:138:B:PHE:HE2	4	0.11
(1,3936)	1:134:B:ILE:H	1:127:B:ARG:HG2	7	0.11
(1,3936)	1:134:B:ILE:H	1:127:B:ARG:HG2	10	0.11
(1,3928)	1:132:B:GLY:H	1:131:B:HIS:HB3	3	0.11
(1,3919)	1:131:B:HIS:H	1:132:B:GLY:HA3	2	0.11
(1,3879)	1:128:B:GLN:H	1:127:B:ARG:HG2	2	0.11
(1,3869)	1:126:B:GLU:H	1:125:B:GLU:HG3	2	0.11
(1,3866)	1:126:B:GLU:H	1:125:B:GLU:HA	5	0.11
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD21	7	0.11
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD22	7	0.11
(1,3850)	1:123:B:LYS:H	1:109:B:LEU:HD23	7	0.11
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB1	2	0.11
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB2	2	0.11
(1,3844)	1:123:B:LYS:H	1:105:B:ALA:HB3	2	0.11
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG21	10	0.11
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG22	10	0.11
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG23	10	0.11
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD11	4	0.11
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD12	4	0.11
(1,3821)	1:120:B:ILE:H	1:120:B:ILE:HD13	4	0.11
(1,3805)	1:119:B:GLU:H	1:114:B:LYS:HB2	4	0.11
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	5	0.11
(1,3790)	1:117:B:VAL:H	1:144:B:LEU:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG21	3	0.11
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG22	3	0.11
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG23	3	0.11
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG21	4	0.11
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG22	4	0.11
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG23	4	0.11
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG21	9	0.11
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG22	9	0.11
(1,3787)	1:117:B:VAL:H	1:118:B:VAL:HG23	9	0.11
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	2	0.11
(1,3723)	1:110:B:THR:H	1:122:B:GLY:H	5	0.11
(1,3670)	1:105:B:ALA:H	1:106:B:PRO:HD3	9	0.11
(1,3643)	1:101:B:VAL:H	1:120:B:ILE:HG21	9	0.11
(1,3643)	1:101:B:VAL:H	1:120:B:ILE:HG22	9	0.11
(1,3643)	1:101:B:VAL:H	1:120:B:ILE:HG23	9	0.11
(1,3626)	1:97:B:VAL:H	1:165:B:VAL:H	6	0.11
(1,3592)	1:170:B:PRO:HB2	1:170:B:PRO:HG2	2	0.11
(1,3592)	1:170:B:PRO:HB2	1:170:B:PRO:HG2	5	0.11
(1,3592)	1:170:B:PRO:HB2	1:170:B:PRO:HG2	6	0.11
(1,3592)	1:170:B:PRO:HB2	1:170:B:PRO:HG2	10	0.11
(1,3568)	1:169:B:MET:HA	1:169:B:MET:HB3	6	0.11
(1,3563)	1:168:B:PRO:HB3	1:169:B:MET:HA	2	0.11
(1,3481)	1:159:B:PRO:HA	1:159:B:PRO:HG3	4	0.11
(1,3474)	1:158:B:SER:HB3	1:160:B:GLU:HB3	5	0.11
(1,3455)	1:157:B:LEU:HD11	1:163:B:LEU:HG	7	0.11
(1,3455)	1:157:B:LEU:HD12	1:163:B:LEU:HG	7	0.11
(1,3455)	1:157:B:LEU:HD13	1:163:B:LEU:HG	7	0.11
(1,3436)	1:157:B:LEU:HB2	1:163:B:LEU:HA	5	0.11
(1,3395)	1:155:B:SER:HB2	1:163:B:LEU:HA	9	0.11
(1,3391)	1:155:B:SER:HA	1:165:B:VAL:HA	5	0.11
(1,3391)	1:155:B:SER:HA	1:165:B:VAL:HA	10	0.11
(1,3345)	1:152:B:GLN:HB2	1:168:B:PRO:HD3	9	0.11
(1,3292)	1:148:B:VAL:HG11	1:169:B:MET:HA	3	0.11
(1,3292)	1:148:B:VAL:HG12	1:169:B:MET:HA	3	0.11
(1,3292)	1:148:B:VAL:HG13	1:169:B:MET:HA	3	0.11
(1,3292)	1:148:B:VAL:HG11	1:169:B:MET:HA	10	0.11
(1,3292)	1:148:B:VAL:HG12	1:169:B:MET:HA	10	0.11
(1,3292)	1:148:B:VAL:HG13	1:169:B:MET:HA	10	0.11
(1,3288)	1:148:B:VAL:HG11	1:153:B:VAL:HA	1	0.11
(1,3288)	1:148:B:VAL:HG12	1:153:B:VAL:HA	1	0.11
(1,3288)	1:148:B:VAL:HG13	1:153:B:VAL:HA	1	0.11
(1,3288)	1:148:B:VAL:HG11	1:153:B:VAL:HA	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3288)	1:148:B:VAL:HG12	1:153:B:VAL:HA	6	0.11
(1,3288)	1:148:B:VAL:HG13	1:153:B:VAL:HA	6	0.11
(1,3266)	1:148:B:VAL:HA	1:149:B:ASP:HB3	3	0.11
(1,3249)	1:146:B:PRO:HB3	1:147:B:GLY:HA3	2	0.11
(1,3242)	1:145:B:PRO:HD2	1:146:B:PRO:HB2	4	0.11
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG21	9	0.11
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG22	9	0.11
(1,3194)	1:144:B:LEU:HB2	1:148:B:VAL:HG23	9	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD21	4	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD22	4	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD23	4	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD21	4	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD22	4	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD23	4	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD21	9	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD22	9	0.11
(1,3162)	1:142:B:TYR:HD1	1:144:B:LEU:HD23	9	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD21	9	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD22	9	0.11
(1,3162)	1:142:B:TYR:HD2	1:144:B:LEU:HD23	9	0.11
(1,3161)	1:142:B:TYR:HD1	1:144:B:LEU:HD11	3	0.11
(1,3161)	1:142:B:TYR:HD1	1:144:B:LEU:HD12	3	0.11
(1,3161)	1:142:B:TYR:HD1	1:144:B:LEU:HD13	3	0.11
(1,3161)	1:142:B:TYR:HD2	1:144:B:LEU:HD11	3	0.11
(1,3161)	1:142:B:TYR:HD2	1:144:B:LEU:HD12	3	0.11
(1,3161)	1:142:B:TYR:HD2	1:144:B:LEU:HD13	3	0.11
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE1	7	0.11
(1,3030)	1:128:B:GLN:HA	1:133:B:TYR:HE2	7	0.11
(1,3015)	1:127:B:ARG:HA	1:127:B:ARG:HB3	2	0.11
(1,2977)	1:123:B:LYS:HD2	1:137:B:CYS:HB3	3	0.11
(1,2977)	1:123:B:LYS:HD3	1:137:B:CYS:HB3	4	0.11
(1,2963)	1:123:B:LYS:HA	1:123:B:LYS:HE3	10	0.11
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	5	0.11
(1,2961)	1:123:B:LYS:HA	1:123:B:LYS:HG3	7	0.11
(1,2933)	1:120:B:ILE:HD11	1:140:B:ARG:HB2	9	0.11
(1,2933)	1:120:B:ILE:HD12	1:140:B:ARG:HB2	9	0.11
(1,2933)	1:120:B:ILE:HD13	1:140:B:ARG:HB2	9	0.11
(1,2920)	1:120:B:ILE:HG12	1:121:B:THR:HA	6	0.11
(1,2914)	1:120:B:ILE:HB	1:120:B:ILE:HD11	4	0.11
(1,2914)	1:120:B:ILE:HB	1:120:B:ILE:HD12	4	0.11
(1,2914)	1:120:B:ILE:HB	1:120:B:ILE:HD13	4	0.11
(1,2886)	1:119:B:GLU:HA	1:120:B:ILE:HG13	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2885)	1:119:B:GLU:HA	1:120:B:ILE:HG12	2	0.11
(1,2864)	1:118:B:VAL:HG11	1:142:B:TYR:HB2	6	0.11
(1,2864)	1:118:B:VAL:HG12	1:142:B:TYR:HB2	6	0.11
(1,2864)	1:118:B:VAL:HG13	1:142:B:TYR:HB2	6	0.11
(1,2831)	1:117:B:VAL:HA	1:148:B:VAL:HB	5	0.11
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG21	8	0.11
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG22	8	0.11
(1,2794)	1:115:B:ASP:HB2	1:117:B:VAL:HG23	8	0.11
(1,2783)	1:113:B:THR:HG21	1:150:B:PRO:HB3	2	0.11
(1,2783)	1:113:B:THR:HG22	1:150:B:PRO:HB3	2	0.11
(1,2783)	1:113:B:THR:HG23	1:150:B:PRO:HB3	2	0.11
(1,2783)	1:113:B:THR:HG21	1:150:B:PRO:HB3	10	0.11
(1,2783)	1:113:B:THR:HG22	1:150:B:PRO:HB3	10	0.11
(1,2783)	1:113:B:THR:HG23	1:150:B:PRO:HB3	10	0.11
(1,2749)	1:112:B:LYS:HG2	1:121:B:THR:HB	9	0.11
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG21	10	0.11
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG22	10	0.11
(1,2713)	1:111:B:VAL:HG11	1:118:B:VAL:HG23	10	0.11
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG21	10	0.11
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG22	10	0.11
(1,2713)	1:111:B:VAL:HG12	1:118:B:VAL:HG23	10	0.11
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG21	10	0.11
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG22	10	0.11
(1,2713)	1:111:B:VAL:HG13	1:118:B:VAL:HG23	10	0.11
(1,2708)	1:111:B:VAL:HG11	1:112:B:LYS:HE2	6	0.11
(1,2708)	1:111:B:VAL:HG12	1:112:B:LYS:HE2	6	0.11
(1,2708)	1:111:B:VAL:HG13	1:112:B:LYS:HE2	6	0.11
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD21	6	0.11
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD22	6	0.11
(1,2652)	1:109:B:LEU:HD11	1:157:B:LEU:HD23	6	0.11
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD21	6	0.11
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD22	6	0.11
(1,2652)	1:109:B:LEU:HD12	1:157:B:LEU:HD23	6	0.11
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD21	6	0.11
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD22	6	0.11
(1,2652)	1:109:B:LEU:HD13	1:157:B:LEU:HD23	6	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD21	1	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD22	1	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD23	1	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD21	10	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD22	10	0.11
(1,2647)	1:109:B:LEU:HG	1:157:B:LEU:HD23	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2643)	1:109:B:LEU:HB3	1:121:B:THR:HB	8	0.11
(1,2629)	1:108:B:GLU:HG3	1:123:B:LYS:HE3	8	0.11
(1,2617)	1:108:B:GLU:HA	1:108:B:GLU:HG2	10	0.11
(1,2583)	1:105:B:ALA:HB1	1:123:B:LYS:HA	3	0.11
(1,2583)	1:105:B:ALA:HB2	1:123:B:LYS:HA	3	0.11
(1,2583)	1:105:B:ALA:HB3	1:123:B:LYS:HA	3	0.11
(1,2578)	1:105:B:ALA:HB1	1:107:B:ASP:HB3	5	0.11
(1,2578)	1:105:B:ALA:HB2	1:107:B:ASP:HB3	5	0.11
(1,2578)	1:105:B:ALA:HB3	1:107:B:ASP:HB3	5	0.11
(1,2568)	1:105:B:ALA:HA	1:108:B:GLU:HB3	1	0.11
(1,2554)	1:101:B:VAL:HG21	1:157:B:LEU:HD21	3	0.11
(1,2554)	1:101:B:VAL:HG21	1:157:B:LEU:HD22	3	0.11
(1,2554)	1:101:B:VAL:HG21	1:157:B:LEU:HD23	3	0.11
(1,2554)	1:101:B:VAL:HG22	1:157:B:LEU:HD21	3	0.11
(1,2554)	1:101:B:VAL:HG22	1:157:B:LEU:HD22	3	0.11
(1,2554)	1:101:B:VAL:HG22	1:157:B:LEU:HD23	3	0.11
(1,2554)	1:101:B:VAL:HG23	1:157:B:LEU:HD21	3	0.11
(1,2554)	1:101:B:VAL:HG23	1:157:B:LEU:HD22	3	0.11
(1,2554)	1:101:B:VAL:HG23	1:157:B:LEU:HD23	3	0.11
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD11	7	0.11
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD12	7	0.11
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD13	7	0.11
(1,2457)	1:98:B:SER:HA	1:162:B:THR:HG21	9	0.11
(1,2457)	1:98:B:SER:HA	1:162:B:THR:HG22	9	0.11
(1,2457)	1:98:B:SER:HA	1:162:B:THR:HG23	9	0.11
(1,2442)	1:97:B:VAL:HG21	1:166:B:GLU:HA	4	0.11
(1,2442)	1:97:B:VAL:HG22	1:166:B:GLU:HA	4	0.11
(1,2442)	1:97:B:VAL:HG23	1:166:B:GLU:HA	4	0.11
(1,2442)	1:97:B:VAL:HG21	1:166:B:GLU:HA	8	0.11
(1,2442)	1:97:B:VAL:HG22	1:166:B:GLU:HA	8	0.11
(1,2442)	1:97:B:VAL:HG23	1:166:B:GLU:HA	8	0.11
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD1	1	0.11
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD2	1	0.11
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD1	1	0.11
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD2	1	0.11
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD1	1	0.11
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD2	1	0.11
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD1	3	0.11
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD2	3	0.11
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD1	3	0.11
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD2	3	0.11
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD1	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD2	3	0.11
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG21	6	0.11
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG22	6	0.11
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG23	6	0.11
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG21	9	0.11
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG22	9	0.11
(1,2413)	1:97:B:VAL:HB	1:165:B:VAL:HG23	9	0.11
(1,2388)	1:96:B:ARG:HG2	1:166:B:GLU:HG2	8	0.11
(1,2382)	1:96:B:ARG:HB3	1:166:B:GLU:HA	5	0.11
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG21	4	0.11
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG22	4	0.11
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG23	4	0.11
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG21	7	0.11
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG22	7	0.11
(1,2369)	1:96:B:ARG:HA	1:165:B:VAL:HG23	7	0.11
(1,2352)	1:95:B:TRP:HB2	1:168:B:PRO:HB2	3	0.11
(1,2291)	1:91:B:THR:HA	1:91:B:THR:HB	8	0.11
(1,2244)	1:136:B:ARG:HG2	1:138:A:PHE:HA	8	0.11
(1,2218)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	2	0.11
(1,2218)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	2	0.11
(1,2218)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	2	0.11
(1,2213)	1:134:A:ILE:HA	1:140:B:ARG:HD3	7	0.11
(1,2155)	1:131:A:HIS:HB2	1:142:B:TYR:HD1	2	0.11
(1,2155)	1:131:A:HIS:HB2	1:142:B:TYR:HD2	2	0.11
(1,2112)	1:136:B:ARG:HG2	1:138:A:PHE:HA	8	0.11
(1,2086)	1:134:A:ILE:HG21	1:138:B:PHE:HB3	2	0.11
(1,2086)	1:134:A:ILE:HG22	1:138:B:PHE:HB3	2	0.11
(1,2086)	1:134:A:ILE:HG23	1:138:B:PHE:HB3	2	0.11
(1,2081)	1:134:A:ILE:HA	1:140:B:ARG:HD3	7	0.11
(1,2023)	1:131:A:HIS:HB2	1:142:B:TYR:HD1	2	0.11
(1,2023)	1:131:A:HIS:HB2	1:142:B:TYR:HD2	2	0.11
(1,1982)	1:167:A:ALA:H	1:166:A:GLU:HB3	10	0.11
(1,1958)	1:165:A:VAL:H	1:166:A:GLU:HB3	7	0.11
(1,1909)	1:161:A:GLY:H	1:160:A:GLU:HB3	2	0.11
(1,1888)	1:158:A:SER:H	1:162:A:THR:H	1	0.11
(1,1870)	1:157:A:LEU:H	1:157:A:LEU:HB3	9	0.11
(1,1849)	1:155:A:SER:H	1:156:A:SER:HA	3	0.11
(1,1816)	1:153:A:VAL:H	1:149:A:ASP:HB2	7	0.11
(1,1803)	1:152:A:GLN:HE21	1:168:A:PRO:HD2	4	0.11
(1,1784)	1:152:A:GLN:H	1:149:A:ASP:HB3	6	0.11
(1,1762)	1:149:A:ASP:H	1:152:A:GLN:HB2	7	0.11
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	2	0.11
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	2	0.11
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG11	7	0.11
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG12	7	0.11
(1,1730)	1:144:A:LEU:H	1:148:A:VAL:HG13	7	0.11
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	1	0.11
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	1	0.11
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	1	0.11
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	2	0.11
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	2	0.11
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	2	0.11
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD11	7	0.11
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD12	7	0.11
(1,1690)	1:140:A:ARG:H	1:99:A:LEU:HD13	7	0.11
(1,1668)	1:135:A:SER:H	1:135:A:SER:HB3	5	0.11
(1,1657)	1:134:A:ILE:H	1:133:A:TYR:HB3	8	0.11
(1,1643)	1:132:A:GLY:H	1:130:A:GLU:HB3	9	0.11
(1,1627)	1:129:A:ASP:H	1:132:A:GLY:H	9	0.11
(1,1622)	1:129:A:ASP:H	1:129:A:ASP:HB3	8	0.11
(1,1616)	1:128:A:GLN:HE21	1:128:A:GLN:HG2	3	0.11
(1,1613)	1:128:A:GLN:HE21	1:128:A:GLN:HA	6	0.11
(1,1611)	1:128:A:GLN:HE22	1:128:A:GLN:H	1	0.11
(1,1600)	1:128:A:GLN:H	1:127:A:ARG:HD2	5	0.11
(1,1598)	1:128:A:GLN:H	1:127:A:ARG:HG2	6	0.11
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD1	6	0.11
(1,1596)	1:127:A:ARG:H	1:133:A:TYR:HD2	6	0.11
(1,1581)	1:125:A:GLU:H	1:108:A:GLU:HG3	1	0.11
(1,1580)	1:125:A:GLU:H	1:108:A:GLU:HG2	8	0.11
(1,1576)	1:124:A:HIS:H	1:136:A:ARG:HA	1	0.11
(1,1576)	1:124:A:HIS:H	1:136:A:ARG:HA	8	0.11
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD11	7	0.11
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD12	7	0.11
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD13	7	0.11
(1,1567)	1:123:A:LYS:H	1:109:A:LEU:HG	9	0.11
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB1	4	0.11
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB2	4	0.11
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB3	4	0.11
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG21	3	0.11
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG22	3	0.11
(1,1556)	1:121:A:THR:H	1:121:A:THR:HG23	3	0.11
(1,1546)	1:120:A:ILE:H	1:142:A:TYR:H	9	0.11
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD11	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD12	10	0.11
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD13	10	0.11
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG21	4	0.11
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG22	4	0.11
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG23	4	0.11
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG21	7	0.11
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG22	7	0.11
(1,1506)	1:117:A:VAL:H	1:118:A:VAL:HG23	7	0.11
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD11	8	0.11
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD12	8	0.11
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD13	8	0.11
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD11	10	0.11
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD12	10	0.11
(1,1439)	1:110:A:THR:H	1:120:A:ILE:HD13	10	0.11
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD11	1	0.11
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD12	1	0.11
(1,1421)	1:108:A:GLU:H	1:109:A:LEU:HD13	1	0.11
(1,1391)	1:105:A:ALA:H	1:108:A:GLU:HB3	2	0.11
(1,1389)	1:105:A:ALA:H	1:106:A:PRO:HD3	4	0.11
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD21	7	0.11
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD22	7	0.11
(1,1384)	1:103:A:HIS:H	1:109:A:LEU:HD23	7	0.11
(1,1345)	1:97:A:VAL:H	1:165:A:VAL:H	2	0.11
(1,1311)	1:170:A:PRO:HB2	1:170:A:PRO:HG2	5	0.11
(1,1311)	1:170:A:PRO:HB2	1:170:A:PRO:HG2	6	0.11
(1,1311)	1:170:A:PRO:HB2	1:170:A:PRO:HG2	8	0.11
(1,1282)	1:168:A:PRO:HB3	1:169:A:MET:HA	5	0.11
(1,1282)	1:168:A:PRO:HB3	1:169:A:MET:HA	10	0.11
(1,1280)	1:168:A:PRO:HB2	1:170:A:PRO:HD3	6	0.11
(1,1276)	1:168:A:PRO:HA	1:169:A:MET:HG2	1	0.11
(1,1248)	1:165:A:VAL:HG21	1:167:A:ALA:HA	2	0.11
(1,1248)	1:165:A:VAL:HG22	1:167:A:ALA:HA	2	0.11
(1,1248)	1:165:A:VAL:HG23	1:167:A:ALA:HA	2	0.11
(1,1192)	1:158:A:SER:HB2	1:162:A:THR:HB	8	0.11
(1,1172)	1:157:A:LEU:HD11	1:163:A:LEU:HB2	10	0.11
(1,1172)	1:157:A:LEU:HD12	1:163:A:LEU:HB2	10	0.11
(1,1172)	1:157:A:LEU:HD13	1:163:A:LEU:HB2	10	0.11
(1,1155)	1:157:A:LEU:HB2	1:163:A:LEU:HA	10	0.11
(1,1149)	1:157:A:LEU:HA	1:163:A:LEU:HB3	2	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD11	1	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD12	1	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD13	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD11	2	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD12	2	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD13	2	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD11	8	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD12	8	0.11
(1,1144)	1:157:A:LEU:HA	1:157:A:LEU:HD13	8	0.11
(1,1027)	1:149:A:ASP:HA	1:150:A:PRO:HG3	6	0.11
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG21	3	0.11
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG22	3	0.11
(1,938)	1:144:A:LEU:HD21	1:148:A:VAL:HG23	3	0.11
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG21	3	0.11
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG22	3	0.11
(1,938)	1:144:A:LEU:HD22	1:148:A:VAL:HG23	3	0.11
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG21	3	0.11
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG22	3	0.11
(1,938)	1:144:A:LEU:HD23	1:148:A:VAL:HG23	3	0.11
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	7	0.11
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	7	0.11
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	7	0.11
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG11	1	0.11
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG12	1	0.11
(1,882)	1:142:A:TYR:HD1	1:165:A:VAL:HG13	1	0.11
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG11	1	0.11
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG12	1	0.11
(1,882)	1:142:A:TYR:HD2	1:165:A:VAL:HG13	1	0.11
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	1	0.11
(1,842)	1:141:A:LYS:HA	1:141:A:LYS:HB2	6	0.11
(1,779)	1:131:A:HIS:HA	1:131:A:HIS:HE1	7	0.11
(1,759)	1:128:A:GLN:HG2	1:133:A:TYR:HA	1	0.11
(1,759)	1:128:A:GLN:HG2	1:133:A:TYR:HA	4	0.11
(1,742)	1:127:A:ARG:HB2	1:127:A:ARG:HD2	1	0.11
(1,737)	1:127:A:ARG:HA	1:127:A:ARG:HD3	10	0.11
(1,734)	1:127:A:ARG:HA	1:127:A:ARG:HB3	4	0.11
(1,734)	1:127:A:ARG:HA	1:127:A:ARG:HB3	6	0.11
(1,734)	1:127:A:ARG:HA	1:127:A:ARG:HB3	8	0.11
(1,734)	1:127:A:ARG:HA	1:127:A:ARG:HB3	10	0.11
(1,729)	1:126:A:GLU:HG3	1:133:A:TYR:HB3	10	0.11
(1,719)	1:126:A:GLU:HG2	1:133:A:TYR:HD1	2	0.11
(1,719)	1:126:A:GLU:HG2	1:133:A:TYR:HD2	2	0.11
(1,708)	1:126:A:GLU:HA	1:134:A:ILE:HG21	6	0.11
(1,708)	1:126:A:GLU:HA	1:134:A:ILE:HG22	6	0.11
(1,708)	1:126:A:GLU:HA	1:134:A:ILE:HG23	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:125:A:GLU:HA	1:135:A:SER:HB3	2	0.11
(1,694)	1:123:A:LYS:HD2	1:137:A:CYS:HA	9	0.11
(1,692)	1:123:A:LYS:HG3	1:137:A:CYS:HB2	10	0.11
(1,671)	1:121:A:THR:HG21	1:137:A:CYS:HB3	2	0.11
(1,671)	1:121:A:THR:HG22	1:137:A:CYS:HB3	2	0.11
(1,671)	1:121:A:THR:HG23	1:137:A:CYS:HB3	2	0.11
(1,664)	1:121:A:THR:HA	1:139:A:THR:HA	10	0.11
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD1	6	0.11
(1,650)	1:120:A:ILE:HG21	1:142:A:TYR:HD2	6	0.11
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD1	6	0.11
(1,650)	1:120:A:ILE:HG22	1:142:A:TYR:HD2	6	0.11
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD1	6	0.11
(1,650)	1:120:A:ILE:HG23	1:142:A:TYR:HD2	6	0.11
(1,649)	1:120:A:ILE:HG21	1:140:A:ARG:HA	6	0.11
(1,649)	1:120:A:ILE:HG22	1:140:A:ARG:HA	6	0.11
(1,649)	1:120:A:ILE:HG23	1:140:A:ARG:HA	6	0.11
(1,648)	1:120:A:ILE:HG21	1:139:A:THR:HA	8	0.11
(1,648)	1:120:A:ILE:HG22	1:139:A:THR:HA	8	0.11
(1,648)	1:120:A:ILE:HG23	1:139:A:THR:HA	8	0.11
(1,647)	1:120:A:ILE:HG21	1:122:A:GLY:HA3	8	0.11
(1,647)	1:120:A:ILE:HG22	1:122:A:GLY:HA3	8	0.11
(1,647)	1:120:A:ILE:HG23	1:122:A:GLY:HA3	8	0.11
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	6	0.11
(1,639)	1:120:A:ILE:HG12	1:121:A:THR:HA	7	0.11
(1,636)	1:120:A:ILE:HB	1:140:A:ARG:HD3	6	0.11
(1,604)	1:119:A:GLU:HA	1:120:A:ILE:HG12	9	0.11
(1,571)	1:118:A:VAL:HB	1:142:A:TYR:HD1	8	0.11
(1,571)	1:118:A:VAL:HB	1:142:A:TYR:HD2	8	0.11
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD21	10	0.11
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD22	10	0.11
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD23	10	0.11
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	1	0.11
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	1	0.11
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	1	0.11
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG11	6	0.11
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG12	6	0.11
(1,551)	1:117:A:VAL:HA	1:148:A:VAL:HG13	6	0.11
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG21	7	0.11
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG22	7	0.11
(1,513)	1:115:A:ASP:HB2	1:117:A:VAL:HG23	7	0.11
(1,502)	1:113:A:THR:HG21	1:150:A:PRO:HB3	5	0.11
(1,502)	1:113:A:THR:HG22	1:150:A:PRO:HB3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:113:A:THR:HG23	1:150:A:PRO:HB3	5	0.11
(1,502)	1:113:A:THR:HG21	1:150:A:PRO:HB3	10	0.11
(1,502)	1:113:A:THR:HG22	1:150:A:PRO:HB3	10	0.11
(1,502)	1:113:A:THR:HG23	1:150:A:PRO:HB3	10	0.11
(1,484)	1:113:A:THR:HA	1:118:A:VAL:HG11	4	0.11
(1,484)	1:113:A:THR:HA	1:118:A:VAL:HG12	4	0.11
(1,484)	1:113:A:THR:HA	1:118:A:VAL:HG13	4	0.11
(1,395)	1:110:A:THR:HB	1:112:A:LYS:HG2	1	0.11
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD21	8	0.11
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD22	8	0.11
(1,371)	1:109:A:LEU:HD11	1:157:A:LEU:HD23	8	0.11
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD21	8	0.11
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD22	8	0.11
(1,371)	1:109:A:LEU:HD12	1:157:A:LEU:HD23	8	0.11
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD21	8	0.11
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD22	8	0.11
(1,371)	1:109:A:LEU:HD13	1:157:A:LEU:HD23	8	0.11
(1,332)	1:107:A:ASP:HA	1:108:A:GLU:HG3	3	0.11
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD11	2	0.11
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD12	2	0.11
(1,289)	1:105:A:ALA:HA	1:157:A:LEU:HD13	2	0.11
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD11	10	0.11
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD12	10	0.11
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD13	10	0.11
(1,271)	1:101:A:VAL:HG21	1:102:A:ASN:HA	8	0.11
(1,271)	1:101:A:VAL:HG22	1:102:A:ASN:HA	8	0.11
(1,271)	1:101:A:VAL:HG23	1:102:A:ASN:HA	8	0.11
(1,261)	1:100:A:ASP:HA	1:162:A:THR:HA	8	0.11
(1,236)	1:99:A:LEU:HD11	1:164:A:THR:HA	3	0.11
(1,236)	1:99:A:LEU:HD12	1:164:A:THR:HA	3	0.11
(1,236)	1:99:A:LEU:HD13	1:164:A:THR:HA	3	0.11
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	4	0.11
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	4	0.11
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	4	0.11
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD11	9	0.11
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD12	9	0.11
(1,216)	1:99:A:LEU:HB3	1:109:A:LEU:HD13	9	0.11
(1,186)	1:98:A:SER:HB2	1:164:A:THR:HA	10	0.11
(1,161)	1:97:A:VAL:HG21	1:166:A:GLU:HA	4	0.11
(1,161)	1:97:A:VAL:HG22	1:166:A:GLU:HA	4	0.11
(1,161)	1:97:A:VAL:HG23	1:166:A:GLU:HA	4	0.11
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD1	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD2	1	0.11
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD1	1	0.11
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD2	1	0.11
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD1	1	0.11
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD2	1	0.11
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD1	4	0.11
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD2	4	0.11
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD1	4	0.11
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD2	4	0.11
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD1	4	0.11
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD2	4	0.11
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD1	5	0.11
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD2	5	0.11
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD1	5	0.11
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD2	5	0.11
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD1	5	0.11
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD2	5	0.11
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG21	8	0.11
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG22	8	0.11
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG23	8	0.11
(1,102)	1:96:A:ARG:HB3	1:166:A:GLU:HB3	4	0.11
(1,101)	1:96:A:ARG:HB3	1:166:A:GLU:HA	5	0.11
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG21	3	0.11
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG22	3	0.11
(1,100)	1:96:A:ARG:HB3	1:164:A:THR:HG23	3	0.11
(1,60)	1:95:A:TRP:HB2	1:95:A:TRP:HE3	8	0.11
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	2	0.11
(1,45)	1:94:A:ARG:HG2	1:168:A:PRO:HB2	8	0.11
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB1	1	0.11
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB2	1	0.11
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB3	1	0.11
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB1	10	0.11
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB2	10	0.11
(1,11)	1:91:A:THR:HB	1:92:A:ALA:HB3	10	0.11
(1,4278)	1:169:B:MET:H	1:169:B:MET:HA	6	0.1
(1,4207)	1:162:B:THR:H	1:161:B:GLY:HA2	7	0.1
(1,4197)	1:162:B:THR:H	1:102:B:ASN:HB3	9	0.1
(1,4183)	1:161:B:GLY:H	1:102:B:ASN:HB3	5	0.1
(1,4130)	1:155:B:SER:H	1:156:B:SER:HA	7	0.1
(1,4037)	1:148:B:VAL:H	1:170:B:PRO:HG3	10	0.1
(1,4034)	1:148:B:VAL:H	1:149:B:ASP:H	4	0.1
(1,4034)	1:148:B:VAL:H	1:149:B:ASP:H	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3928)	1:132:B:GLY:H	1:131:B:HIS:HB3	1	0.1
(1,3928)	1:132:B:GLY:H	1:131:B:HIS:HB3	6	0.1
(1,3924)	1:132:B:GLY:H	1:130:B:GLU:HB3	6	0.1
(1,3915)	1:131:B:HIS:H	1:129:B:ASP:HB3	5	0.1
(1,3910)	1:129:B:ASP:H	1:133:B:TYR:HB2	5	0.1
(1,3905)	1:129:B:ASP:H	1:131:B:HIS:HA	9	0.1
(1,3894)	1:128:B:GLN:HE21	1:128:B:GLN:HA	6	0.1
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD1	8	0.1
(1,3877)	1:127:B:ARG:H	1:133:B:TYR:HD2	8	0.1
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG21	1	0.1
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG22	1	0.1
(1,3837)	1:121:B:THR:H	1:121:B:THR:HG23	1	0.1
(1,3816)	1:120:B:ILE:H	1:112:B:LYS:HG3	10	0.1
(1,3798)	1:118:B:VAL:H	1:142:B:TYR:HB2	10	0.1
(1,3770)	1:114:B:LYS:H	1:119:B:GLU:H	5	0.1
(1,3726)	1:111:B:VAL:H	1:110:B:THR:HB	9	0.1
(1,3670)	1:105:B:ALA:H	1:106:B:PRO:HD3	2	0.1
(1,3644)	1:101:B:VAL:H	1:162:B:THR:HA	1	0.1
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG21	9	0.1
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG22	9	0.1
(1,3600)	1:94:B:ARG:H	1:91:B:THR:HG23	9	0.1
(1,3585)	1:169:B:MET:HG3	1:170:B:PRO:HD2	5	0.1
(1,3453)	1:157:B:LEU:HD11	1:163:B:LEU:HB2	7	0.1
(1,3453)	1:157:B:LEU:HD12	1:163:B:LEU:HB2	7	0.1
(1,3453)	1:157:B:LEU:HD13	1:163:B:LEU:HB2	7	0.1
(1,3436)	1:157:B:LEU:HB2	1:163:B:LEU:HA	10	0.1
(1,3429)	1:157:B:LEU:HA	1:162:B:THR:HB	9	0.1
(1,3425)	1:157:B:LEU:HA	1:157:B:LEU:HD11	7	0.1
(1,3425)	1:157:B:LEU:HA	1:157:B:LEU:HD12	7	0.1
(1,3425)	1:157:B:LEU:HA	1:157:B:LEU:HD13	7	0.1
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD21	9	0.1
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD22	9	0.1
(1,3403)	1:155:B:SER:HB3	1:157:B:LEU:HD23	9	0.1
(1,3341)	1:152:B:GLN:HA	1:168:B:PRO:HG3	1	0.1
(1,3278)	1:148:B:VAL:HB	1:150:B:PRO:HA	1	0.1
(1,3049)	1:129:B:ASP:HA	1:134:B:ILE:HG21	1	0.1
(1,3049)	1:129:B:ASP:HA	1:134:B:ILE:HG22	1	0.1
(1,3049)	1:129:B:ASP:HA	1:134:B:ILE:HG23	1	0.1
(1,3043)	1:128:B:GLN:HG3	1:133:B:TYR:HD1	4	0.1
(1,3043)	1:128:B:GLN:HG3	1:133:B:TYR:HD2	4	0.1
(1,3027)	1:128:B:GLN:HA	1:128:B:GLN:HG3	5	0.1
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD11	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD12	4	0.1
(1,3022)	1:127:B:ARG:HA	1:134:B:ILE:HD13	4	0.1
(1,3015)	1:127:B:ARG:HA	1:127:B:ARG:HB3	10	0.1
(1,2977)	1:123:B:LYS:HD3	1:137:B:CYS:HB3	9	0.1
(1,2916)	1:120:B:ILE:HB	1:140:B:ARG:HD2	10	0.1
(1,2900)	1:119:B:GLU:HG2	1:141:B:LYS:HE3	7	0.1
(1,2886)	1:119:B:GLU:HA	1:120:B:ILE:HG13	3	0.1
(1,2885)	1:119:B:GLU:HA	1:120:B:ILE:HG12	6	0.1
(1,2831)	1:117:B:VAL:HA	1:148:B:VAL:HB	7	0.1
(1,2830)	1:117:B:VAL:HA	1:144:B:LEU:HD21	6	0.1
(1,2830)	1:117:B:VAL:HA	1:144:B:LEU:HD22	6	0.1
(1,2830)	1:117:B:VAL:HA	1:144:B:LEU:HD23	6	0.1
(1,2809)	1:116:B:GLY:HA2	1:148:B:VAL:HB	10	0.1
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG21	1	0.1
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG22	1	0.1
(1,2802)	1:116:B:GLY:HA2	1:118:B:VAL:HG23	1	0.1
(1,2704)	1:111:B:VAL:HB	1:112:B:LYS:HA	9	0.1
(1,2578)	1:105:B:ALA:HB1	1:107:B:ASP:HB3	8	0.1
(1,2578)	1:105:B:ALA:HB2	1:107:B:ASP:HB3	8	0.1
(1,2578)	1:105:B:ALA:HB3	1:107:B:ASP:HB3	8	0.1
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD11	2	0.1
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD12	2	0.1
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD13	2	0.1
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD11	5	0.1
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD12	5	0.1
(1,2497)	1:99:B:LEU:HB3	1:109:B:LEU:HD13	5	0.1
(1,2430)	1:97:B:VAL:HG21	1:98:B:SER:HB2	3	0.1
(1,2430)	1:97:B:VAL:HG22	1:98:B:SER:HB2	3	0.1
(1,2430)	1:97:B:VAL:HG23	1:98:B:SER:HB2	3	0.1
(1,2424)	1:97:B:VAL:HG11	1:142:B:TYR:HE1	7	0.1
(1,2424)	1:97:B:VAL:HG11	1:142:B:TYR:HE2	7	0.1
(1,2424)	1:97:B:VAL:HG12	1:142:B:TYR:HE1	7	0.1
(1,2424)	1:97:B:VAL:HG12	1:142:B:TYR:HE2	7	0.1
(1,2424)	1:97:B:VAL:HG13	1:142:B:TYR:HE1	7	0.1
(1,2424)	1:97:B:VAL:HG13	1:142:B:TYR:HE2	7	0.1
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD1	2	0.1
(1,2422)	1:97:B:VAL:HG11	1:142:B:TYR:HD2	2	0.1
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD1	2	0.1
(1,2422)	1:97:B:VAL:HG12	1:142:B:TYR:HD2	2	0.1
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD1	2	0.1
(1,2422)	1:97:B:VAL:HG13	1:142:B:TYR:HD2	2	0.1
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG11	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG12	7	0.1
(1,2400)	1:97:B:VAL:HA	1:97:B:VAL:HG13	7	0.1
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG21	9	0.1
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG22	9	0.1
(1,2389)	1:96:B:ARG:HG3	1:97:B:VAL:HG23	9	0.1
(1,2336)	1:95:B:TRP:HA	1:96:B:ARG:HG3	8	0.1
(1,2330)	1:94:B:ARG:HD3	1:168:B:PRO:HA	9	0.1
(1,2329)	1:94:B:ARG:HD2	1:168:B:PRO:HA	9	0.1
(1,2316)	1:94:B:ARG:HB2	1:94:B:ARG:HG3	8	0.1
(1,2304)	1:94:B:ARG:HA	1:94:B:ARG:HB3	5	0.1
(1,2279)	1:143:B:THR:H	1:132:A:GLY:HA2	1	0.1
(1,2234)	1:135:A:SER:HB2	1:139:B:THR:HG21	4	0.1
(1,2234)	1:135:A:SER:HB2	1:139:B:THR:HG22	4	0.1
(1,2234)	1:135:A:SER:HB2	1:139:B:THR:HG23	4	0.1
(1,2215)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	3	0.1
(1,2146)	1:143:B:THR:H	1:132:A:GLY:HA2	1	0.1
(1,2102)	1:135:A:SER:HB2	1:139:B:THR:HG21	4	0.1
(1,2102)	1:135:A:SER:HB2	1:139:B:THR:HG22	4	0.1
(1,2102)	1:135:A:SER:HB2	1:139:B:THR:HG23	4	0.1
(1,2083)	1:134:A:ILE:HG12	1:140:B:ARG:HB3	3	0.1
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD11	7	0.1
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD12	7	0.1
(1,1938)	1:164:A:THR:H	1:157:A:LEU:HD13	7	0.1
(1,1834)	1:154:A:SER:H	1:155:A:SER:HB2	8	0.1
(1,1806)	1:152:A:GLN:HE22	1:149:A:ASP:HB2	1	0.1
(1,1804)	1:152:A:GLN:HE21	1:169:A:MET:HA	3	0.1
(1,1783)	1:152:A:GLN:H	1:149:A:ASP:HA	6	0.1
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD11	9	0.1
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD12	9	0.1
(1,1726)	1:144:A:LEU:H	1:144:A:LEU:HD13	9	0.1
(1,1668)	1:135:A:SER:H	1:135:A:SER:HB3	2	0.1
(1,1637)	1:131:A:HIS:H	1:130:A:GLU:HG3	2	0.1
(1,1616)	1:128:A:GLN:HE21	1:128:A:GLN:HG2	7	0.1
(1,1585)	1:126:A:GLU:H	1:125:A:GLU:HA	7	0.1
(1,1580)	1:125:A:GLU:H	1:108:A:GLU:HG2	6	0.1
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD21	8	0.1
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD22	8	0.1
(1,1569)	1:123:A:LYS:H	1:109:A:LEU:HD23	8	0.1
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD11	1	0.1
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD12	1	0.1
(1,1568)	1:123:A:LYS:H	1:109:A:LEU:HD13	1	0.1
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB1	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB2	2	0.1
(1,1563)	1:123:A:LYS:H	1:105:A:ALA:HB3	2	0.1
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG21	7	0.1
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG22	7	0.1
(1,1554)	1:121:A:THR:H	1:120:A:ILE:HG23	7	0.1
(1,1553)	1:121:A:THR:H	1:120:A:ILE:HG13	10	0.1
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD11	8	0.1
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD12	8	0.1
(1,1540)	1:120:A:ILE:H	1:120:A:ILE:HD13	8	0.1
(1,1517)	1:118:A:VAL:H	1:142:A:TYR:HB2	2	0.1
(1,1505)	1:117:A:VAL:H	1:117:A:VAL:HG21	9	0.1
(1,1505)	1:117:A:VAL:H	1:117:A:VAL:HG22	9	0.1
(1,1505)	1:117:A:VAL:H	1:117:A:VAL:HG23	9	0.1
(1,1458)	1:112:A:LYS:H	1:112:A:LYS:HB3	9	0.1
(1,1442)	1:110:A:THR:H	1:122:A:GLY:H	8	0.1
(1,1311)	1:170:A:PRO:HB2	1:170:A:PRO:HG2	4	0.1
(1,1217)	1:161:A:GLY:HA3	1:163:A:LEU:HA	6	0.1
(1,1198)	1:159:A:PRO:HA	1:159:A:PRO:HB3	2	0.1
(1,1157)	1:157:A:LEU:HB3	1:157:A:LEU:HG	6	0.1
(1,1079)	1:153:A:VAL:HB	1:154:A:SER:HA	9	0.1
(1,997)	1:148:A:VAL:HB	1:150:A:PRO:HA	3	0.1
(1,992)	1:148:A:VAL:HA	1:170:A:PRO:HB3	2	0.1
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG21	8	0.1
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG22	8	0.1
(1,913)	1:144:A:LEU:HB2	1:148:A:VAL:HG23	8	0.1
(1,857)	1:141:A:LYS:HG2	1:143:A:THR:HA	5	0.1
(1,853)	1:141:A:LYS:HG2	1:141:A:LYS:HE3	3	0.1
(1,782)	1:131:A:HIS:HB2	1:132:A:GLY:HA2	7	0.1
(1,776)	1:130:A:GLU:HG3	1:131:A:HIS:HD2	6	0.1
(1,719)	1:126:A:GLU:HG2	1:133:A:TYR:HD1	7	0.1
(1,719)	1:126:A:GLU:HG2	1:133:A:TYR:HD2	7	0.1
(1,712)	1:126:A:GLU:HB3	1:133:A:TYR:HB2	4	0.1
(1,654)	1:120:A:ILE:HD11	1:140:A:ARG:HD2	8	0.1
(1,654)	1:120:A:ILE:HD12	1:140:A:ARG:HD2	8	0.1
(1,654)	1:120:A:ILE:HD13	1:140:A:ARG:HD2	8	0.1
(1,649)	1:120:A:ILE:HG21	1:140:A:ARG:HA	9	0.1
(1,649)	1:120:A:ILE:HG22	1:140:A:ARG:HA	9	0.1
(1,649)	1:120:A:ILE:HG23	1:140:A:ARG:HA	9	0.1
(1,613)	1:119:A:GLU:HB3	1:121:A:THR:HB	6	0.1
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD1	5	0.1
(1,585)	1:118:A:VAL:HG11	1:142:A:TYR:HD2	5	0.1
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD1	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:118:A:VAL:HG12	1:142:A:TYR:HD2	5	0.1
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD1	5	0.1
(1,585)	1:118:A:VAL:HG13	1:142:A:TYR:HD2	5	0.1
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD21	7	0.1
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD22	7	0.1
(1,566)	1:118:A:VAL:HA	1:144:A:LEU:HD23	7	0.1
(1,562)	1:117:A:VAL:HG11	1:142:A:TYR:HB3	2	0.1
(1,562)	1:117:A:VAL:HG12	1:142:A:TYR:HB3	2	0.1
(1,562)	1:117:A:VAL:HG13	1:142:A:TYR:HB3	2	0.1
(1,553)	1:117:A:VAL:HB	1:143:A:THR:HA	10	0.1
(1,517)	1:115:A:ASP:HB3	1:150:A:PRO:HG2	6	0.1
(1,466)	1:112:A:LYS:HG3	1:119:A:GLU:HA	3	0.1
(1,453)	1:112:A:LYS:HA	1:114:A:LYS:HB3	5	0.1
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG21	5	0.1
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG22	5	0.1
(1,432)	1:111:A:VAL:HG11	1:118:A:VAL:HG23	5	0.1
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG21	5	0.1
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG22	5	0.1
(1,432)	1:111:A:VAL:HG12	1:118:A:VAL:HG23	5	0.1
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG21	5	0.1
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG22	5	0.1
(1,432)	1:111:A:VAL:HG13	1:118:A:VAL:HG23	5	0.1
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD11	3	0.1
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD12	3	0.1
(1,288)	1:105:A:ALA:HA	1:109:A:LEU:HD13	3	0.1
(1,248)	1:99:A:LEU:HD21	1:140:A:ARG:HD2	1	0.1
(1,248)	1:99:A:LEU:HD22	1:140:A:ARG:HD2	1	0.1
(1,248)	1:99:A:LEU:HD23	1:140:A:ARG:HD2	1	0.1
(1,143)	1:97:A:VAL:HG11	1:142:A:TYR:HE1	2	0.1
(1,143)	1:97:A:VAL:HG11	1:142:A:TYR:HE2	2	0.1
(1,143)	1:97:A:VAL:HG12	1:142:A:TYR:HE1	2	0.1
(1,143)	1:97:A:VAL:HG12	1:142:A:TYR:HE2	2	0.1
(1,143)	1:97:A:VAL:HG13	1:142:A:TYR:HE1	2	0.1
(1,143)	1:97:A:VAL:HG13	1:142:A:TYR:HE2	2	0.1
(1,143)	1:97:A:VAL:HG11	1:142:A:TYR:HE1	9	0.1
(1,143)	1:97:A:VAL:HG11	1:142:A:TYR:HE2	9	0.1
(1,143)	1:97:A:VAL:HG12	1:142:A:TYR:HE1	9	0.1
(1,143)	1:97:A:VAL:HG12	1:142:A:TYR:HE2	9	0.1
(1,143)	1:97:A:VAL:HG13	1:142:A:TYR:HE1	9	0.1
(1,143)	1:97:A:VAL:HG13	1:142:A:TYR:HE2	9	0.1
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD1	9	0.1
(1,141)	1:97:A:VAL:HG11	1:142:A:TYR:HD2	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD1	9	0.1
(1,141)	1:97:A:VAL:HG12	1:142:A:TYR:HD2	9	0.1
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD1	9	0.1
(1,141)	1:97:A:VAL:HG13	1:142:A:TYR:HD2	9	0.1
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG21	7	0.1
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG22	7	0.1
(1,132)	1:97:A:VAL:HB	1:165:A:VAL:HG23	7	0.1
(1,116)	1:96:A:ARG:HD3	1:166:A:GLU:HB3	9	0.1

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

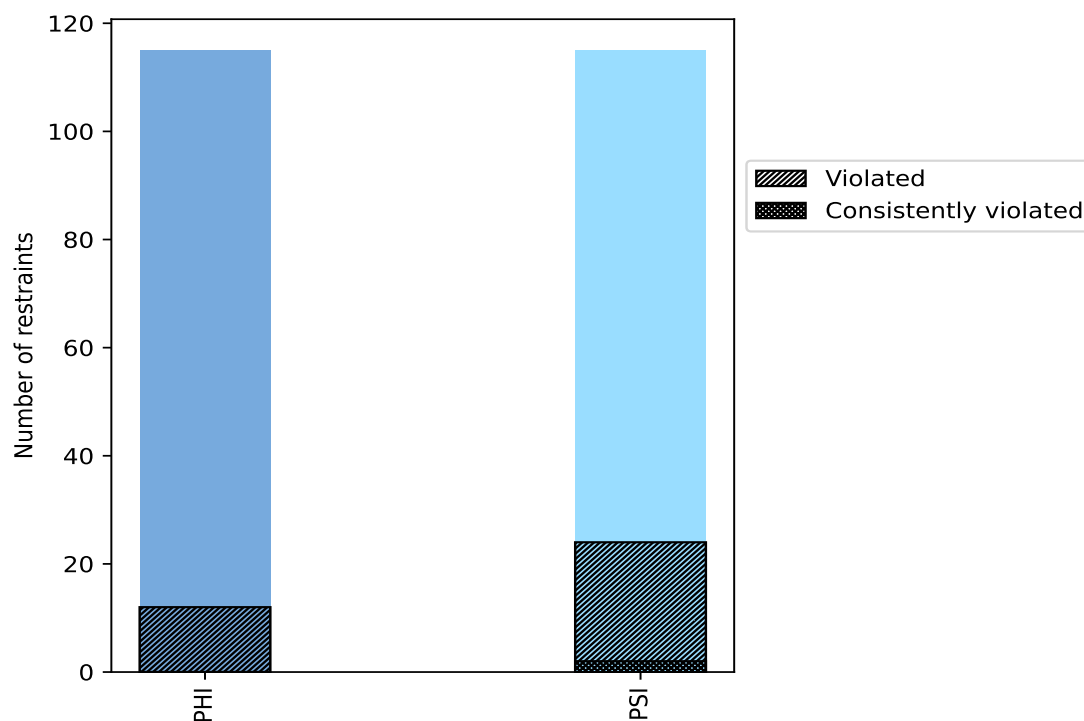
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	115	50.0	12	10.4	5.2	0	0.0	0.0
PSI	115	50.0	24	20.9	10.4	2	1.7	0.9
Total	230	100.0	36	15.7	15.7	2	0.9	0.9

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

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



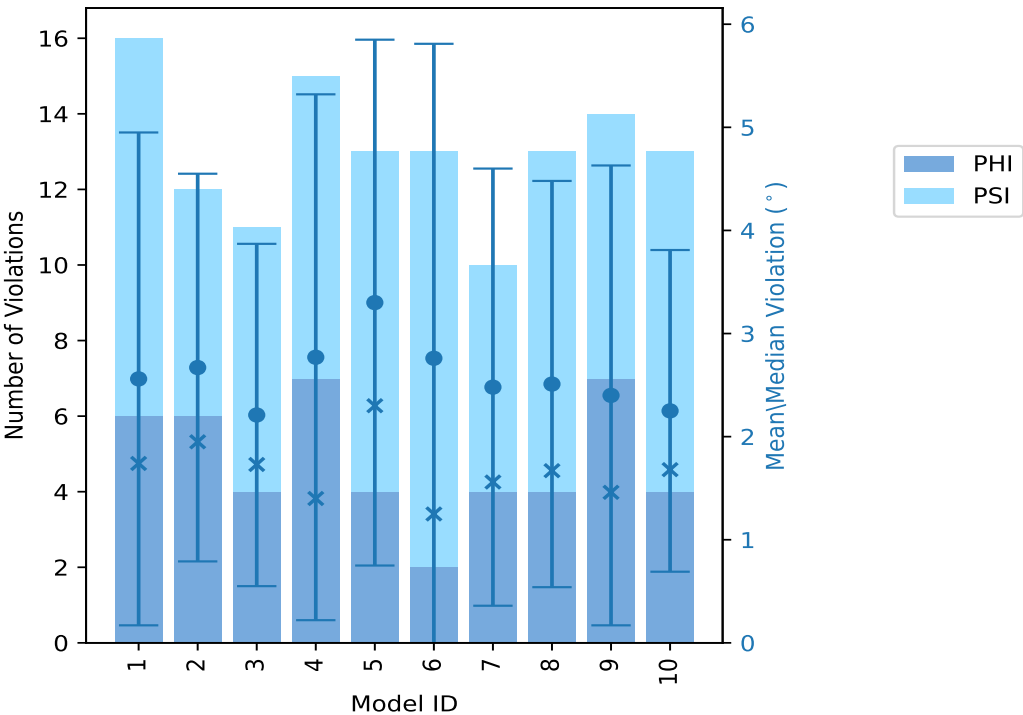
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	6	10	16	2.56	9.21	2.39	1.74
2	6	6	12	2.67	7.82	1.88	1.95
3	4	7	11	2.21	7.02	1.66	1.73
4	7	8	15	2.77	9.05	2.55	1.4
5	4	9	13	3.3	9.77	2.55	2.3
6	2	11	13	2.76	10.01	3.05	1.25
7	4	6	10	2.48	7.7	2.12	1.56
8	4	9	13	2.51	7.46	1.97	1.67
9	7	7	14	2.4	8.65	2.23	1.46
10	4	9	13	2.25	7.26	1.56	1.68

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

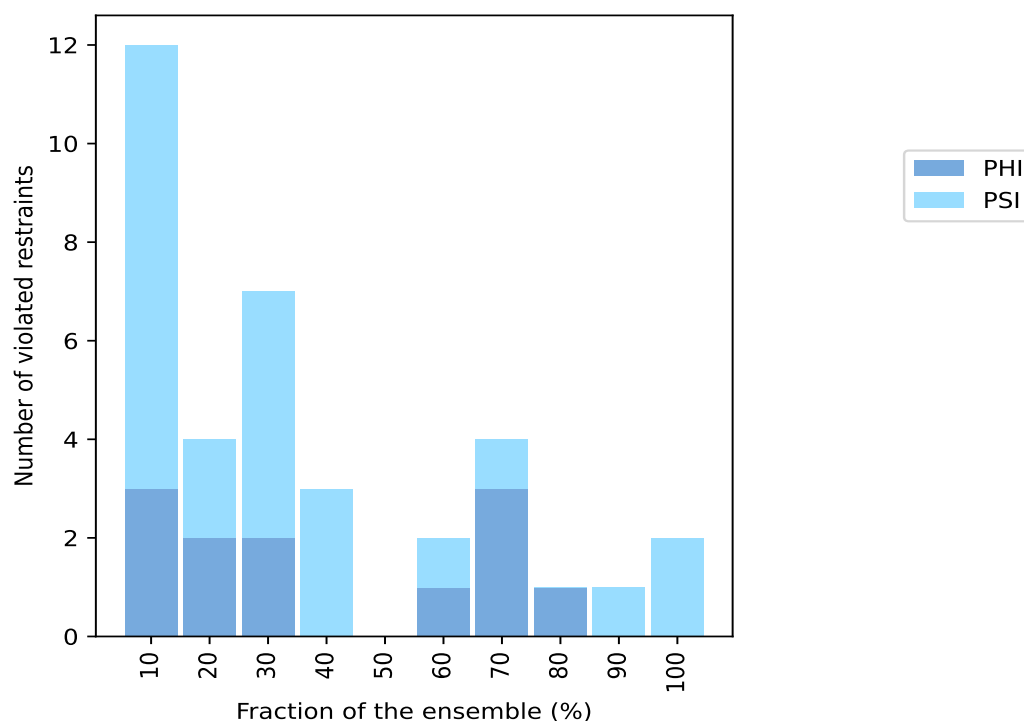
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
3	9	12	1	10.0
2	2	4	2	20.0
2	5	7	3	30.0
0	3	3	4	40.0
0	0	0	5	50.0
1	1	2	6	60.0
3	1	4	7	70.0
1	0	1	8	80.0
0	1	1	9	90.0
0	2	2	10	100.0

¹ Number of models with violations

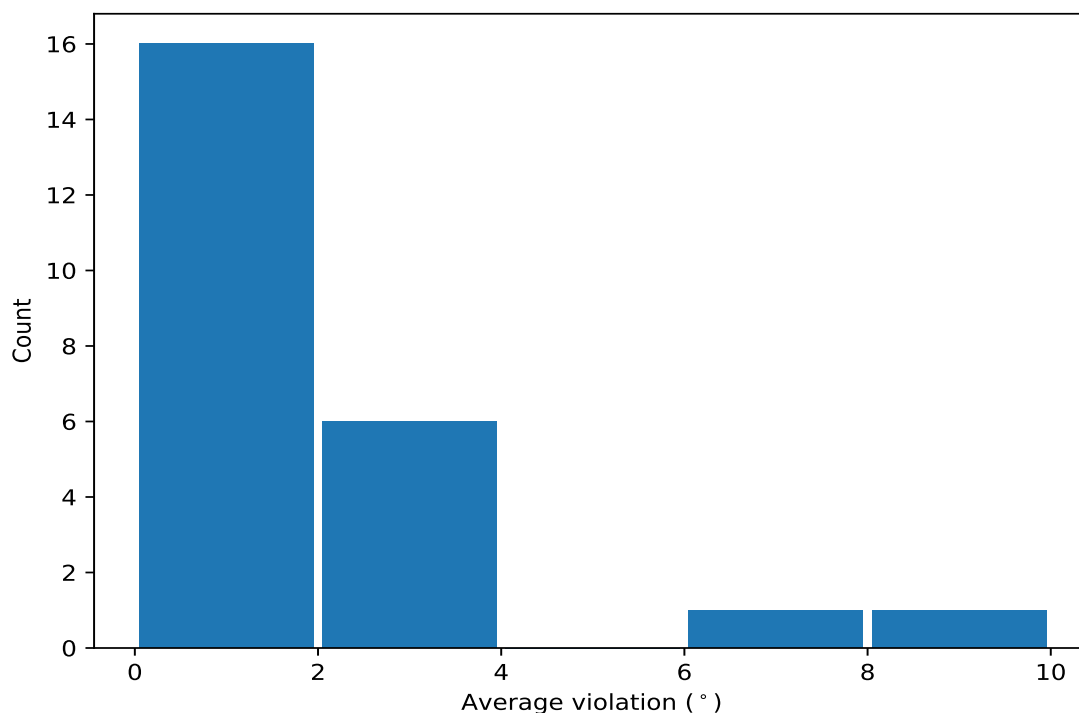
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	10	8.08	0.98	7.94
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	10	6.86	2.25	7.08
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	9	1.72	0.53	1.73
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	8	2.18	0.49	2.26
(1,58)	1:132:A:GLY:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	7	2.5	1.21	1.91
(1,87)	1:150:A:PRO:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	7	1.64	0.43	1.61
(1,16)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:GLU:N	7	1.58	0.3	1.66
(1,146)	1:116:B:GLY:C	1:117:B:VAL:N	1:117:B:VAL:CA	1:117:B:VAL:C	7	1.46	0.12	1.51
(1,30)	1:116:A:GLY:C	1:117:A:VAL:N	1:117:A:VAL:CA	1:117:A:VAL:C	6	1.83	0.4	1.89
(1,132)	1:107:B:ASP:N	1:107:B:ASP:CA	1:107:B:ASP:C	1:108:B:GLU:N	6	1.46	0.35	1.34
(1,163)	1:126:B:GLU:N	1:126:B:GLU:CA	1:126:B:GLU:C	1:127:B:ARG:N	4	2.15	0.59	1.96
(1,144)	1:115:B:ASP:N	1:115:B:ASP:CA	1:115:B:ASP:C	1:116:B:GLY:N	4	2.0	0.74	1.85
(1,28)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLY:N	4	1.53	0.22	1.54

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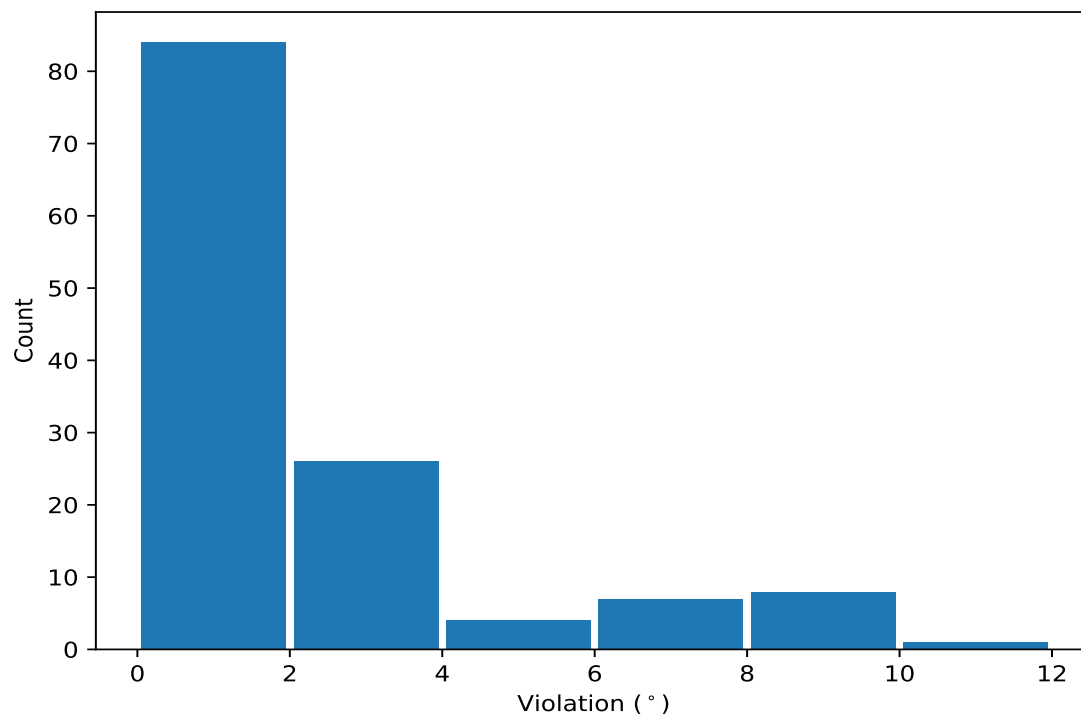
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,57)	1:131:A:HIS:N	1:131:A:HIS:CA	1:131:A:HIS:C	1:132:A:GLY:N	3	2.2	1.0	1.81
(1,115)	1:168:A:PRO:N	1:168:A:PRO:CA	1:168:A:PRO:C	1:169:A:MET:N	3	2.06	1.14	1.27
(1,47)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ARG:N	3	1.55	0.52	1.21
(1,105)	1:161:A:GLY:N	1:161:A:GLY:CA	1:161:A:GLY:C	1:162:A:THR:N	3	1.39	0.28	1.47
(1,203)	1:150:B:PRO:C	1:151:B:THR:N	1:151:B:THR:CA	1:151:B:THR:C	3	1.36	0.17	1.36
(1,221)	1:161:B:GLY:N	1:161:B:GLY:CA	1:161:B:GLY:C	1:162:B:THR:N	3	1.27	0.21	1.16
(1,201)	1:149:B:ASP:C	1:150:B:PRO:N	1:150:B:PRO:CA	1:150:B:PRO:C	3	1.19	0.15	1.12
(1,174)	1:132:B:GLY:C	1:133:B:TYR:N	1:133:B:TYR:CA	1:133:B:TYR:C	2	1.77	0.2	1.77
(1,112)	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	1:166:A:GLU:N	2	1.34	0.31	1.34
(1,42)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	2	1.23	0.1	1.23
(1,79)	1:143:A:THR:N	1:143:A:THR:CA	1:143:A:THR:C	1:144:A:LEU:N	2	1.08	0.01	1.08

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

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

restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	6	10.01
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	5	9.77
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	6	9.52
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	1	9.21
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	4	9.05
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	9	8.65
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	4	8.48
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	1	8.31
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	5	8.06
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	2	7.82
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	7	7.7
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	8	7.46
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	10	7.26
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	3	7.02
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	9	6.7
(1,81)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:PRO:N	8	6.6
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	2	5.54
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	7	5.46
(1,58)	1:132:A:GLY:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	5	4.46
(1,58)	1:132:A:GLY:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	4	4.31
(1,115)	1:168:A:PRO:N	1:168:A:PRO:CA	1:168:A:PRO:C	1:169:A:MET:N	4	3.67
(1,57)	1:131:A:HIS:N	1:131:A:HIS:CA	1:131:A:HIS:C	1:132:A:GLY:N	6	3.57
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	3	3.51
(1,197)	1:144:B:LEU:N	1:144:B:LEU:CA	1:144:B:LEU:C	1:145:B:PRO:N	10	3.28
(1,144)	1:115:B:ASP:N	1:115:B:ASP:CA	1:115:B:ASP:C	1:116:B:GLY:N	5	3.09
(1,163)	1:126:B:GLU:N	1:126:B:GLU:CA	1:126:B:GLU:C	1:127:B:ARG:N	1	3.06
(1,158)	1:122:B:GLY:C	1:123:B:LYS:N	1:123:B:LYS:CA	1:123:B:LYS:C	4	2.82
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	10	2.69
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	5	2.66
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	8	2.54
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	2	2.46
(1,87)	1:150:A:PRO:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	9	2.46
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	5	2.42
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	9	2.35
(1,163)	1:126:B:GLU:N	1:126:B:GLU:CA	1:126:B:GLU:C	1:127:B:ARG:N	5	2.3
(1,47)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ARG:N	10	2.29
(1,30)	1:116:A:GLY:C	1:117:A:VAL:N	1:117:A:VAL:CA	1:117:A:VAL:C	5	2.27
(1,144)	1:115:B:ASP:N	1:115:B:ASP:CA	1:115:B:ASP:C	1:116:B:GLY:N	2	2.23
(1,132)	1:107:B:ASP:N	1:107:B:ASP:CA	1:107:B:ASP:C	1:108:B:GLU:N	5	2.21
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	2	2.17
(1,59)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ILE:N	4	2.15
(1,30)	1:116:A:GLY:C	1:117:A:VAL:N	1:117:A:VAL:CA	1:117:A:VAL:C	8	2.14
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	8	2.12
(1,58)	1:132:A:GLY:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	3	2.09
(1,44)	1:123:A:LYS:C	1:124:A:HIS:N	1:124:A:HIS:CA	1:124:A:HIS:C	1	2.05
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	1	2.02
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	1	1.99
(1,174)	1:132:B:GLY:C	1:133:B:TYR:N	1:133:B:TYR:CA	1:133:B:TYR:C	9	1.97
(1,87)	1:150:A:PRO:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	2	1.97
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	3	1.96
(1,16)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:GLU:N	2	1.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,58)	1:132:A:GLY:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	7	1.91
(1,30)	1:116:A:GLY:C	1:117:A:VAL:N	1:117:A:VAL:CA	1:117:A:VAL:C	2	1.9
(1,16)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:GLU:N	1	1.9
(1,30)	1:116:A:GLY:C	1:117:A:VAL:N	1:117:A:VAL:CA	1:117:A:VAL:C	10	1.88
(1,28)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLY:N	9	1.83
(1,57)	1:131:A:HIS:N	1:131:A:HIS:CA	1:131:A:HIS:C	1:132:A:GLY:N	10	1.81
(1,16)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:GLU:N	8	1.79
(1,45)	1:124:A:HIS:N	1:124:A:HIS:CA	1:124:A:HIS:C	1:125:A:GLU:N	1	1.78
(1,30)	1:116:A:GLY:C	1:117:A:VAL:N	1:117:A:VAL:CA	1:117:A:VAL:C	3	1.77
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	3	1.73
(1,58)	1:132:A:GLY:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1	1.69
(1,105)	1:161:A:GLY:N	1:161:A:GLY:CA	1:161:A:GLY:C	1:162:A:THR:N	10	1.68
(1,87)	1:150:A:PRO:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	8	1.67
(1,112)	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	1:166:A:GLU:N	6	1.66
(1,16)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:GLU:N	10	1.66
(1,163)	1:126:B:GLU:N	1:126:B:GLU:CA	1:126:B:GLU:C	1:127:B:ARG:N	6	1.63
(1,169)	1:129:B:ASP:N	1:129:B:ASP:CA	1:129:B:ASP:C	1:130:B:GLU:N	8	1.62
(1,163)	1:126:B:GLU:N	1:126:B:GLU:CA	1:126:B:GLU:C	1:127:B:ARG:N	8	1.61
(1,87)	1:150:A:PRO:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	7	1.61
(1,58)	1:132:A:GLY:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	2	1.59
(1,146)	1:116:B:GLY:C	1:117:B:VAL:N	1:117:B:VAL:CA	1:117:B:VAL:C	10	1.58
(1,203)	1:150:B:PRO:C	1:151:B:THR:N	1:151:B:THR:CA	1:151:B:THR:C	2	1.57
(1,174)	1:132:B:GLY:C	1:133:B:TYR:N	1:133:B:TYR:CA	1:133:B:TYR:C	7	1.57
(1,221)	1:161:B:GLY:N	1:161:B:GLY:CA	1:161:B:GLY:C	1:162:B:THR:N	7	1.56
(1,146)	1:116:B:GLY:C	1:117:B:VAL:N	1:117:B:VAL:CA	1:117:B:VAL:C	7	1.56
(1,28)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLY:N	8	1.55
(1,172)	1:130:B:GLU:C	1:131:B:HIS:N	1:131:B:HIS:CA	1:131:B:HIS:C	1	1.54
(1,146)	1:116:B:GLY:C	1:117:B:VAL:N	1:117:B:VAL:CA	1:117:B:VAL:C	4	1.53
(1,28)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLY:N	2	1.53
(1,146)	1:116:B:GLY:C	1:117:B:VAL:N	1:117:B:VAL:CA	1:117:B:VAL:C	3	1.51
(1,144)	1:115:B:ASP:N	1:115:B:ASP:CA	1:115:B:ASP:C	1:116:B:GLY:N	6	1.47
(1,105)	1:161:A:GLY:N	1:161:A:GLY:CA	1:161:A:GLY:C	1:162:A:THR:N	5	1.47
(1,16)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:GLU:N	5	1.47
(1,132)	1:107:B:ASP:N	1:107:B:ASP:CA	1:107:B:ASP:C	1:108:B:GLU:N	9	1.46
(1,146)	1:116:B:GLY:C	1:117:B:VAL:N	1:117:B:VAL:CA	1:117:B:VAL:C	9	1.45
(1,104)	1:160:A:GLU:N	1:160:A:GLU:CA	1:160:A:GLU:C	1:161:A:GLY:N	3	1.45
(1,87)	1:150:A:PRO:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	5	1.45
(1,58)	1:132:A:GLY:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	10	1.45
(1,132)	1:107:B:ASP:N	1:107:B:ASP:CA	1:107:B:ASP:C	1:108:B:GLU:N	1	1.43
(1,201)	1:149:B:ASP:C	1:150:B:PRO:N	1:150:B:PRO:CA	1:150:B:PRO:C	4	1.4
(1,203)	1:150:B:PRO:C	1:151:B:THR:N	1:151:B:THR:CA	1:151:B:THR:C	9	1.36
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	10	1.36
(1,146)	1:116:B:GLY:C	1:117:B:VAL:N	1:117:B:VAL:CA	1:117:B:VAL:C	1	1.35
(1,42)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	2	1.32
(1,115)	1:168:A:PRO:N	1:168:A:PRO:CA	1:168:A:PRO:C	1:169:A:MET:N	5	1.27
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	4	1.26
(1,117)	1:96:B:ARG:N	1:96:B:ARG:CA	1:96:B:ARG:C	1:97:B:VAL:N	1	1.26
(1,132)	1:107:B:ASP:N	1:107:B:ASP:CA	1:107:B:ASP:C	1:108:B:GLU:N	6	1.25
(1,115)	1:168:A:PRO:N	1:168:A:PRO:CA	1:168:A:PRO:C	1:169:A:MET:N	10	1.25
(1,57)	1:131:A:HIS:N	1:131:A:HIS:CA	1:131:A:HIS:C	1:132:A:GLY:N	9	1.22
(1,28)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLY:N	1	1.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,146)	1:116:B:GLY:C	1:117:B:VAL:N	1:117:B:VAL:CA	1:117:B:VAL:C	8	1.21
(1,47)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ARG:N	6	1.21
(1,132)	1:107:B:ASP:N	1:107:B:ASP:CA	1:107:B:ASP:C	1:108:B:GLU:N	4	1.2
(1,132)	1:107:B:ASP:N	1:107:B:ASP:CA	1:107:B:ASP:C	1:108:B:GLU:N	8	1.2
(1,144)	1:115:B:ASP:N	1:115:B:ASP:CA	1:115:B:ASP:C	1:116:B:GLY:N	3	1.19
(1,87)	1:150:A:PRO:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	4	1.19
(1,16)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:GLU:N	7	1.18
(1,10)	1:102:A:ASN:N	1:102:A:ASN:CA	1:102:A:ASN:C	1:103:A:HIS:N	7	1.18
(1,221)	1:161:B:GLY:N	1:161:B:GLY:CA	1:161:B:GLY:C	1:162:B:THR:N	6	1.16
(1,203)	1:150:B:PRO:C	1:151:B:THR:N	1:151:B:THR:CA	1:151:B:THR:C	4	1.15
(1,47)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ARG:N	8	1.15
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	6	1.14
(1,87)	1:150:A:PRO:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	1	1.14
(1,42)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	9	1.13
(1,16)	1:107:A:ASP:N	1:107:A:ASP:CA	1:107:A:ASP:C	1:108:A:GLU:N	4	1.13
(1,1)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:VAL:N	6	1.13
(1,201)	1:149:B:ASP:C	1:150:B:PRO:N	1:150:B:PRO:CA	1:150:B:PRO:C	6	1.12
(1,85)	1:149:A:ASP:C	1:150:A:PRO:N	1:150:A:PRO:CA	1:150:A:PRO:C	4	1.1
(1,221)	1:161:B:GLY:N	1:161:B:GLY:CA	1:161:B:GLY:C	1:162:B:THR:N	4	1.09
(1,173)	1:131:B:HIS:N	1:131:B:HIS:CA	1:131:B:HIS:C	1:132:B:GLY:N	7	1.08
(1,79)	1:143:A:THR:N	1:143:A:THR:CA	1:143:A:THR:C	1:144:A:LEU:N	10	1.08
(1,79)	1:143:A:THR:N	1:143:A:THR:CA	1:143:A:THR:C	1:144:A:LEU:N	1	1.07
(1,228)	1:165:B:VAL:N	1:165:B:VAL:CA	1:165:B:VAL:C	1:166:B:GLU:N	3	1.06
(1,201)	1:149:B:ASP:C	1:150:B:PRO:N	1:150:B:PRO:CA	1:150:B:PRO:C	9	1.05
(1,112)	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	1:166:A:GLU:N	3	1.03
(1,30)	1:116:A:GLY:C	1:117:A:VAL:N	1:117:A:VAL:CA	1:117:A:VAL:C	6	1.03
(1,105)	1:161:A:GLY:N	1:161:A:GLY:CA	1:161:A:GLY:C	1:162:A:THR:N	9	1.02
(1,193)	1:142:B:TYR:N	1:142:B:TYR:CA	1:142:B:TYR:C	1:143:B:THR:N	9	1.0