



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 03:49 AM UTC

PDB ID : 2LCP / pdb_00002lcp
BMRB ID : 4378
Title : NMR structure of calcium loaded, un-myristoylated human NCS-1
Authors : Heidarsson, P.O.; Bjerrum-Bohr, I.J.; Bellucci, L.; Gitte, J.; Corni, S.; Poulsen, F.M.; Finn, B.E.; Di Felice, R.; Kragelund, B.
Deposited on : 2011-05-05

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

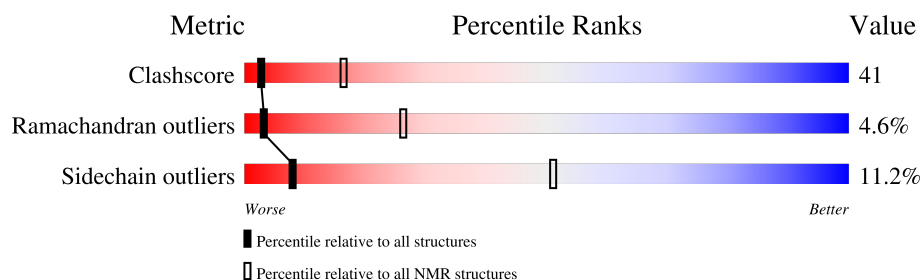
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 58%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	190	36% 52% 5% 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:9-A:184 (176)	1.84	2

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3051 atoms, of which 1505 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Neuronal calcium sensor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	190	Total	C	H	N	O	S	0
			3048	987	1505	248	302	6	

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	3	Total	Ca
			3	3

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: Neuronal calcium sensor 1

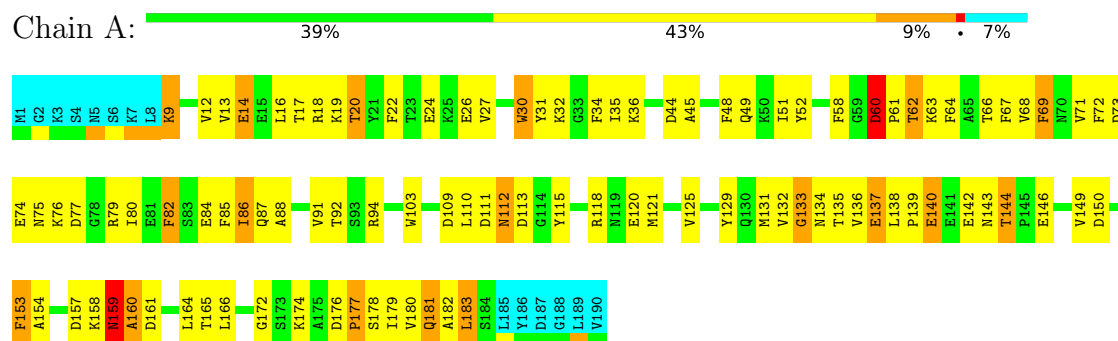


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

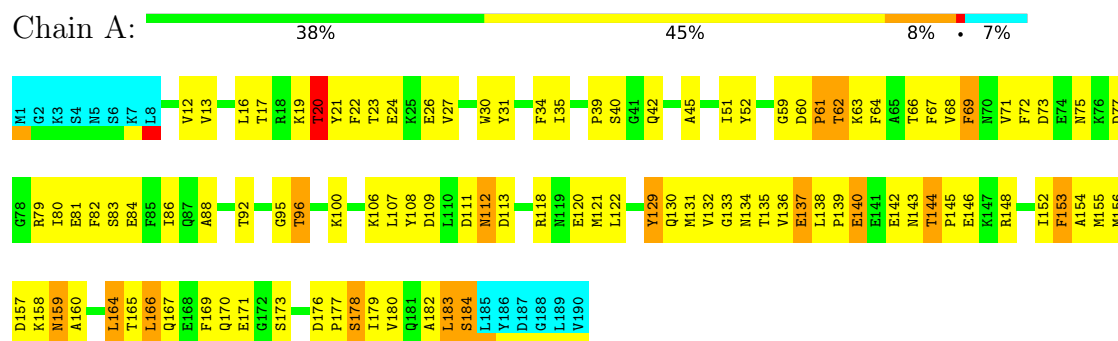
4.2.1 Score per residue for model 1

- Molecule 1: Neuronal calcium sensor 1



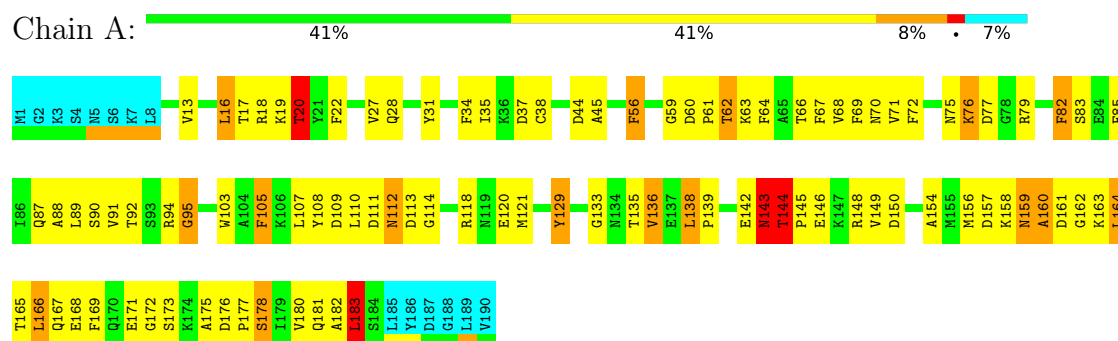
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Neuronal calcium sensor 1



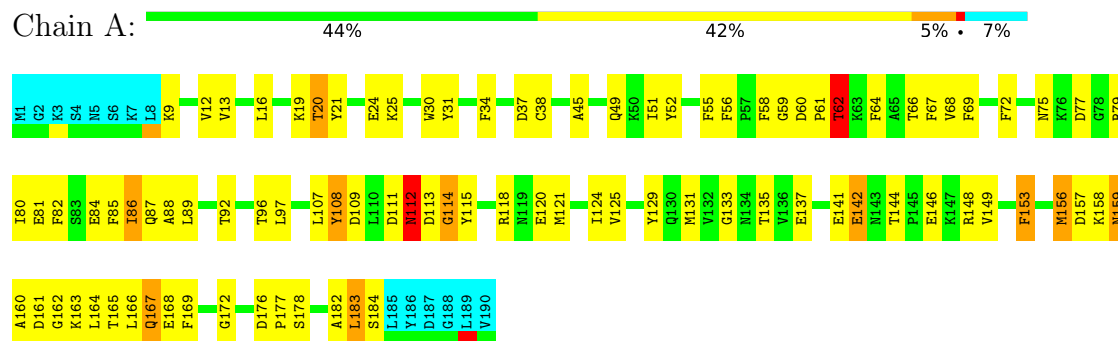
4.2.3 Score per residue for model 3

- Molecule 1: Neuronal calcium sensor 1



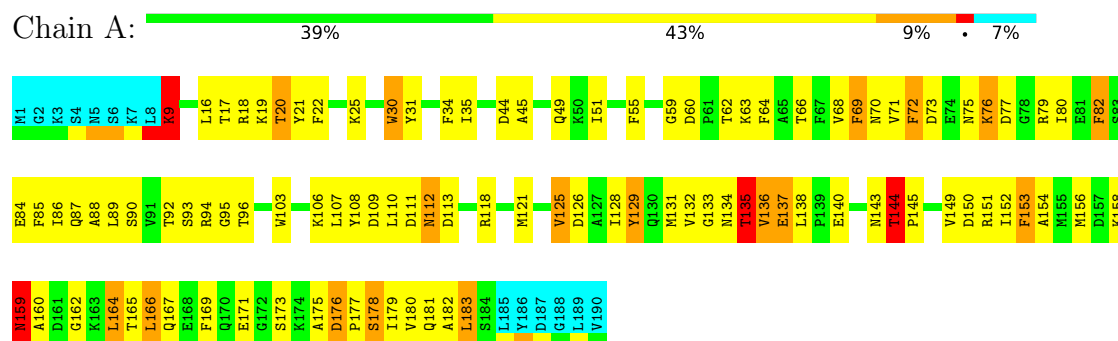
4.2.4 Score per residue for model 4

- Molecule 1: Neuronal calcium sensor 1



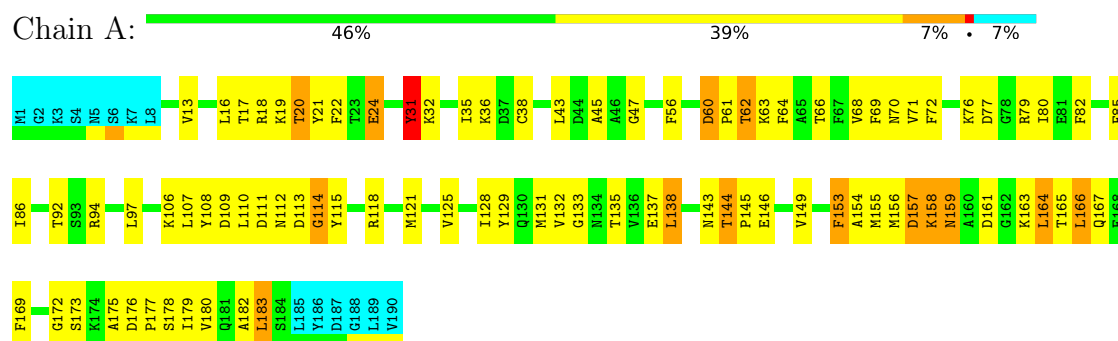
4.2.5 Score per residue for model 5

- Molecule 1: Neuronal calcium sensor 1



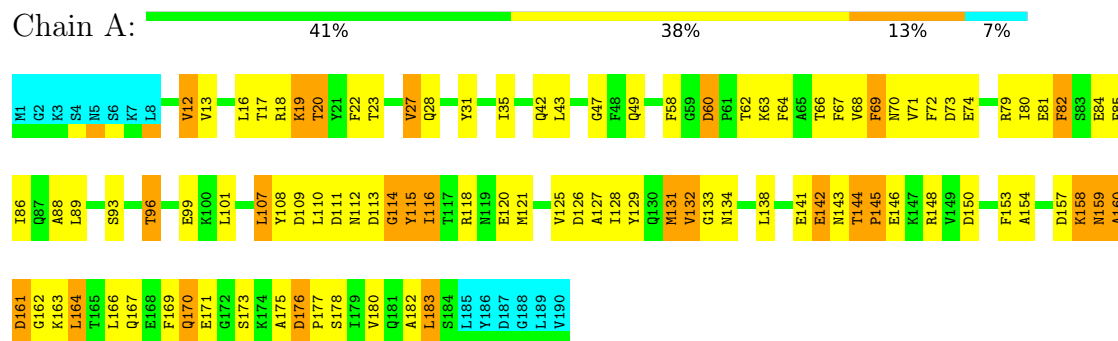
4.2.6 Score per residue for model 6

- Molecule 1: Neuronal calcium sensor 1



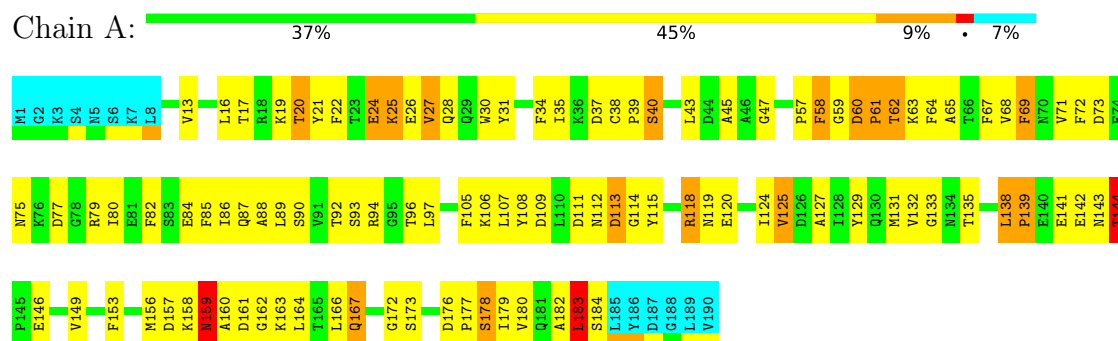
4.2.7 Score per residue for model 7

- Molecule 1: Neuronal calcium sensor 1



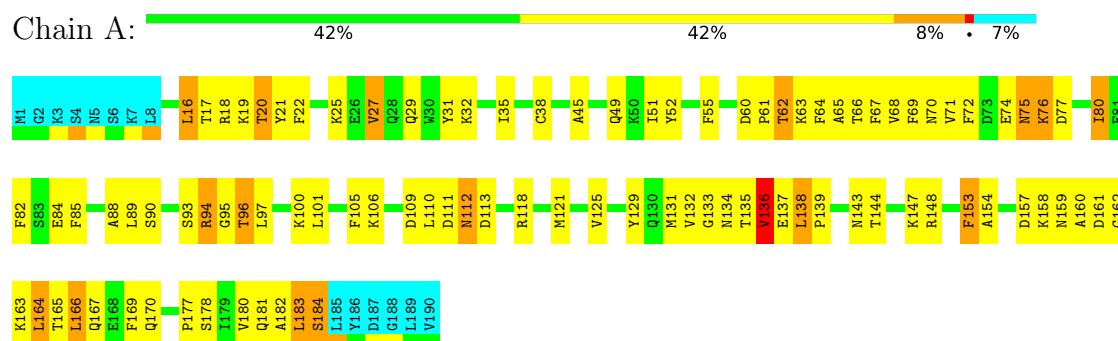
4.2.8 Score per residue for model 8

- Molecule 1: Neuronal calcium sensor 1



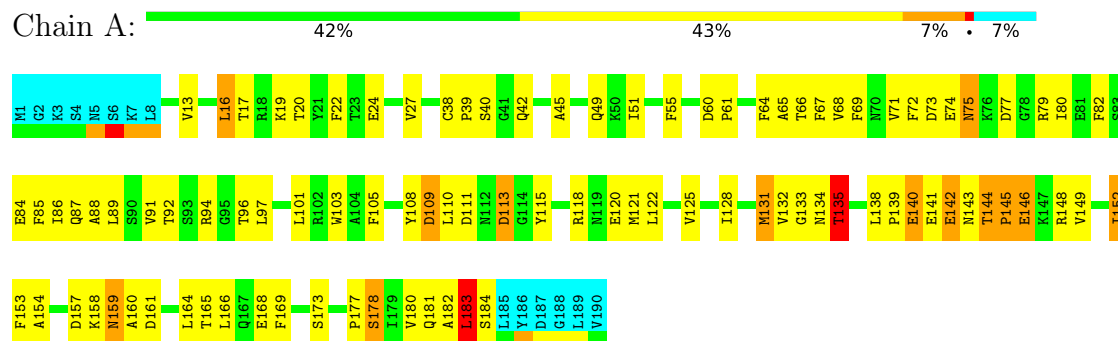
4.2.9 Score per residue for model 9

- Molecule 1: Neuronal calcium sensor 1



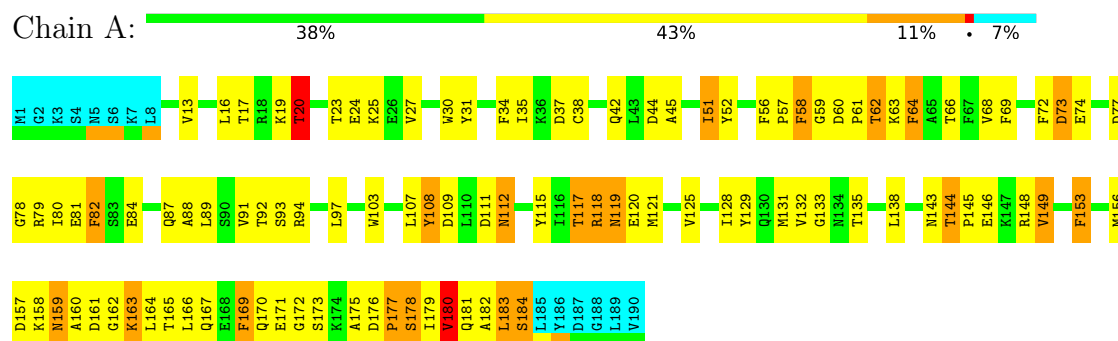
4.2.10 Score per residue for model 10

- Molecule 1: Neuronal calcium sensor 1



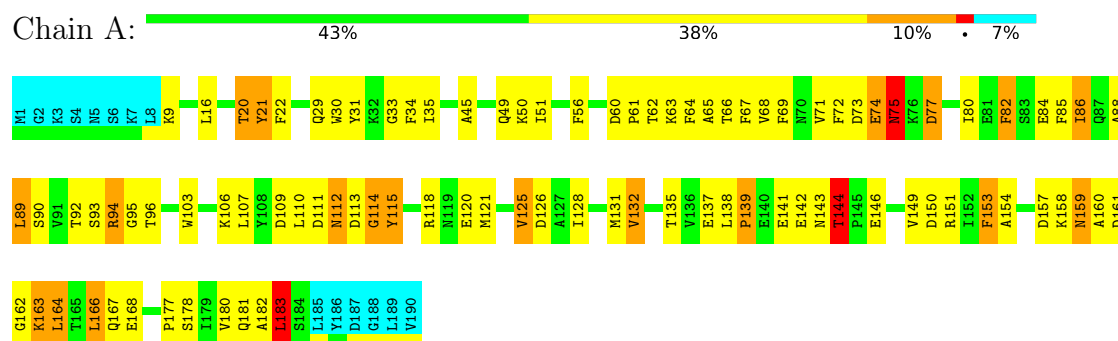
4.2.11 Score per residue for model 11

- Molecule 1: Neuronal calcium sensor 1



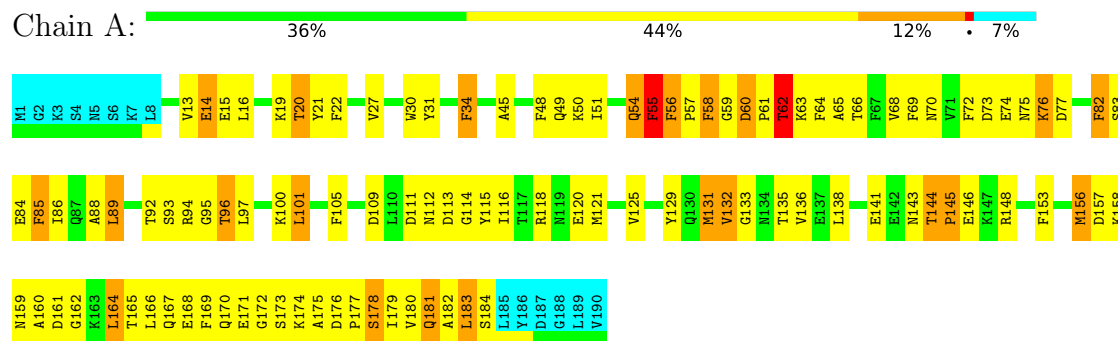
4.2.12 Score per residue for model 12

- Molecule 1: Neuronal calcium sensor 1



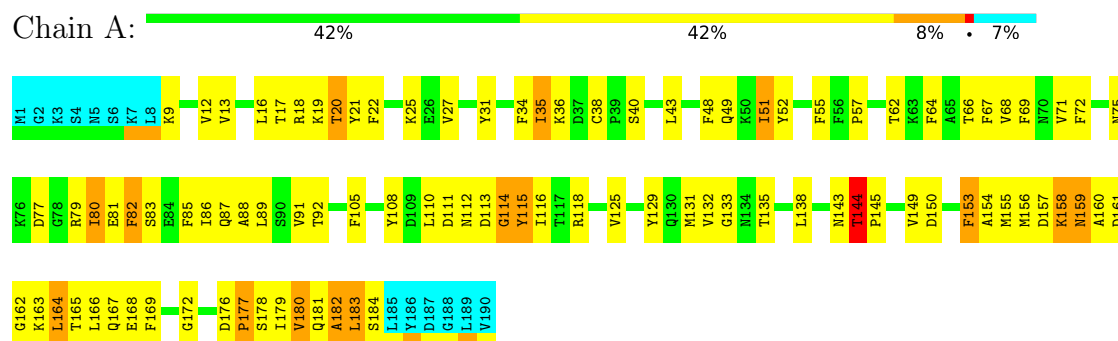
4.2.13 Score per residue for model 13

- Molecule 1: Neuronal calcium sensor 1



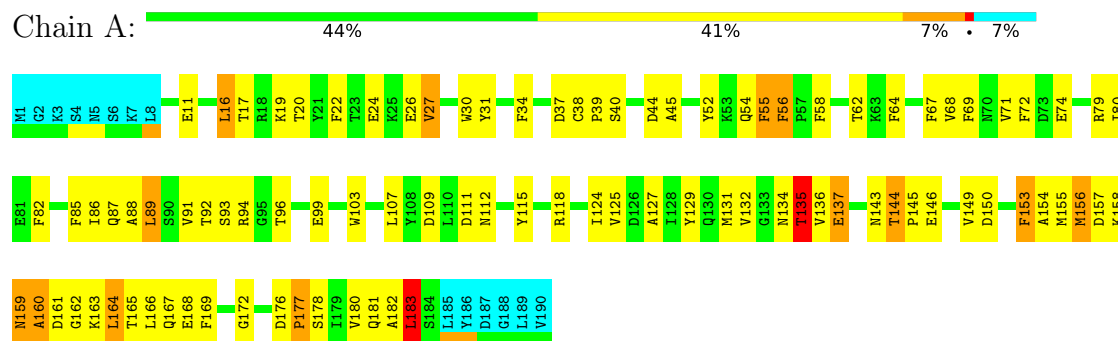
4.2.14 Score per residue for model 14

- Molecule 1: Neuronal calcium sensor 1



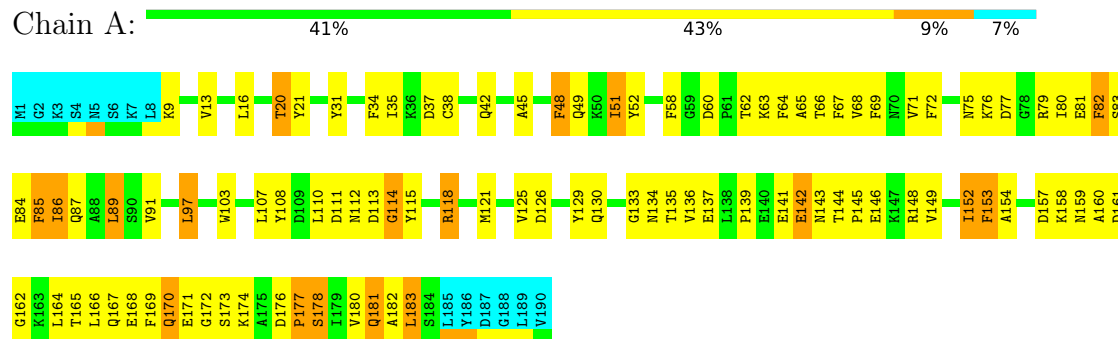
4.2.15 Score per residue for model 15

- Molecule 1: Neuronal calcium sensor 1



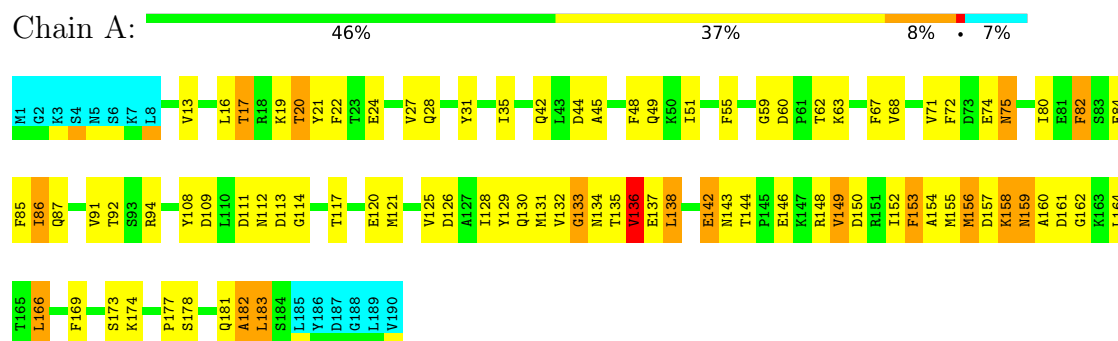
4.2.16 Score per residue for model 16

- Molecule 1: Neuronal calcium sensor 1



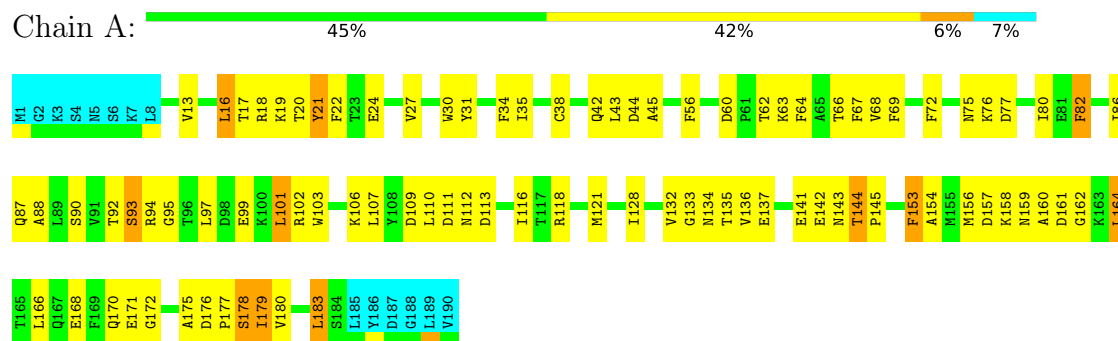
4.2.17 Score per residue for model 17

- Molecule 1: Neuronal calcium sensor 1



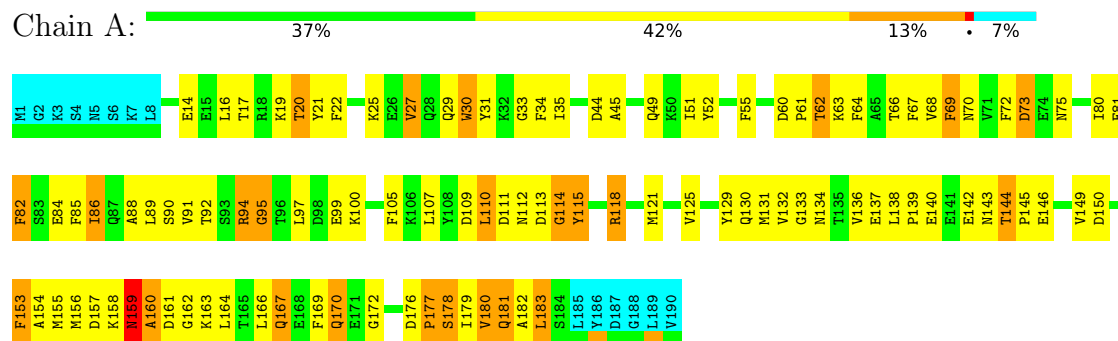
4.2.18 Score per residue for model 18

- Molecule 1: Neuronal calcium sensor 1



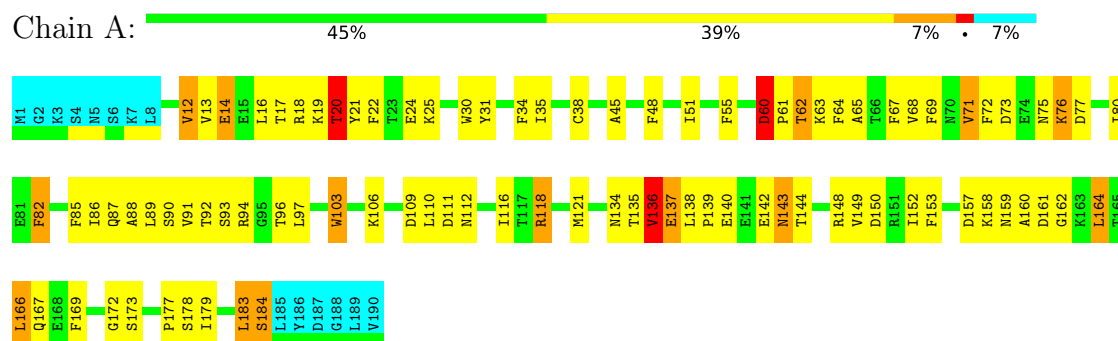
4.2.19 Score per residue for model 19

- Molecule 1: Neuronal calcium sensor 1



4.2.20 Score per residue for model 20

• Molecule 1: Neuronal calcium sensor 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
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	1477
Number of shifts mapped to atoms	1477
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.43±0.01	0±0/1469 (0.0± 0.0%)	1.18±0.01	1±1/1982 (0.1± 0.1%)
All	All	1.43	1/29380 (0.0%)	1.18	20/39640 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	138	LEU	N-CA	5.07	1.50	1.45	6	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	PHE	CA-CB-CG	-6.40	107.40	113.80	13	3
1	A	153	PHE	CA-CB-CG	-5.89	107.91	113.80	2	7
1	A	105	PHE	CA-CB-CG	-5.63	108.17	113.80	3	1
1	A	85	PHE	CA-CB-CG	-5.57	108.23	113.80	13	2
1	A	114	GLY	N-CA-C	-5.42	108.25	114.69	6	3
1	A	55	PHE	CA-CB-CG	-5.22	108.58	113.80	13	1
1	A	162	GLY	N-CA-C	-5.18	108.91	115.08	5	1
1	A	77	ASP	CA-CB-CG	-5.15	107.45	112.60	12	1
1	A	48	PHE	CA-CB-CG	-5.03	108.77	113.80	16	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1437	1391	1391	116±13
All	All	28800	27820	27820	2311

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:PHE:CZ	1:A:88:ALA:HB2	0.96	1.96	7	10
1:A:153:PHE:CZ	1:A:164:LEU:HD12	0.95	1.96	4	1
1:A:183:LEU:H	1:A:183:LEU:HD22	0.93	1.24	9	7
1:A:49:GLN:NE2	1:A:66:THR:HG22	0.91	1.80	7	1
1:A:183:LEU:HD13	1:A:183:LEU:N	0.88	1.83	5	4
1:A:166:LEU:H	1:A:166:LEU:HD13	0.88	1.29	12	1
1:A:156:MET:HE2	1:A:179:ILE:HD11	0.87	1.44	13	1
1:A:166:LEU:H	1:A:166:LEU:HD23	0.87	1.28	9	6
1:A:183:LEU:HD23	1:A:183:LEU:N	0.85	1.86	20	5
1:A:153:PHE:CE2	1:A:164:LEU:HD13	0.84	2.08	20	1
1:A:97:LEU:H	1:A:97:LEU:HD22	0.83	1.32	6	1
1:A:85:PHE:CE1	1:A:89:LEU:HD11	0.83	2.08	8	2
1:A:88:ALA:O	1:A:92:THR:HG23	0.83	1.74	19	1
1:A:67:PHE:O	1:A:71:VAL:HG22	0.83	1.73	3	2
1:A:183:LEU:HD22	1:A:183:LEU:N	0.81	1.90	13	7
1:A:67:PHE:CZ	1:A:124:ILE:HD11	0.80	2.11	8	1
1:A:128:ILE:O	1:A:132:VAL:HG22	0.80	1.76	10	3
1:A:182:ALA:C	1:A:183:LEU:HD13	0.79	2.03	13	4
1:A:64:PHE:O	1:A:68:VAL:HG23	0.79	1.77	15	12
1:A:156:MET:SD	1:A:179:ILE:HD11	0.78	2.18	5	2
1:A:62:THR:O	1:A:66:THR:HG23	0.78	1.79	18	6
1:A:13:VAL:O	1:A:17:THR:HG23	0.77	1.79	10	9
1:A:153:PHE:CD1	1:A:164:LEU:HD11	0.76	2.14	1	1
1:A:110:LEU:C	1:A:110:LEU:HD13	0.76	2.06	9	4
1:A:183:LEU:HD22	1:A:183:LEU:H	0.75	1.41	14	2
1:A:182:ALA:C	1:A:183:LEU:HD12	0.74	2.07	10	1
1:A:121:MET:O	1:A:125:VAL:HG23	0.74	1.83	11	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:THR:O	1:A:144:THR:HG23	0.74	1.81	4	2
1:A:153:PHE:CZ	1:A:164:LEU:HD11	0.73	2.19	16	1
1:A:72:PHE:CE2	1:A:88:ALA:HB2	0.73	2.19	18	4
1:A:136:VAL:O	1:A:136:VAL:HG13	0.73	1.82	5	2
1:A:107:LEU:O	1:A:107:LEU:HD23	0.73	1.84	11	5
1:A:172:GLY:O	1:A:176:ASP:N	0.72	2.22	6	9
1:A:85:PHE:CZ	1:A:89:LEU:HD11	0.72	2.18	8	1
1:A:153:PHE:CE1	1:A:164:LEU:HD21	0.72	2.19	19	6
1:A:89:LEU:C	1:A:89:LEU:HD13	0.72	2.09	4	3
1:A:31:TYR:CD1	1:A:82:PHE:CE2	0.72	2.78	12	1
1:A:60:ASP:N	1:A:61:PRO:CD	0.72	2.53	11	2
1:A:62:THR:O	1:A:66:THR:HG22	0.71	1.84	2	1
1:A:128:ILE:O	1:A:132:VAL:HG12	0.71	1.85	18	2
1:A:45:ALA:HB2	1:A:69:PHE:CZ	0.71	2.21	8	11
1:A:166:LEU:HD23	1:A:166:LEU:N	0.71	1.99	9	5
1:A:97:LEU:HD22	1:A:97:LEU:N	0.70	2.00	6	1
1:A:138:LEU:N	1:A:138:LEU:HD23	0.70	2.02	11	4
1:A:110:LEU:C	1:A:110:LEU:HD23	0.70	2.12	20	2
1:A:97:LEU:HD23	1:A:97:LEU:N	0.69	2.02	13	2
1:A:159:ASN:ND2	1:A:161:ASP:N	0.69	2.40	1	1
1:A:45:ALA:HB2	1:A:69:PHE:CD1	0.69	2.21	3	1
1:A:64:PHE:CD1	1:A:64:PHE:N	0.69	2.59	11	1
1:A:20:THR:HG23	1:A:22:PHE:H	0.69	1.48	7	2
1:A:183:LEU:N	1:A:183:LEU:HD22	0.69	2.02	1	2
1:A:118:ARG:NE	1:A:153:PHE:CD1	0.69	2.60	4	2
1:A:69:PHE:CD2	1:A:70:ASN:N	0.69	2.61	5	1
1:A:138:LEU:HD23	1:A:138:LEU:H	0.69	1.48	11	3
1:A:113:ASP:N	1:A:113:ASP:OD1	0.69	2.23	10	4
1:A:119:ASN:ND2	1:A:120:GLU:N	0.68	2.41	11	1
1:A:121:MET:SD	1:A:153:PHE:CE2	0.68	2.87	10	4
1:A:64:PHE:CD1	1:A:65:ALA:N	0.68	2.61	9	4
1:A:31:TYR:CG	1:A:32:LYS:N	0.68	2.62	6	1
1:A:131:MET:N	1:A:131:MET:SD	0.68	2.67	10	1
1:A:143:ASN:ND2	1:A:181:GLN:NE2	0.68	2.41	10	1
1:A:159:ASN:H	1:A:159:ASN:ND2	0.68	1.86	5	1
1:A:21:TYR:CD1	1:A:21:TYR:N	0.68	2.60	18	2
1:A:183:LEU:HD12	1:A:183:LEU:N	0.68	2.04	10	2
1:A:85:PHE:CZ	1:A:89:LEU:HD23	0.68	2.24	16	1
1:A:159:ASN:O	1:A:160:ALA:HB3	0.68	1.89	10	14
1:A:108:TYR:CD1	1:A:121:MET:SD	0.67	2.87	16	3
1:A:183:LEU:HD13	1:A:183:LEU:H	0.67	1.47	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:PHE:CE1	1:A:131:MET:SD	0.67	2.88	8	1
1:A:148:ARG:O	1:A:152:ILE:HD13	0.67	1.89	16	2
1:A:19:LYS:NZ	1:A:87:GLN:NE2	0.67	2.41	20	1
1:A:64:PHE:CD1	1:A:131:MET:SD	0.67	2.86	2	1
1:A:153:PHE:CD1	1:A:164:LEU:HD21	0.67	2.24	17	4
1:A:183:LEU:H	1:A:183:LEU:CD2	0.67	2.03	19	8
1:A:108:TYR:CE1	1:A:121:MET:SD	0.67	2.87	3	4
1:A:61:PRO:O	1:A:63:LYS:N	0.67	2.28	13	4
1:A:54:GLN:NE2	1:A:55:PHE:CE2	0.66	2.64	13	1
1:A:183:LEU:H	1:A:183:LEU:HD12	0.66	1.51	17	1
1:A:129:TYR:CE1	1:A:144:THR:HG21	0.65	2.26	7	1
1:A:121:MET:SD	1:A:153:PHE:CD2	0.65	2.89	2	3
1:A:181:GLN:O	1:A:182:ALA:HB3	0.65	1.91	9	1
1:A:37:ASP:OD1	1:A:38:CYS:N	0.65	2.30	8	4
1:A:42:GLN:HE22	1:A:79:ARG:NH2	0.65	1.89	2	2
1:A:108:TYR:CE1	1:A:121:MET:CE	0.65	2.80	4	3
1:A:97:LEU:H	1:A:97:LEU:CD2	0.64	2.04	6	3
1:A:75:ASN:CG	1:A:75:ASN:O	0.64	2.40	12	1
1:A:158:LYS:O	1:A:160:ALA:N	0.64	2.30	19	16
1:A:118:ARG:H	1:A:118:ARG:CD	0.64	2.05	11	3
1:A:97:LEU:HD12	1:A:97:LEU:H	0.64	1.51	8	2
1:A:42:GLN:NE2	1:A:79:ARG:CZ	0.64	2.61	16	3
1:A:166:LEU:H	1:A:166:LEU:CD2	0.64	2.04	9	5
1:A:155:MET:SD	1:A:156:MET:SD	0.64	2.96	14	1
1:A:13:VAL:HG13	1:A:24:GLU:CD	0.64	2.18	18	1
1:A:161:ASP:OD1	1:A:162:GLY:N	0.64	2.31	8	12
1:A:111:ASP:OD1	1:A:112:ASN:N	0.64	2.30	7	12
1:A:97:LEU:HD12	1:A:97:LEU:N	0.64	2.07	8	2
1:A:16:LEU:HD23	1:A:16:LEU:O	0.64	1.93	5	1
1:A:159:ASN:HD22	1:A:159:ASN:N	0.64	1.90	6	2
1:A:82:PHE:CD1	1:A:82:PHE:C	0.63	2.77	13	13
1:A:183:LEU:H	1:A:183:LEU:CD1	0.63	2.04	17	3
1:A:183:LEU:N	1:A:183:LEU:CD1	0.63	2.55	5	6
1:A:111:ASP:O	1:A:112:ASN:C	0.63	2.41	1	16
1:A:75:ASN:O	1:A:77:ASP:N	0.63	2.31	13	6
1:A:111:ASP:O	1:A:113:ASP:N	0.63	2.30	4	7
1:A:129:TYR:O	1:A:133:GLY:N	0.63	2.31	19	15
1:A:118:ARG:H	1:A:118:ARG:NE	0.63	1.91	10	6
1:A:183:LEU:N	1:A:183:LEU:HD13	0.63	2.08	14	4
1:A:52:TYR:CD2	1:A:131:MET:SD	0.63	2.91	15	1
1:A:48:PHE:CE2	1:A:85:PHE:CD2	0.63	2.87	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:PHE:CZ	1:A:107:LEU:HD11	0.63	2.29	4	5
1:A:72:PHE:CZ	1:A:88:ALA:CB	0.63	2.80	18	7
1:A:166:LEU:HD12	1:A:166:LEU:H	0.63	1.51	8	6
1:A:183:LEU:N	1:A:183:LEU:CD2	0.63	2.60	20	12
1:A:48:PHE:CE2	1:A:85:PHE:CE2	0.63	2.87	13	1
1:A:110:LEU:HD13	1:A:110:LEU:O	0.63	1.93	10	3
1:A:143:ASN:HD22	1:A:143:ASN:N	0.63	1.91	3	1
1:A:135:THR:O	1:A:137:GLU:N	0.62	2.32	9	4
1:A:164:LEU:HD13	1:A:165:THR:N	0.62	2.09	9	7
1:A:159:ASN:HD22	1:A:160:ALA:N	0.62	1.93	8	2
1:A:63:LYS:O	1:A:67:PHE:CD1	0.62	2.52	2	9
1:A:141:GLU:O	1:A:142:GLU:CB	0.62	2.47	10	3
1:A:16:LEU:O	1:A:20:THR:HG22	0.62	1.94	13	3
1:A:51:ILE:HD12	1:A:52:TYR:N	0.62	2.09	1	2
1:A:118:ARG:NH2	1:A:157:ASP:CB	0.62	2.62	9	4
1:A:97:LEU:H	1:A:97:LEU:HD23	0.62	1.53	16	1
1:A:42:GLN:NE2	1:A:79:ARG:NH2	0.62	2.47	2	1
1:A:61:PRO:O	1:A:65:ALA:HB3	0.62	1.95	12	2
1:A:153:PHE:CZ	1:A:164:LEU:HD21	0.62	2.29	11	1
1:A:64:PHE:CD2	1:A:131:MET:SD	0.62	2.93	5	3
1:A:146:GLU:O	1:A:149:VAL:HG22	0.62	1.95	8	7
1:A:129:TYR:C	1:A:129:TYR:CD1	0.62	2.78	2	2
1:A:21:TYR:OH	1:A:96:THR:HG23	0.61	1.95	20	1
1:A:159:ASN:HD21	1:A:161:ASP:N	0.61	1.92	1	1
1:A:159:ASN:HD21	1:A:161:ASP:CG	0.61	2.03	1	3
1:A:121:MET:CE	1:A:153:PHE:CE2	0.61	2.83	20	1
1:A:153:PHE:CE1	1:A:164:LEU:HD11	0.61	2.30	1	1
1:A:159:ASN:HD22	1:A:159:ASN:H	0.61	1.39	6	1
1:A:121:MET:HE1	1:A:153:PHE:CZ	0.61	2.29	9	2
1:A:158:LYS:C	1:A:159:ASN:ND2	0.61	2.58	19	1
1:A:69:PHE:CG	1:A:70:ASN:N	0.61	2.67	5	2
1:A:110:LEU:HD23	1:A:111:ASP:H	0.61	1.55	6	1
1:A:115:TYR:CD1	1:A:115:TYR:N	0.61	2.68	19	4
1:A:49:GLN:OE1	1:A:66:THR:HG22	0.61	1.94	9	1
1:A:159:ASN:ND2	1:A:159:ASN:C	0.61	2.58	1	1
1:A:110:LEU:HD23	1:A:110:LEU:N	0.61	2.10	5	1
1:A:109:ASP:OD2	1:A:112:ASN:N	0.61	2.33	8	1
1:A:112:ASN:OD1	1:A:113:ASP:N	0.61	2.34	13	1
1:A:110:LEU:HD23	1:A:110:LEU:O	0.61	1.96	18	2
1:A:38:CYS:O	1:A:40:SER:N	0.61	2.34	10	1
1:A:129:TYR:CE1	1:A:146:GLU:OE2	0.61	2.54	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:ASN:ND2	1:A:161:ASP:H	0.61	1.94	11	2
1:A:109:ASP:OD1	1:A:112:ASN:N	0.60	2.34	13	4
1:A:166:LEU:HD22	1:A:166:LEU:N	0.60	2.11	14	3
1:A:183:LEU:H	1:A:183:LEU:HD13	0.60	1.56	14	1
1:A:21:TYR:CD2	1:A:93:SER:OG	0.60	2.54	9	1
1:A:143:ASN:O	1:A:144:THR:C	0.60	2.44	15	9
1:A:14:GLU:OE2	1:A:18:ARG:NE	0.60	2.35	1	1
1:A:159:ASN:C	1:A:161:ASP:H	0.60	2.05	15	2
1:A:118:ARG:H	1:A:118:ARG:HE	0.60	1.39	14	3
1:A:155:MET:C	1:A:155:MET:SD	0.60	2.84	19	3
1:A:143:ASN:ND2	1:A:183:LEU:O	0.60	2.34	20	2
1:A:135:THR:O	1:A:138:LEU:HD23	0.60	1.96	13	1
1:A:30:TRP:O	1:A:34:PHE:CE2	0.60	2.55	15	6
1:A:118:ARG:NH2	1:A:157:ASP:CG	0.60	2.60	12	2
1:A:42:GLN:NE2	1:A:79:ARG:NH1	0.60	2.49	10	1
1:A:182:ALA:O	1:A:184:SER:N	0.60	2.35	10	1
1:A:158:LYS:CG	1:A:159:ASN:H	0.60	2.10	19	2
1:A:19:LYS:NZ	1:A:87:GLN:HE22	0.60	1.92	20	1
1:A:158:LYS:O	1:A:159:ASN:C	0.60	2.44	19	18
1:A:49:GLN:NE2	1:A:66:THR:OG1	0.60	2.35	5	7
1:A:71:VAL:O	1:A:106:LYS:NZ	0.60	2.34	5	1
1:A:16:LEU:HD22	1:A:20:THR:OG1	0.60	1.97	6	1
1:A:22:PHE:CD2	1:A:26:GLU:OE1	0.60	2.55	1	3
1:A:44:ASP:OD1	1:A:79:ARG:NE	0.60	2.35	15	2
1:A:56:PHE:CD1	1:A:56:PHE:N	0.60	2.69	3	4
1:A:75:ASN:ND2	1:A:77:ASP:OD2	0.60	2.35	5	2
1:A:118:ARG:NH2	1:A:157:ASP:OD2	0.60	2.35	20	2
1:A:69:PHE:CE2	1:A:70:ASN:OD1	0.60	2.55	7	2
1:A:105:PHE:CZ	1:A:166:LEU:CD1	0.59	2.85	3	2
1:A:139:PRO:O	1:A:143:ASN:N	0.59	2.35	3	4
1:A:71:VAL:HG13	1:A:72:PHE:N	0.59	2.10	9	7
1:A:111:ASP:O	1:A:112:ASN:ND2	0.59	2.35	6	2
1:A:153:PHE:CZ	1:A:164:LEU:CD1	0.59	2.84	16	1
1:A:138:LEU:N	1:A:138:LEU:CD2	0.59	2.65	11	3
1:A:44:ASP:OD1	1:A:79:ARG:NH1	0.59	2.35	5	1
1:A:75:ASN:O	1:A:75:ASN:ND2	0.59	2.35	12	1
1:A:63:LYS:O	1:A:67:PHE:CG	0.59	2.56	19	4
1:A:108:TYR:CE1	1:A:121:MET:HE3	0.59	2.31	4	2
1:A:24:GLU:H	1:A:24:GLU:CD	0.59	2.04	8	3
1:A:20:THR:O	1:A:21:TYR:CG	0.59	2.56	12	2
1:A:42:GLN:NE2	1:A:43:LEU:C	0.59	2.60	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:ASP:OD1	1:A:163:LYS:N	0.59	2.36	19	1
1:A:30:TRP:O	1:A:34:PHE:CD1	0.59	2.55	20	4
1:A:64:PHE:CG	1:A:131:MET:SD	0.59	2.95	2	2
1:A:115:TYR:CD2	1:A:165:THR:HG22	0.59	2.32	4	2
1:A:72:PHE:CD1	1:A:72:PHE:C	0.59	2.80	5	2
1:A:150:ASP:O	1:A:154:ALA:HB2	0.59	1.98	19	8
1:A:110:LEU:HD23	1:A:110:LEU:H	0.59	1.57	5	1
1:A:20:THR:O	1:A:21:TYR:CD2	0.59	2.56	13	3
1:A:170:GLN:NE2	1:A:170:GLN:C	0.59	2.61	19	1
1:A:27:VAL:HG13	1:A:86:ILE:HD11	0.59	1.74	14	3
1:A:66:THR:O	1:A:70:ASN:ND2	0.59	2.36	3	1
1:A:51:ILE:O	1:A:55:PHE:CD2	0.59	2.56	17	7
1:A:159:ASN:ND2	1:A:161:ASP:OD1	0.59	2.35	1	2
1:A:142:GLU:C	1:A:144:THR:H	0.59	2.06	19	4
1:A:157:ASP:C	1:A:159:ASN:ND2	0.59	2.61	6	2
1:A:91:VAL:O	1:A:95:GLY:N	0.59	2.35	3	1
1:A:113:ASP:OD1	1:A:114:GLY:N	0.59	2.36	12	5
1:A:118:ARG:NH1	1:A:162:GLY:C	0.59	2.61	8	1
1:A:180:VAL:O	1:A:182:ALA:N	0.59	2.36	13	7
1:A:73:ASP:OD2	1:A:78:GLY:N	0.59	2.36	11	1
1:A:55:PHE:CD1	1:A:55:PHE:N	0.59	2.71	15	3
1:A:142:GLU:OE2	1:A:148:ARG:NH2	0.59	2.35	20	2
1:A:16:LEU:O	1:A:20:THR:OG1	0.59	2.21	15	12
1:A:30:TRP:O	1:A:34:PHE:CD2	0.59	2.56	15	4
1:A:139:PRO:O	1:A:140:GLU:C	0.59	2.46	10	5
1:A:159:ASN:O	1:A:160:ALA:CB	0.59	2.51	4	11
1:A:166:LEU:HD12	1:A:166:LEU:N	0.59	2.12	8	8
1:A:73:ASP:OD2	1:A:76:LYS:N	0.59	2.36	5	1
1:A:136:VAL:O	1:A:137:GLU:C	0.59	2.46	18	3
1:A:60:ASP:N	1:A:131:MET:O	0.59	2.36	7	2
1:A:118:ARG:NH1	1:A:157:ASP:OD2	0.59	2.36	15	3
1:A:96:THR:C	1:A:100:LYS:NZ	0.58	2.61	2	1
1:A:45:ALA:HB2	1:A:69:PHE:CE2	0.58	2.33	11	10
1:A:19:LYS:O	1:A:21:TYR:N	0.58	2.36	6	2
1:A:157:ASP:O	1:A:159:ASN:ND2	0.58	2.36	8	2
1:A:119:ASN:ND2	1:A:119:ASN:C	0.58	2.61	11	1
1:A:68:VAL:O	1:A:72:PHE:N	0.58	2.36	1	14
1:A:72:PHE:CG	1:A:72:PHE:O	0.58	2.56	3	1
1:A:142:GLU:O	1:A:144:THR:N	0.58	2.36	3	4
1:A:16:LEU:O	1:A:19:LYS:N	0.58	2.36	11	3
1:A:112:ASN:O	1:A:115:TYR:N	0.58	2.35	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:PRO:O	1:A:149:VAL:HG22	0.58	1.98	16	1
1:A:19:LYS:O	1:A:20:THR:CB	0.58	2.51	2	2
1:A:30:TRP:O	1:A:34:PHE:CE1	0.58	2.55	4	4
1:A:20:THR:C	1:A:21:TYR:CG	0.58	2.80	13	7
1:A:79:ARG:NH1	1:A:81:GLU:OE2	0.58	2.36	4	1
1:A:157:ASP:OD1	1:A:159:ASN:ND2	0.58	2.36	6	1
1:A:86:ILE:HD13	1:A:86:ILE:O	0.58	1.97	12	2
1:A:159:ASN:ND2	1:A:168:GLU:OE2	0.58	2.36	12	2
1:A:178:SER:OG	1:A:181:GLN:NE2	0.58	2.36	5	1
1:A:22:PHE:CZ	1:A:93:SER:OG	0.58	2.55	18	2
1:A:159:ASN:OD1	1:A:160:ALA:N	0.58	2.35	13	1
1:A:99:GLU:OE1	1:A:102:ARG:NH2	0.58	2.36	18	1
1:A:31:TYR:O	1:A:35:ILE:CG1	0.58	2.51	14	14
1:A:112:ASN:CG	1:A:112:ASN:O	0.58	2.46	12	5
1:A:118:ARG:NE	1:A:157:ASP:OD2	0.58	2.36	3	1
1:A:143:ASN:C	1:A:144:THR:HG22	0.58	2.23	3	1
1:A:159:ASN:O	1:A:161:ASP:N	0.58	2.36	3	3
1:A:56:PHE:CD1	1:A:137:GLU:OE2	0.58	2.56	6	1
1:A:74:GLU:N	1:A:84:GLU:OE2	0.58	2.37	11	2
1:A:109:ASP:OD1	1:A:113:ASP:N	0.58	2.36	10	1
1:A:115:TYR:CE1	1:A:165:THR:OG1	0.58	2.55	11	1
1:A:67:PHE:CE2	1:A:124:ILE:HD12	0.58	2.34	4	1
1:A:132:VAL:O	1:A:138:LEU:HD21	0.58	1.98	13	1
1:A:20:THR:C	1:A:22:PHE:H	0.58	2.07	3	11
1:A:114:GLY:O	1:A:115:TYR:CD1	0.58	2.56	13	1
1:A:156:MET:O	1:A:159:ASN:ND2	0.58	2.36	5	1
1:A:73:ASP:OD2	1:A:77:ASP:N	0.58	2.36	11	1
1:A:121:MET:HE1	1:A:153:PHE:CE2	0.58	2.33	20	1
1:A:128:ILE:HD12	1:A:183:LEU:HD11	0.58	1.76	11	1
1:A:112:ASN:O	1:A:112:ASN:ND2	0.58	2.36	4	2
1:A:96:THR:N	1:A:99:GLU:OE1	0.58	2.36	7	1
1:A:85:PHE:CE1	1:A:89:LEU:HD23	0.58	2.33	13	4
1:A:58:PHE:O	1:A:135:THR:HG22	0.58	1.98	13	1
1:A:164:LEU:HD12	1:A:169:PHE:CE2	0.57	2.34	7	1
1:A:182:ALA:C	1:A:184:SER:N	0.57	2.60	10	1
1:A:143:ASN:O	1:A:145:PRO:N	0.57	2.36	15	1
1:A:135:THR:O	1:A:136:VAL:C	0.57	2.46	20	8
1:A:125:VAL:HG11	1:A:146:GLU:OE1	0.57	1.99	11	2
1:A:22:PHE:CE2	1:A:93:SER:OG	0.57	2.55	12	2
1:A:126:ASP:OD2	1:A:130:GLN:NE2	0.57	2.36	16	1
1:A:91:VAL:HG11	1:A:103:TRP:HE1	0.57	1.58	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:PHE:CD1	1:A:69:PHE:C	0.57	2.81	19	2
1:A:183:LEU:O	1:A:184:SER:CB	0.57	2.52	14	2
1:A:142:GLU:CD	1:A:148:ARG:NH1	0.57	2.62	3	1
1:A:32:LYS:O	1:A:36:LYS:NZ	0.57	2.37	1	1
1:A:31:TYR:CD1	1:A:82:PHE:CZ	0.57	2.92	4	3
1:A:177:PRO:O	1:A:178:SER:CB	0.57	2.51	14	19
1:A:176:ASP:OD1	1:A:176:ASP:N	0.57	2.37	5	1
1:A:20:THR:HG21	1:A:27:VAL:HG11	0.57	1.74	8	2
1:A:135:THR:C	1:A:137:GLU:N	0.57	2.62	9	2
1:A:138:LEU:HD12	1:A:138:LEU:H	0.57	1.59	17	1
1:A:19:LYS:C	1:A:20:THR:HG1	0.57	2.07	19	3
1:A:121:MET:C	1:A:121:MET:SD	0.57	2.88	19	1
1:A:166:LEU:HD22	1:A:167:GLN:N	0.57	2.15	12	1
1:A:85:PHE:C	1:A:85:PHE:CD1	0.56	2.82	9	8
1:A:89:LEU:HD13	1:A:89:LEU:O	0.56	2.00	3	6
1:A:84:GLU:O	1:A:88:ALA:HB3	0.56	2.00	5	3
1:A:42:GLN:NE2	1:A:79:ARG:NE	0.56	2.53	11	3
1:A:59:GLY:O	1:A:131:MET:HE1	0.56	2.00	8	1
1:A:153:PHE:CZ	1:A:164:LEU:CD2	0.56	2.87	11	1
1:A:131:MET:SD	1:A:131:MET:C	0.56	2.88	13	2
1:A:67:PHE:CE2	1:A:110:LEU:HD22	0.56	2.35	14	1
1:A:156:MET:O	1:A:156:MET:SD	0.56	2.63	17	2
1:A:61:PRO:C	1:A:63:LYS:H	0.56	2.07	8	4
1:A:79:ARG:NH2	1:A:81:GLU:OE2	0.56	2.38	4	1
1:A:110:LEU:HD23	1:A:111:ASP:N	0.56	2.16	6	1
1:A:131:MET:O	1:A:131:MET:SD	0.56	2.63	12	2
1:A:145:PRO:CD	1:A:182:ALA:O	0.56	2.54	15	1
1:A:127:ALA:O	1:A:131:MET:SD	0.56	2.63	7	1
1:A:153:PHE:O	1:A:157:ASP:N	0.56	2.39	13	3
1:A:37:ASP:O	1:A:38:CYS:SG	0.56	2.63	15	2
1:A:159:ASN:ND2	1:A:161:ASP:OD2	0.56	2.39	12	1
1:A:67:PHE:C	1:A:67:PHE:CD1	0.56	2.82	10	2
1:A:136:VAL:O	1:A:136:VAL:CG1	0.56	2.54	5	2
1:A:42:GLN:HE21	1:A:43:LEU:C	0.56	2.09	18	1
1:A:75:ASN:C	1:A:77:ASP:N	0.56	2.62	9	5
1:A:157:ASP:O	1:A:158:LYS:C	0.56	2.49	20	7
1:A:109:ASP:OD1	1:A:109:ASP:O	0.56	2.24	10	1
1:A:157:ASP:CG	1:A:162:GLY:H	0.56	2.08	11	1
1:A:108:TYR:OH	1:A:182:ALA:HB2	0.56	2.00	14	1
1:A:142:GLU:CG	1:A:143:ASN:N	0.56	2.69	18	2
1:A:121:MET:O	1:A:125:VAL:HG13	0.56	1.99	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:THR:O	1:A:138:LEU:CD1	0.56	2.54	12	2
1:A:17:THR:CG2	1:A:24:GLU:OE1	0.56	2.54	18	1
1:A:118:ARG:HH22	1:A:157:ASP:CG	0.56	2.09	12	3
1:A:27:VAL:HG23	1:A:86:ILE:HD11	0.56	1.78	17	1
1:A:138:LEU:H	1:A:138:LEU:CD1	0.56	2.14	17	1
1:A:19:LYS:O	1:A:20:THR:OG1	0.55	2.24	11	11
1:A:61:PRO:C	1:A:63:LYS:N	0.55	2.62	13	4
1:A:75:ASN:HD21	1:A:77:ASP:CG	0.55	2.09	18	3
1:A:118:ARG:HH21	1:A:157:ASP:CB	0.55	2.14	2	1
1:A:144:THR:O	1:A:144:THR:CG2	0.55	2.53	4	2
1:A:143:ASN:CG	1:A:181:GLN:NE2	0.55	2.65	10	1
1:A:132:VAL:O	1:A:132:VAL:HG12	0.55	2.01	1	5
1:A:131:MET:O	1:A:135:THR:HG21	0.55	2.01	6	1
1:A:118:ARG:HH22	1:A:157:ASP:CB	0.55	2.15	1	2
1:A:96:THR:CB	1:A:99:GLU:OE1	0.55	2.55	7	1
1:A:149:VAL:HG12	1:A:153:PHE:CD2	0.55	2.37	10	1
1:A:16:LEU:O	1:A:20:THR:CG2	0.55	2.54	12	3
1:A:31:TYR:CD1	1:A:82:PHE:CD2	0.55	2.94	12	1
1:A:171:GLU:CG	1:A:172:GLY:N	0.55	2.70	16	1
1:A:21:TYR:CE2	1:A:95:GLY:CA	0.55	2.90	18	1
1:A:166:LEU:O	1:A:167:GLN:C	0.55	2.49	15	15
1:A:101:LEU:O	1:A:105:PHE:CG	0.55	2.60	10	1
1:A:107:LEU:HD23	1:A:107:LEU:C	0.55	2.25	12	3
1:A:158:LYS:CG	1:A:159:ASN:N	0.55	2.69	19	2
1:A:118:ARG:CZ	1:A:157:ASP:OD2	0.55	2.54	15	2
1:A:142:GLU:C	1:A:144:THR:N	0.55	2.65	3	3
1:A:97:LEU:HD23	1:A:97:LEU:H	0.55	1.62	4	2
1:A:97:LEU:H	1:A:97:LEU:CD1	0.55	2.15	8	2
1:A:181:GLN:O	1:A:182:ALA:CB	0.55	2.55	9	1
1:A:128:ILE:O	1:A:132:VAL:CG1	0.55	2.55	18	1
1:A:158:LYS:C	1:A:160:ALA:N	0.55	2.62	8	16
1:A:71:VAL:CG2	1:A:110:LEU:O	0.55	2.55	12	1
1:A:110:LEU:C	1:A:110:LEU:CD1	0.55	2.78	9	4
1:A:61:PRO:O	1:A:62:THR:CB	0.55	2.55	4	1
1:A:157:ASP:C	1:A:159:ASN:HD22	0.55	2.10	6	1
1:A:129:TYR:CD1	1:A:144:THR:HG21	0.55	2.37	7	1
1:A:173:SER:OG	1:A:180:VAL:CG2	0.55	2.54	13	2
1:A:96:THR:C	1:A:100:LYS:HZ3	0.55	2.10	2	1
1:A:182:ALA:C	1:A:183:LEU:HD23	0.55	2.26	11	1
1:A:97:LEU:N	1:A:97:LEU:CD2	0.54	2.70	20	6
1:A:19:LYS:C	1:A:21:TYR:H	0.54	2.10	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:ASN:ND2	1:A:161:ASP:CG	0.54	2.65	1	3
1:A:85:PHE:CE1	1:A:89:LEU:HD22	0.54	2.37	7	4
1:A:144:THR:O	1:A:145:PRO:C	0.54	2.50	7	3
1:A:45:ALA:N	1:A:69:PHE:CZ	0.54	2.75	11	1
1:A:61:PRO:O	1:A:65:ALA:CB	0.54	2.56	12	1
1:A:105:PHE:CD1	1:A:169:PHE:CE2	0.54	2.95	19	1
1:A:45:ALA:HB2	1:A:69:PHE:CE1	0.54	2.37	1	2
1:A:109:ASP:CG	1:A:112:ASN:H	0.54	2.10	6	5
1:A:31:TYR:CE1	1:A:82:PHE:CD2	0.54	2.95	12	1
1:A:19:LYS:HZ2	1:A:87:GLN:HE22	0.54	1.44	20	1
1:A:51:ILE:O	1:A:55:PHE:CE2	0.54	2.60	9	4
1:A:75:ASN:O	1:A:76:LYS:C	0.54	2.51	20	8
1:A:93:SER:O	1:A:94:ARG:CB	0.54	2.56	12	2
1:A:125:VAL:HG22	1:A:145:PRO:HG2	0.54	1.79	16	1
1:A:142:GLU:CG	1:A:143:ASN:H	0.54	2.14	18	1
1:A:136:VAL:O	1:A:136:VAL:HG23	0.54	2.03	9	1
1:A:159:ASN:N	1:A:159:ASN:ND2	0.54	2.55	6	1
1:A:129:TYR:O	1:A:133:GLY:CA	0.54	2.55	7	1
1:A:20:THR:O	1:A:21:TYR:CB	0.54	2.55	12	4
1:A:139:PRO:O	1:A:142:GLU:N	0.54	2.41	10	1
1:A:136:VAL:O	1:A:136:VAL:HG12	0.54	2.02	18	1
1:A:128:ILE:O	1:A:132:VAL:N	0.54	2.41	12	2
1:A:58:PHE:CD2	1:A:135:THR:HG23	0.54	2.37	8	1
1:A:42:GLN:CD	1:A:79:ARG:NE	0.54	2.66	11	2
1:A:67:PHE:CD2	1:A:110:LEU:HD13	0.54	2.37	14	2
1:A:181:GLN:CG	1:A:181:GLN:O	0.54	2.56	5	1
1:A:139:PRO:CG	1:A:142:GLU:O	0.54	2.56	16	1
1:A:68:VAL:O	1:A:72:PHE:CB	0.53	2.56	2	9
1:A:91:VAL:HG11	1:A:103:TRP:NE1	0.53	2.18	1	4
1:A:97:LEU:N	1:A:97:LEU:HD22	0.53	2.17	20	3
1:A:20:THR:C	1:A:22:PHE:N	0.53	2.64	3	10
1:A:155:MET:CE	1:A:156:MET:HE2	0.53	2.32	2	1
1:A:180:VAL:C	1:A:182:ALA:N	0.53	2.62	13	3
1:A:61:PRO:O	1:A:65:ALA:N	0.53	2.38	12	1
1:A:71:VAL:HG21	1:A:107:LEU:HA	0.53	1.80	3	1
1:A:59:GLY:O	1:A:131:MET:CE	0.53	2.56	8	1
1:A:141:GLU:OE2	1:A:148:ARG:NH2	0.53	2.41	10	1
1:A:143:ASN:HB3	1:A:183:LEU:HD22	0.53	1.81	18	1
1:A:27:VAL:HG13	1:A:86:ILE:CD1	0.53	2.33	18	3
1:A:143:ASN:C	1:A:144:THR:OG1	0.53	2.52	12	3
1:A:106:LYS:NZ	1:A:112:ASN:ND2	0.53	2.56	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:TRP:CD1	1:A:106:LYS:HZ1	0.53	2.20	18	1
1:A:110:LEU:C	1:A:110:LEU:CD2	0.53	2.81	20	2
1:A:16:LEU:O	1:A:19:LYS:O	0.53	2.26	6	10
1:A:72:PHE:CE1	1:A:88:ALA:HB2	0.53	2.38	13	4
1:A:135:THR:O	1:A:138:LEU:HD22	0.53	2.03	11	2
1:A:166:LEU:HD22	1:A:166:LEU:H	0.53	1.64	14	1
1:A:31:TYR:CE1	1:A:35:ILE:HD11	0.53	2.38	1	2
1:A:64:PHE:CE2	1:A:107:LEU:HD21	0.53	2.38	3	1
1:A:75:ASN:C	1:A:77:ASP:H	0.53	2.12	12	3
1:A:74:GLU:CA	1:A:77:ASP:OD1	0.53	2.56	12	1
1:A:181:GLN:O	1:A:182:ALA:C	0.53	2.50	14	2
1:A:112:ASN:ND2	1:A:112:ASN:C	0.53	2.65	4	1
1:A:106:LYS:HZ3	1:A:106:LYS:HB3	0.53	1.63	5	1
1:A:72:PHE:CE2	1:A:80:ILE:HD11	0.53	2.39	9	2
1:A:112:ASN:O	1:A:113:ASP:CG	0.53	2.52	13	1
1:A:135:THR:O	1:A:135:THR:OG1	0.53	2.27	15	1
1:A:179:ILE:HG22	1:A:180:VAL:N	0.53	2.18	18	1
1:A:133:GLY:O	1:A:134:ASN:ND2	0.53	2.41	19	1
1:A:67:PHE:CD1	1:A:110:LEU:HD13	0.53	2.39	3	1
1:A:129:TYR:CE1	1:A:143:ASN:O	0.53	2.62	17	1
1:A:145:PRO:CG	1:A:183:LEU:HD12	0.53	2.34	19	1
1:A:172:GLY:O	1:A:176:ASP:O	0.52	2.27	13	5
1:A:134:ASN:C	1:A:135:THR:HG22	0.52	2.29	15	2
1:A:20:THR:HG22	1:A:22:PHE:H	0.52	1.64	2	1
1:A:89:LEU:C	1:A:89:LEU:CD1	0.52	2.81	4	6
1:A:145:PRO:CG	1:A:182:ALA:O	0.52	2.56	15	2
1:A:142:GLU:O	1:A:143:ASN:C	0.52	2.51	17	1
1:A:39:PRO:O	1:A:40:SER:CB	0.52	2.55	2	1
1:A:51:ILE:HG22	1:A:52:TYR:N	0.52	2.19	16	2
1:A:118:ARG:NE	1:A:153:PHE:CE1	0.52	2.77	16	2
1:A:20:THR:HG23	1:A:21:TYR:N	0.52	2.18	12	1
1:A:136:VAL:HG13	1:A:137:GLU:N	0.52	2.19	1	2
1:A:118:ARG:HE	1:A:157:ASP:CG	0.52	2.12	3	1
1:A:118:ARG:HH21	1:A:121:MET:HE1	0.52	1.64	5	1
1:A:42:GLN:HE22	1:A:79:ARG:NH1	0.52	2.02	10	1
1:A:115:TYR:CE1	1:A:165:THR:HG22	0.52	2.39	16	2
1:A:141:GLU:CG	1:A:142:GLU:N	0.52	2.71	16	1
1:A:159:ASN:ND2	1:A:159:ASN:N	0.52	2.56	5	3
1:A:118:ARG:NH2	1:A:162:GLY:O	0.52	2.43	7	1
1:A:109:ASP:OD1	1:A:113:ASP:OD1	0.52	2.27	10	1
1:A:182:ALA:C	1:A:184:SER:H	0.52	2.12	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ASP:C	1:A:77:ASP:OD1	0.52	2.53	12	1
1:A:141:GLU:CD	1:A:143:ASN:HD21	0.52	2.12	13	1
1:A:122:LEU:HD22	1:A:146:GLU:OE2	0.52	2.05	2	1
1:A:72:PHE:O	1:A:72:PHE:CD1	0.52	2.62	3	1
1:A:143:ASN:OD1	1:A:148:ARG:NH2	0.52	2.42	11	1
1:A:105:PHE:CZ	1:A:166:LEU:HD11	0.52	2.39	13	1
1:A:75:ASN:OD1	1:A:84:GLU:OE2	0.52	2.28	16	7
1:A:170:GLN:CG	1:A:171:GLU:N	0.52	2.73	2	1
1:A:143:ASN:ND2	1:A:181:GLN:CD	0.52	2.68	10	1
1:A:159:ASN:C	1:A:161:ASP:N	0.52	2.67	3	3
1:A:177:PRO:O	1:A:179:ILE:N	0.52	2.42	6	1
1:A:183:LEU:O	1:A:184:SER:C	0.52	2.52	2	2
1:A:156:MET:HE3	1:A:179:ILE:HG12	0.52	1.82	19	1
1:A:14:GLU:CD	1:A:14:GLU:C	0.52	2.78	13	3
1:A:62:THR:O	1:A:66:THR:CG2	0.52	2.58	2	3
1:A:108:TYR:CZ	1:A:121:MET:HE3	0.52	2.40	4	2
1:A:156:MET:SD	1:A:164:LEU:HD21	0.52	2.45	4	1
1:A:170:GLN:NE2	1:A:170:GLN:O	0.52	2.43	19	1
1:A:172:GLY:C	1:A:179:ILE:HD12	0.51	2.30	13	4
1:A:72:PHE:CZ	1:A:88:ALA:HB1	0.51	2.40	10	3
1:A:141:GLU:O	1:A:183:LEU:O	0.51	2.29	4	1
1:A:159:ASN:O	1:A:160:ALA:C	0.51	2.52	19	2
1:A:16:LEU:C	1:A:20:THR:HG1	0.51	2.13	11	2
1:A:158:LYS:HG3	1:A:159:ASN:H	0.51	1.65	15	2
1:A:159:ASN:OD1	1:A:161:ASP:OD2	0.51	2.29	10	4
1:A:82:PHE:CG	1:A:83:SER:N	0.51	2.77	14	5
1:A:16:LEU:O	1:A:19:LYS:C	0.51	2.53	19	4
1:A:86:ILE:HG23	1:A:87:GLN:N	0.51	2.20	5	3
1:A:169:PHE:O	1:A:173:SER:N	0.51	2.42	6	1
1:A:74:GLU:O	1:A:75:ASN:CB	0.51	2.59	12	4
1:A:121:MET:O	1:A:125:VAL:CG2	0.51	2.55	11	1
1:A:19:LYS:HZ2	1:A:87:GLN:NE2	0.51	2.02	20	1
1:A:166:LEU:H	1:A:166:LEU:CD1	0.51	2.18	8	2
1:A:19:LYS:C	1:A:20:THR:OG1	0.51	2.53	20	7
1:A:110:LEU:H	1:A:110:LEU:CD2	0.51	2.19	5	1
1:A:135:THR:O	1:A:138:LEU:CD2	0.51	2.59	6	1
1:A:131:MET:O	1:A:135:THR:OG1	0.51	2.26	11	3
1:A:159:ASN:OD1	1:A:168:GLU:OE2	0.51	2.29	16	3
1:A:101:LEU:C	1:A:101:LEU:CD1	0.51	2.84	18	2
1:A:85:PHE:CE1	1:A:89:LEU:HD13	0.51	2.40	19	1
1:A:111:ASP:OD1	1:A:111:ASP:C	0.51	2.53	18	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:GLU:CD	1:A:168:GLU:H	0.51	2.14	4	1
1:A:60:ASP:CG	1:A:60:ASP:O	0.51	2.54	12	1
1:A:109:ASP:OD2	1:A:120:GLU:OE1	0.51	2.29	8	5
1:A:62:THR:HG23	1:A:63:LYS:H	0.51	1.64	5	1
1:A:166:LEU:O	1:A:169:PHE:N	0.51	2.43	20	5
1:A:112:ASN:O	1:A:115:TYR:O	0.51	2.28	8	1
1:A:138:LEU:HD12	1:A:138:LEU:O	0.51	2.06	8	1
1:A:51:ILE:CG2	1:A:52:TYR:N	0.51	2.74	16	2
1:A:111:ASP:O	1:A:112:ASN:CG	0.51	2.54	19	3
1:A:169:PHE:O	1:A:173:SER:OG	0.51	2.29	10	9
1:A:107:LEU:O	1:A:107:LEU:HD13	0.51	2.05	7	1
1:A:25:LYS:O	1:A:29:GLN:CD	0.51	2.54	9	1
1:A:158:LYS:C	1:A:159:ASN:HD22	0.51	2.12	19	1
1:A:180:VAL:O	1:A:181:GLN:C	0.51	2.54	13	7
1:A:109:ASP:OD1	1:A:111:ASP:OD1	0.51	2.28	13	10
1:A:109:ASP:OD2	1:A:111:ASP:OD1	0.51	2.29	3	3
1:A:111:ASP:OD2	1:A:113:ASP:OD2	0.51	2.29	6	2
1:A:125:VAL:O	1:A:129:TYR:CB	0.51	2.59	14	3
1:A:180:VAL:HG22	1:A:180:VAL:O	0.51	2.04	9	1
1:A:62:THR:O	1:A:66:THR:OG1	0.51	2.29	12	2
1:A:129:TYR:CZ	1:A:143:ASN:O	0.51	2.64	17	1
1:A:139:PRO:O	1:A:140:GLU:O	0.51	2.29	2	2
1:A:37:ASP:OD1	1:A:37:ASP:C	0.51	2.54	8	4
1:A:58:PHE:O	1:A:134:ASN:CG	0.51	2.54	16	2
1:A:158:LYS:O	1:A:159:ASN:OD1	0.51	2.28	7	1
1:A:161:ASP:OD2	1:A:163:LYS:O	0.50	2.29	7	6
1:A:183:LEU:HD23	1:A:183:LEU:H	0.50	1.65	4	2
1:A:43:LEU:HD21	1:A:47:GLY:C	0.50	2.31	6	3
1:A:71:VAL:CG1	1:A:72:PHE:N	0.50	2.74	9	8
1:A:73:ASP:O	1:A:77:ASP:OD2	0.50	2.29	12	1
1:A:77:ASP:OD2	1:A:81:GLU:OE2	0.50	2.28	14	1
1:A:34:PHE:O	1:A:37:ASP:CG	0.50	2.55	3	1
1:A:133:GLY:O	1:A:134:ASN:O	0.50	2.28	18	1
1:A:103:TRP:CZ3	1:A:107:LEU:HD22	0.50	2.41	18	2
1:A:138:LEU:CD2	1:A:138:LEU:H	0.50	2.17	9	1
1:A:110:LEU:N	1:A:120:GLU:OE2	0.50	2.44	10	1
1:A:75:ASN:OD1	1:A:77:ASP:N	0.50	2.42	14	1
1:A:60:ASP:OD1	1:A:60:ASP:N	0.50	2.41	3	1
1:A:158:LYS:C	1:A:159:ASN:OD1	0.50	2.55	7	1
1:A:166:LEU:O	1:A:170:GLN:CG	0.50	2.59	11	3
1:A:94:ARG:CG	1:A:95:GLY:N	0.50	2.74	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:TYR:O	1:A:34:PHE:CE1	0.50	2.64	13	1
1:A:171:GLU:O	1:A:175:ALA:HB3	0.50	2.06	18	1
1:A:59:GLY:O	1:A:60:ASP:C	0.50	2.55	5	2
1:A:156:MET:O	1:A:168:GLU:OE1	0.50	2.29	3	2
1:A:73:ASP:OD1	1:A:84:GLU:OE1	0.50	2.28	12	3
1:A:20:THR:CG2	1:A:22:PHE:H	0.50	2.19	6	2
1:A:180:VAL:C	1:A:182:ALA:H	0.50	2.14	15	5
1:A:60:ASP:CB	1:A:61:PRO:CD	0.50	2.90	20	3
1:A:111:ASP:OD2	1:A:120:GLU:OE2	0.50	2.30	3	2
1:A:72:PHE:CE2	1:A:88:ALA:HB1	0.50	2.41	5	1
1:A:177:PRO:C	1:A:179:ILE:N	0.50	2.68	6	1
1:A:16:LEU:C	1:A:20:THR:OG1	0.50	2.54	11	3
1:A:93:SER:O	1:A:94:ARG:HB2	0.50	2.06	12	1
1:A:170:GLN:C	1:A:170:GLN:CD	0.50	2.79	19	1
1:A:132:VAL:O	1:A:133:GLY:O	0.50	2.29	17	2
1:A:133:GLY:O	1:A:134:ASN:C	0.50	2.55	19	3
1:A:75:ASN:OD1	1:A:75:ASN:C	0.50	2.55	4	5
1:A:142:GLU:OE2	1:A:183:LEU:C	0.50	2.54	2	1
1:A:111:ASP:OD1	1:A:120:GLU:CD	0.50	2.55	4	1
1:A:112:ASN:O	1:A:112:ASN:CG	0.50	2.54	6	3
1:A:62:THR:HG23	1:A:63:LYS:N	0.50	2.21	5	1
1:A:138:LEU:H	1:A:138:LEU:HD23	0.50	1.66	5	1
1:A:111:ASP:O	1:A:112:ASN:OD1	0.50	2.30	16	5
1:A:167:GLN:O	1:A:171:GLU:OE1	0.50	2.30	7	1
1:A:112:ASN:C	1:A:113:ASP:CG	0.50	2.79	8	1
1:A:153:PHE:CE2	1:A:164:LEU:HD21	0.50	2.41	11	1
1:A:112:ASN:O	1:A:113:ASP:C	0.50	2.55	13	1
1:A:44:ASP:CG	1:A:45:ALA:H	0.50	2.14	19	2
1:A:115:TYR:CE2	1:A:165:THR:OG1	0.50	2.64	1	1
1:A:159:ASN:OD1	1:A:161:ASP:CG	0.50	2.54	8	3
1:A:20:THR:HG21	1:A:27:VAL:CG1	0.50	2.36	19	4
1:A:128:ILE:O	1:A:132:VAL:HG23	0.50	2.06	17	1
1:A:21:TYR:OH	1:A:95:GLY:C	0.50	2.55	2	2
1:A:157:ASP:OD1	1:A:161:ASP:OD1	0.50	2.29	4	4
1:A:118:ARG:N	1:A:118:ARG:CD	0.50	2.74	16	8
1:A:170:GLN:OE1	1:A:171:GLU:OE2	0.50	2.30	7	1
1:A:111:ASP:CG	1:A:113:ASP:OD1	0.50	2.54	8	1
1:A:42:GLN:HE22	1:A:79:ARG:CZ	0.50	2.20	16	2
1:A:57:PRO:C	1:A:59:GLY:H	0.50	2.15	11	1
1:A:159:ASN:C	1:A:159:ASN:HD22	0.50	2.14	11	1
1:A:15:GLU:O	1:A:19:LYS:N	0.50	2.45	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:MET:SD	1:A:155:MET:C	0.50	2.94	14	1
1:A:16:LEU:O	1:A:20:THR:CB	0.50	2.60	15	1
1:A:143:ASN:CB	1:A:183:LEU:HD22	0.50	2.36	18	1
1:A:111:ASP:C	1:A:112:ASN:OD1	0.50	2.55	20	1
1:A:58:PHE:O	1:A:134:ASN:OD1	0.49	2.30	16	3
1:A:61:PRO:O	1:A:62:THR:OG1	0.49	2.30	9	5
1:A:142:GLU:OE1	1:A:183:LEU:O	0.49	2.30	2	1
1:A:109:ASP:CG	1:A:111:ASP:OD1	0.49	2.55	11	4
1:A:56:PHE:O	1:A:60:ASP:CG	0.49	2.55	4	1
1:A:159:ASN:OD1	1:A:161:ASP:OD1	0.49	2.29	7	1
1:A:59:GLY:O	1:A:131:MET:SD	0.49	2.70	8	1
1:A:59:GLY:C	1:A:60:ASP:CG	0.49	2.80	8	1
1:A:157:ASP:OD2	1:A:161:ASP:OD1	0.49	2.30	8	1
1:A:90:SER:O	1:A:93:SER:OG	0.49	2.29	20	2
1:A:21:TYR:CD2	1:A:95:GLY:N	0.49	2.79	12	1
1:A:62:THR:O	1:A:62:THR:OG1	0.49	2.30	13	1
1:A:64:PHE:CE1	1:A:107:LEU:HD11	0.49	2.41	15	1
1:A:148:ARG:HG2	1:A:152:ILE:HD12	0.49	1.84	17	1
1:A:113:ASP:OD1	1:A:113:ASP:C	0.49	2.55	18	4
1:A:157:ASP:OD1	1:A:163:LYS:O	0.49	2.30	4	3
1:A:75:ASN:CG	1:A:77:ASP:OD1	0.49	2.56	5	1
1:A:68:VAL:O	1:A:70:ASN:N	0.49	2.45	6	1
1:A:157:ASP:OD1	1:A:157:ASP:O	0.49	2.30	6	2
1:A:164:LEU:HD13	1:A:164:LEU:C	0.49	2.31	6	4
1:A:106:LYS:O	1:A:109:ASP:O	0.49	2.30	8	3
1:A:142:GLU:OE1	1:A:182:ALA:O	0.49	2.30	8	2
1:A:82:PHE:CD1	1:A:82:PHE:O	0.49	2.65	10	1
1:A:109:ASP:O	1:A:109:ASP:CG	0.49	2.54	10	1
1:A:72:PHE:O	1:A:74:GLU:CD	0.49	2.55	15	1
1:A:48:PHE:CZ	1:A:72:PHE:CE2	0.49	3.01	16	1
1:A:133:GLY:O	1:A:134:ASN:CG	0.49	2.55	19	1
1:A:157:ASP:CG	1:A:162:GLY:C	0.49	2.81	19	1
1:A:158:LYS:C	1:A:160:ALA:H	0.49	2.15	8	6
1:A:34:PHE:O	1:A:37:ASP:OD1	0.49	2.29	8	2
1:A:17:THR:O	1:A:18:ARG:C	0.49	2.56	5	7
1:A:109:ASP:OD1	1:A:120:GLU:OE1	0.49	2.31	8	3
1:A:112:ASN:O	1:A:112:ASN:OD1	0.49	2.31	12	6
1:A:42:GLN:CD	1:A:79:ARG:CZ	0.49	2.86	2	1
1:A:66:THR:O	1:A:70:ASN:CG	0.49	2.55	9	3
1:A:159:ASN:OD1	1:A:168:GLU:CD	0.49	2.56	3	2
1:A:60:ASP:O	1:A:61:PRO:C	0.49	2.55	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD13	1:A:20:THR:OG1	0.49	2.07	10	1
1:A:145:PRO:HD3	1:A:183:LEU:HD22	0.49	1.84	11	1
1:A:159:ASN:HD22	1:A:161:ASP:H	0.49	1.50	11	1
1:A:112:ASN:O	1:A:113:ASP:OD1	0.49	2.31	13	1
1:A:81:GLU:O	1:A:82:PHE:C	0.49	2.55	19	5
1:A:146:GLU:OE1	1:A:146:GLU:C	0.49	2.56	3	1
1:A:126:ASP:OD1	1:A:146:GLU:OE2	0.49	2.29	7	1
1:A:74:GLU:C	1:A:75:ASN:CG	0.49	2.79	13	4
1:A:111:ASP:C	1:A:112:ASN:CG	0.49	2.80	9	2
1:A:60:ASP:O	1:A:64:PHE:CD2	0.49	2.66	11	1
1:A:39:PRO:O	1:A:40:SER:C	0.49	2.54	15	1
1:A:158:LYS:O	1:A:161:ASP:OD1	0.49	2.31	17	2
1:A:16:LEU:O	1:A:16:LEU:HD23	0.49	2.06	18	1
1:A:60:ASP:CG	1:A:130:GLN:OE1	0.49	2.56	19	1
1:A:94:ARG:O	1:A:95:GLY:O	0.49	2.31	19	1
1:A:138:LEU:H	1:A:138:LEU:CD2	0.49	2.20	1	1
1:A:60:ASP:O	1:A:62:THR:N	0.49	2.45	2	2
1:A:75:ASN:ND2	1:A:77:ASP:CG	0.49	2.71	18	3
1:A:109:ASP:CG	1:A:120:GLU:OE1	0.49	2.56	7	3
1:A:35:ILE:O	1:A:38:CYS:O	0.49	2.31	14	3
1:A:138:LEU:HD23	1:A:142:GLU:CD	0.49	2.32	10	1
1:A:143:ASN:CG	1:A:181:GLN:HE22	0.49	2.14	10	1
1:A:159:ASN:CG	1:A:168:GLU:OE2	0.49	2.55	13	1
1:A:21:TYR:OH	1:A:99:GLU:OE1	0.49	2.31	19	1
1:A:94:ARG:O	1:A:95:GLY:C	0.49	2.56	3	2
1:A:59:GLY:O	1:A:131:MET:O	0.49	2.30	4	1
1:A:115:TYR:CG	1:A:165:THR:HG22	0.49	2.43	4	1
1:A:159:ASN:OD1	1:A:168:GLU:OE1	0.49	2.30	4	2
1:A:75:ASN:OD1	1:A:77:ASP:CG	0.49	2.55	5	1
1:A:111:ASP:CG	1:A:113:ASP:OD2	0.49	2.56	16	2
1:A:112:ASN:C	1:A:114:GLY:H	0.49	2.16	16	3
1:A:135:THR:C	1:A:137:GLU:H	0.49	2.16	9	1
1:A:134:ASN:O	1:A:135:THR:O	0.49	2.30	10	1
1:A:60:ASP:O	1:A:64:PHE:CE2	0.49	2.65	11	1
1:A:107:LEU:C	1:A:109:ASP:N	0.49	2.66	12	1
1:A:144:THR:O	1:A:144:THR:OG1	0.49	2.30	15	1
1:A:109:ASP:OD1	1:A:120:GLU:OE2	0.49	2.30	17	1
1:A:156:MET:O	1:A:168:GLU:OE2	0.49	2.31	18	1
1:A:116:ILE:O	1:A:164:LEU:CB	0.49	2.61	14	2
1:A:16:LEU:O	1:A:16:LEU:HD13	0.49	2.08	9	1
1:A:169:PHE:CE1	1:A:179:ILE:HG22	0.49	2.43	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASP:OD2	1:A:130:GLN:OE1	0.49	2.30	16	1
1:A:136:VAL:CG1	1:A:137:GLU:N	0.49	2.76	1	2
1:A:157:ASP:O	1:A:157:ASP:OD1	0.49	2.31	7	5
1:A:73:ASP:OD1	1:A:84:GLU:OE2	0.49	2.30	2	2
1:A:77:ASP:OD1	1:A:79:ARG:O	0.49	2.30	8	5
1:A:74:GLU:N	1:A:77:ASP:OD1	0.49	2.46	12	1
1:A:42:GLN:CD	1:A:42:GLN:C	0.49	2.80	18	1
1:A:157:ASP:OD2	1:A:162:GLY:O	0.49	2.30	19	1
1:A:143:ASN:ND2	1:A:184:SER:O	0.49	2.45	20	1
1:A:112:ASN:OD1	1:A:112:ASN:C	0.49	2.56	12	1
1:A:42:GLN:O	1:A:42:GLN:CG	0.49	2.61	17	1
1:A:156:MET:O	1:A:159:ASN:OD1	0.49	2.31	17	1
1:A:176:ASP:O	1:A:177:PRO:O	0.48	2.30	19	7
1:A:142:GLU:OE1	1:A:181:GLN:O	0.48	2.31	3	1
1:A:69:PHE:CD2	1:A:70:ASN:OD1	0.48	2.65	13	2
1:A:40:SER:O	1:A:40:SER:OG	0.48	2.30	10	1
1:A:153:PHE:CE1	1:A:164:LEU:CD2	0.48	2.95	19	2
1:A:135:THR:O	1:A:138:LEU:HD12	0.48	2.08	20	1
1:A:111:ASP:OD1	1:A:111:ASP:N	0.48	2.46	1	2
1:A:178:SER:O	1:A:181:GLN:OE1	0.48	2.30	1	1
1:A:118:ARG:CD	1:A:118:ARG:N	0.48	2.76	3	3
1:A:24:GLU:OE1	1:A:24:GLU:C	0.48	2.56	4	1
1:A:12:VAL:O	1:A:16:LEU:CB	0.48	2.61	14	2
1:A:132:VAL:C	1:A:134:ASN:H	0.48	2.17	7	1
1:A:20:THR:C	1:A:21:TYR:CD1	0.48	2.92	12	1
1:A:54:GLN:OE1	1:A:54:GLN:C	0.48	2.55	13	1
1:A:157:ASP:OD2	1:A:162:GLY:C	0.48	2.55	19	1
1:A:74:GLU:C	1:A:76:LYS:N	0.48	2.70	9	1
1:A:109:ASP:O	1:A:112:ASN:OD1	0.48	2.30	9	1
1:A:157:ASP:C	1:A:159:ASN:N	0.48	2.68	10	3
1:A:181:GLN:O	1:A:182:ALA:O	0.48	2.30	14	1
1:A:73:ASP:OD2	1:A:77:ASP:OD1	0.48	2.31	20	4
1:A:164:LEU:CD1	1:A:164:LEU:C	0.48	2.87	3	2
1:A:16:LEU:HD23	1:A:16:LEU:C	0.48	2.32	5	1
1:A:181:GLN:O	1:A:183:LEU:N	0.48	2.46	17	1
1:A:101:LEU:C	1:A:101:LEU:HD13	0.48	2.33	18	1
1:A:143:ASN:O	1:A:143:ASN:OD1	0.48	2.31	20	1
1:A:87:GLN:O	1:A:90:SER:OG	0.48	2.30	5	4
1:A:183:LEU:N	1:A:183:LEU:HD12	0.48	2.24	6	2
1:A:24:GLU:CD	1:A:24:GLU:N	0.48	2.71	8	1
1:A:143:ASN:O	1:A:144:THR:OG1	0.48	2.27	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LYS:O	1:A:29:GLN:OE1	0.48	2.30	9	1
1:A:21:TYR:OH	1:A:99:GLU:CD	0.48	2.57	19	1
1:A:19:LYS:HZ1	1:A:87:GLN:NE2	0.48	2.05	20	1
1:A:34:PHE:O	1:A:37:ASP:OD2	0.48	2.31	3	1
1:A:89:LEU:O	1:A:92:THR:OG1	0.48	2.30	3	6
1:A:23:THR:O	1:A:27:VAL:HG13	0.48	2.08	7	2
1:A:159:ASN:HD22	1:A:160:ALA:H	0.48	1.51	8	1
1:A:129:TYR:CD2	1:A:144:THR:OG1	0.48	2.66	9	1
1:A:77:ASP:C	1:A:77:ASP:OD1	0.48	2.56	14	2
1:A:166:LEU:HD13	1:A:166:LEU:N	0.48	2.12	12	1
1:A:124:ILE:O	1:A:127:ALA:HB3	0.48	2.09	15	1
1:A:16:LEU:CD2	1:A:20:THR:OG1	0.48	2.61	17	1
1:A:132:VAL:O	1:A:133:GLY:C	0.48	2.55	2	2
1:A:164:LEU:HD13	1:A:168:GLU:OE1	0.48	2.09	18	1
1:A:61:PRO:O	1:A:62:THR:HG22	0.48	2.08	20	1
1:A:183:LEU:O	1:A:184:SER:O	0.48	2.31	20	1
1:A:115:TYR:CE2	1:A:165:THR:HG22	0.48	2.44	15	4
1:A:75:ASN:CG	1:A:77:ASP:CG	0.48	2.81	5	1
1:A:143:ASN:O	1:A:144:THR:O	0.48	2.32	11	2
1:A:159:ASN:CG	1:A:161:ASP:OD2	0.48	2.56	11	1
1:A:134:ASN:O	1:A:134:ASN:OD1	0.48	2.31	19	1
1:A:171:GLU:O	1:A:175:ALA:CB	0.48	2.62	13	5
1:A:21:TYR:CE2	1:A:95:GLY:N	0.48	2.82	12	1
1:A:149:VAL:HG22	1:A:153:PHE:CD2	0.48	2.44	17	1
1:A:144:THR:O	1:A:146:GLU:OE2	0.48	2.31	19	1
1:A:142:GLU:CD	1:A:183:LEU:O	0.48	2.57	2	1
1:A:166:LEU:N	1:A:166:LEU:CD2	0.48	2.77	16	3
1:A:118:ARG:NE	1:A:118:ARG:N	0.48	2.61	14	2
1:A:139:PRO:CG	1:A:143:ASN:OD1	0.48	2.61	20	1
1:A:54:GLN:OE1	1:A:54:GLN:O	0.47	2.32	13	1
1:A:132:VAL:O	1:A:136:VAL:HG12	0.47	2.09	15	1
1:A:137:GLU:CG	1:A:137:GLU:O	0.47	2.62	15	1
1:A:181:GLN:O	1:A:183:LEU:HD12	0.47	2.08	17	1
1:A:110:LEU:O	1:A:112:ASN:ND2	0.47	2.47	19	1
1:A:84:GLU:O	1:A:88:ALA:CB	0.47	2.61	5	4
1:A:88:ALA:O	1:A:92:THR:OG1	0.47	2.31	2	1
1:A:155:MET:HE3	1:A:156:MET:HE2	0.47	1.85	2	1
1:A:68:VAL:O	1:A:69:PHE:C	0.47	2.54	6	3
1:A:129:TYR:OH	1:A:143:ASN:O	0.47	2.30	17	1
1:A:143:ASN:N	1:A:143:ASN:ND2	0.47	2.60	3	1
1:A:166:LEU:HD23	1:A:170:GLN:NE2	0.47	2.24	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:PRO:O	1:A:62:THR:CG2	0.47	2.62	20	1
1:A:13:VAL:HG11	1:A:24:GLU:OE2	0.47	2.10	1	1
1:A:151:ARG:CG	1:A:152:ILE:N	0.47	2.77	5	1
1:A:82:PHE:C	1:A:82:PHE:CD1	0.47	2.90	11	1
1:A:141:GLU:CG	1:A:142:GLU:H	0.47	2.23	16	1
1:A:153:PHE:O	1:A:154:ALA:C	0.47	2.57	10	10
1:A:71:VAL:HG23	1:A:72:PHE:N	0.47	2.23	2	1
1:A:169:PHE:O	1:A:173:SER:CB	0.47	2.63	5	8
1:A:67:PHE:CG	1:A:110:LEU:HD13	0.47	2.44	3	2
1:A:93:SER:O	1:A:94:ARG:CG	0.47	2.63	15	5
1:A:129:TYR:CD1	1:A:144:THR:OG1	0.47	2.64	14	1
1:A:158:LYS:HG3	1:A:159:ASN:N	0.47	2.25	19	1
1:A:157:ASP:OD2	1:A:162:GLY:CA	0.47	2.63	4	1
1:A:118:ARG:CD	1:A:153:PHE:CE1	0.47	2.97	16	1
1:A:13:VAL:CG1	1:A:24:GLU:OE1	0.47	2.62	2	1
1:A:148:ARG:O	1:A:152:ILE:CG1	0.47	2.63	2	1
1:A:97:LEU:N	1:A:97:LEU:CD1	0.47	2.76	8	2
1:A:134:ASN:O	1:A:135:THR:HG23	0.47	2.09	9	2
1:A:72:PHE:CD1	1:A:72:PHE:O	0.47	2.67	12	1
1:A:125:VAL:CG1	1:A:146:GLU:OE2	0.47	2.63	17	1
1:A:126:ASP:O	1:A:130:GLN:CB	0.47	2.63	17	1
1:A:16:LEU:O	1:A:17:THR:C	0.47	2.54	11	5
1:A:112:ASN:OD1	1:A:112:ASN:O	0.47	2.33	11	1
1:A:9:LYS:N	1:A:9:LYS:CD	0.47	2.78	12	1
1:A:48:PHE:CZ	1:A:85:PHE:CE2	0.47	3.03	13	1
1:A:69:PHE:O	1:A:73:ASP:CB	0.47	2.63	13	1
1:A:96:THR:HG22	1:A:97:LEU:HD23	0.47	1.85	13	1
1:A:99:GLU:O	1:A:103:TRP:CD1	0.47	2.67	15	1
1:A:16:LEU:HD23	1:A:20:THR:OG1	0.47	2.10	17	1
1:A:19:LYS:O	1:A:19:LYS:CG	0.47	2.63	20	1
1:A:108:TYR:OH	1:A:149:VAL:HG11	0.47	2.10	4	1
1:A:60:ASP:O	1:A:64:PHE:CD1	0.47	2.68	9	1
1:A:79:ARG:O	1:A:81:GLU:OE2	0.47	2.32	14	1
1:A:87:GLN:O	1:A:91:VAL:HG23	0.47	2.09	11	5
1:A:24:GLU:C	1:A:24:GLU:CD	0.47	2.82	4	1
1:A:20:THR:CG2	1:A:21:TYR:N	0.47	2.77	12	1
1:A:89:LEU:HD13	1:A:89:LEU:C	0.47	2.34	12	2
1:A:115:TYR:CE2	1:A:165:THR:CG2	0.47	2.98	15	1
1:A:159:ASN:ND2	1:A:160:ALA:N	0.46	2.61	8	1
1:A:183:LEU:CD1	1:A:183:LEU:C	0.46	2.88	8	2
1:A:107:LEU:C	1:A:109:ASP:H	0.46	2.17	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASP:CG	1:A:64:PHE:H	0.46	2.18	18	1
1:A:31:TYR:CD1	1:A:31:TYR:C	0.46	2.92	6	1
1:A:129:TYR:CE2	1:A:144:THR:OG1	0.46	2.67	9	1
1:A:134:ASN:O	1:A:135:THR:CG2	0.46	2.64	9	2
1:A:157:ASP:O	1:A:160:ALA:N	0.46	2.47	11	1
1:A:74:GLU:O	1:A:84:GLU:OE2	0.46	2.33	12	1
1:A:85:PHE:O	1:A:89:LEU:CB	0.46	2.63	4	4
1:A:42:GLN:NE2	1:A:79:ARG:CD	0.46	2.79	7	1
1:A:177:PRO:O	1:A:178:SER:OG	0.46	2.30	7	7
1:A:82:PHE:O	1:A:86:ILE:HG22	0.46	2.10	14	2
1:A:57:PRO:C	1:A:59:GLY:N	0.46	2.74	11	3
1:A:60:ASP:O	1:A:64:PHE:CE1	0.46	2.68	9	1
1:A:182:ALA:O	1:A:183:LEU:C	0.46	2.58	10	1
1:A:67:PHE:CD2	1:A:110:LEU:HD23	0.46	2.45	1	2
1:A:156:MET:C	1:A:158:LYS:H	0.46	2.19	6	1
1:A:114:GLY:C	1:A:115:TYR:CD1	0.46	2.94	7	2
1:A:94:ARG:O	1:A:100:LYS:NZ	0.46	2.48	9	1
1:A:180:VAL:O	1:A:180:VAL:CG2	0.46	2.64	9	1
1:A:163:LYS:HZ2	1:A:163:LYS:HB3	0.46	1.70	11	1
1:A:143:ASN:O	1:A:183:LEU:HD12	0.46	2.11	16	1
1:A:51:ILE:O	1:A:55:PHE:CD1	0.46	2.69	20	1
1:A:116:ILE:HG22	1:A:121:MET:HE2	0.46	1.87	20	1
1:A:86:ILE:CG2	1:A:87:GLN:N	0.46	2.78	4	5
1:A:60:ASP:N	1:A:60:ASP:OD1	0.46	2.48	4	1
1:A:121:MET:HE3	1:A:149:VAL:HG21	0.46	1.86	3	1
1:A:52:TYR:CE2	1:A:131:MET:CE	0.46	2.98	4	1
1:A:149:VAL:O	1:A:150:ASP:C	0.46	2.56	20	7
1:A:68:VAL:C	1:A:70:ASN:N	0.46	2.72	6	1
1:A:118:ARG:HH12	1:A:162:GLY:C	0.46	2.19	8	1
1:A:119:ASN:CG	1:A:120:GLU:N	0.46	2.74	8	1
1:A:101:LEU:O	1:A:105:PHE:CB	0.46	2.64	9	1
1:A:44:ASP:C	1:A:69:PHE:CE1	0.46	2.94	11	1
1:A:112:ASN:C	1:A:112:ASN:OD1	0.46	2.58	11	1
1:A:142:GLU:O	1:A:183:LEU:CB	0.46	2.64	4	1
1:A:157:ASP:CG	1:A:161:ASP:OD1	0.46	2.58	8	1
1:A:38:CYS:O	1:A:38:CYS:SG	0.46	2.74	9	2
1:A:61:PRO:C	1:A:62:THR:CG2	0.46	2.89	13	1
1:A:118:ARG:HE	1:A:118:ARG:H	0.46	1.54	13	1
1:A:184:SER:O	1:A:184:SER:OG	0.46	2.33	13	1
1:A:183:LEU:O	1:A:184:SER:OG	0.46	2.35	14	1
1:A:67:PHE:CE2	1:A:107:LEU:HD12	0.46	2.46	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:164:LEU:C	1:A:164:LEU:CD1	0.45	2.89	6	3
1:A:16:LEU:CA	1:A:20:THR:OG1	0.45	2.64	8	2
1:A:64:PHE:H	1:A:131:MET:CG	0.45	2.24	10	1
1:A:103:TRP:CH2	1:A:107:LEU:CD1	0.45	2.99	11	1
1:A:108:TYR:CZ	1:A:121:MET:CE	0.45	3.00	11	1
1:A:107:LEU:O	1:A:109:ASP:N	0.45	2.49	12	1
1:A:136:VAL:C	1:A:138:LEU:H	0.45	2.19	13	1
1:A:35:ILE:HG22	1:A:40:SER:O	0.45	2.12	14	1
1:A:71:VAL:CG1	1:A:110:LEU:O	0.45	2.65	1	1
1:A:139:PRO:O	1:A:143:ASN:CA	0.45	2.64	3	2
1:A:145:PRO:HD3	1:A:183:LEU:HD12	0.45	1.87	5	1
1:A:20:THR:O	1:A:22:PHE:CD2	0.45	2.69	10	1
1:A:97:LEU:CD2	1:A:97:LEU:H	0.45	2.24	13	1
1:A:27:VAL:CG1	1:A:28:GLN:N	0.45	2.79	17	1
1:A:75:ASN:OD1	1:A:77:ASP:OD1	0.45	2.34	18	1
1:A:21:TYR:HH	1:A:99:GLU:CD	0.45	2.19	19	1
1:A:144:THR:O	1:A:146:GLU:CD	0.45	2.59	19	1
1:A:13:VAL:O	1:A:16:LEU:N	0.45	2.49	20	1
1:A:23:THR:OG1	1:A:26:GLU:OE1	0.45	2.29	2	1
1:A:60:ASP:OD1	1:A:60:ASP:C	0.45	2.60	6	1
1:A:175:ALA:C	1:A:176:ASP:OD1	0.45	2.59	6	1
1:A:149:VAL:O	1:A:153:PHE:N	0.45	2.50	11	1
1:A:74:GLU:C	1:A:77:ASP:OD1	0.45	2.59	12	1
1:A:67:PHE:N	1:A:67:PHE:CD1	0.45	2.82	18	1
1:A:75:ASN:CG	1:A:84:GLU:OE2	0.45	2.59	19	1
1:A:161:ASP:OD1	1:A:163:LYS:O	0.45	2.35	6	1
1:A:72:PHE:O	1:A:74:GLU:N	0.45	2.49	11	1
1:A:144:THR:CB	1:A:145:PRO:CD	0.45	2.94	18	2
1:A:45:ALA:HB2	1:A:69:PHE:CD2	0.45	2.47	15	1
1:A:27:VAL:O	1:A:31:TYR:CB	0.45	2.64	18	1
1:A:39:PRO:O	1:A:40:SER:OG	0.45	2.31	2	2
1:A:109:ASP:OD1	1:A:109:ASP:C	0.45	2.57	2	4
1:A:165:THR:O	1:A:168:GLU:OE2	0.45	2.34	4	1
1:A:13:VAL:O	1:A:17:THR:CG2	0.45	2.64	7	1
1:A:119:ASN:C	1:A:119:ASN:HD22	0.45	2.17	11	1
1:A:139:PRO:CB	1:A:142:GLU:O	0.45	2.64	16	1
1:A:68:VAL:HG23	1:A:69:PHE:N	0.45	2.26	18	2
1:A:71:VAL:HG21	1:A:109:ASP:O	0.45	2.12	12	1
1:A:31:TYR:CE1	1:A:35:ILE:CD1	0.45	3.00	1	2
1:A:111:ASP:OD1	1:A:120:GLU:OE2	0.45	2.35	4	1
1:A:45:ALA:CB	1:A:69:PHE:CE2	0.45	3.00	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:PHE:CZ	1:A:77:ASP:O	0.45	2.70	12	1
1:A:73:ASP:O	1:A:77:ASP:CG	0.45	2.60	12	1
1:A:92:THR:O	1:A:93:SER:C	0.45	2.60	20	2
1:A:121:MET:SD	1:A:125:VAL:CG2	0.45	3.05	13	1
1:A:112:ASN:C	1:A:112:ASN:HD22	0.45	2.18	4	1
1:A:132:VAL:CG2	1:A:137:GLU:O	0.45	2.65	12	1
1:A:79:ARG:CZ	1:A:81:GLU:OE2	0.45	2.64	4	1
1:A:112:ASN:C	1:A:114:GLY:N	0.45	2.74	13	4
1:A:73:ASP:OD1	1:A:73:ASP:C	0.45	2.59	7	1
1:A:64:PHE:CG	1:A:65:ALA:N	0.45	2.85	8	4
1:A:112:ASN:CG	1:A:113:ASP:N	0.45	2.75	13	1
1:A:133:GLY:O	1:A:135:THR:HG23	0.45	2.12	13	1
1:A:75:ASN:O	1:A:76:LYS:CG	0.44	2.65	3	1
1:A:175:ALA:O	1:A:176:ASP:CG	0.44	2.60	6	1
1:A:114:GLY:O	1:A:166:LEU:CD1	0.44	2.64	8	1
1:A:9:LYS:O	1:A:13:VAL:HG23	0.44	2.12	1	1
1:A:85:PHE:CE1	1:A:89:LEU:CD1	0.44	2.92	8	1
1:A:124:ILE:O	1:A:125:VAL:C	0.44	2.59	8	2
1:A:132:VAL:O	1:A:132:VAL:CG1	0.44	2.64	8	2
1:A:117:THR:OG1	1:A:119:ASN:OD1	0.44	2.30	11	1
1:A:138:LEU:HD12	1:A:138:LEU:N	0.44	2.26	17	1
1:A:64:PHE:CD2	1:A:65:ALA:N	0.44	2.86	20	1
1:A:166:LEU:CD2	1:A:167:GLN:N	0.44	2.80	12	1
1:A:64:PHE:CE2	1:A:131:MET:SD	0.44	3.10	13	2
1:A:156:MET:HE1	1:A:179:ILE:HD11	0.44	1.88	8	1
1:A:42:GLN:NE2	1:A:79:ARG:HH11	0.44	2.10	10	1
1:A:156:MET:HE1	1:A:179:ILE:HD13	0.44	1.89	11	1
1:A:50:LYS:O	1:A:51:ILE:C	0.44	2.60	12	2
1:A:20:THR:CG2	1:A:27:VAL:HG11	0.44	2.43	3	1
1:A:124:ILE:O	1:A:127:ALA:N	0.44	2.50	8	2
1:A:128:ILE:O	1:A:132:VAL:HG13	0.44	2.13	10	1
1:A:86:ILE:CD1	1:A:90:SER:OG	0.44	2.65	12	1
1:A:121:MET:SD	1:A:153:PHE:CZ	0.44	3.10	20	1
1:A:61:PRO:C	1:A:62:THR:OG1	0.44	2.60	6	1
1:A:27:VAL:CG2	1:A:28:GLN:N	0.44	2.81	7	2
1:A:143:ASN:HD22	1:A:148:ARG:NH1	0.44	2.10	7	1
1:A:96:THR:HG22	1:A:97:LEU:CD2	0.44	2.43	13	1
1:A:52:TYR:CE2	1:A:131:MET:HE3	0.44	2.48	4	1
1:A:62:THR:OG1	1:A:65:ALA:HB3	0.44	2.11	8	1
1:A:13:VAL:O	1:A:14:GLU:C	0.44	2.58	20	1
1:A:19:LYS:C	1:A:21:TYR:N	0.44	2.72	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:PRO:C	1:A:179:ILE:H	0.44	2.21	6	2
1:A:45:ALA:CB	1:A:69:PHE:CD2	0.44	3.01	13	1
1:A:132:VAL:O	1:A:135:THR:OG1	0.44	2.31	13	1
1:A:43:LEU:HD12	1:A:43:LEU:N	0.44	2.28	14	1
1:A:136:VAL:O	1:A:137:GLU:CB	0.43	2.66	1	2
1:A:177:PRO:C	1:A:178:SER:OG	0.43	2.60	2	5
1:A:20:THR:C	1:A:21:TYR:CD2	0.43	2.96	4	3
1:A:110:LEU:N	1:A:110:LEU:CD2	0.43	2.78	5	1
1:A:134:ASN:O	1:A:138:LEU:HD13	0.43	2.13	7	1
1:A:105:PHE:CZ	1:A:112:ASN:OD1	0.43	2.71	8	1
1:A:35:ILE:O	1:A:38:CYS:C	0.43	2.61	11	1
1:A:132:VAL:O	1:A:138:LEU:CB	0.43	2.66	11	1
1:A:129:TYR:CG	1:A:144:THR:OG1	0.43	2.71	14	1
1:A:175:ALA:C	1:A:176:ASP:CG	0.43	2.86	7	2
1:A:103:TRP:CH2	1:A:107:LEU:HD13	0.43	2.49	11	1
1:A:44:ASP:OD1	1:A:79:ARG:CD	0.43	2.67	3	2
1:A:73:ASP:OD2	1:A:79:ARG:N	0.43	2.50	10	1
1:A:128:ILE:O	1:A:132:VAL:CG2	0.43	2.60	10	1
1:A:162:GLY:C	1:A:163:LYS:CD	0.43	2.92	12	1
1:A:30:TRP:O	1:A:31:TYR:C	0.43	2.58	13	2
1:A:172:GLY:O	1:A:176:ASP:C	0.43	2.61	16	2
1:A:72:PHE:CZ	1:A:88:ALA:CA	0.43	3.01	18	1
1:A:125:VAL:CG2	1:A:126:ASP:N	0.43	2.81	5	2
1:A:71:VAL:HG21	1:A:106:LYS:O	0.43	2.13	6	1
1:A:118:ARG:H	1:A:118:ARG:CZ	0.43	2.26	7	1
1:A:42:GLN:OE1	1:A:79:ARG:CZ	0.43	2.66	11	1
1:A:42:GLN:NE2	1:A:44:ASP:OD1	0.43	2.46	18	1
1:A:58:PHE:HB2	1:A:135:THR:HG23	0.43	1.91	4	1
1:A:61:PRO:O	1:A:62:THR:C	0.43	2.61	13	2
1:A:52:TYR:O	1:A:56:PHE:N	0.43	2.51	11	1
1:A:77:ASP:OD1	1:A:77:ASP:C	0.43	2.61	16	2
1:A:157:ASP:O	1:A:157:ASP:CG	0.43	2.61	16	1
1:A:183:LEU:CD2	1:A:183:LEU:N	0.43	2.78	19	1
1:A:153:PHE:CE2	1:A:164:LEU:HD22	0.43	2.49	20	1
1:A:148:ARG:O	1:A:149:VAL:C	0.43	2.60	20	2
1:A:111:ASP:CG	1:A:120:GLU:OE2	0.43	2.61	4	1
1:A:71:VAL:O	1:A:72:PHE:C	0.43	2.59	12	1
1:A:21:TYR:OH	1:A:95:GLY:CA	0.43	2.67	2	1
1:A:173:SER:OG	1:A:180:VAL:HG13	0.43	2.14	7	1
1:A:183:LEU:C	1:A:183:LEU:HD12	0.43	2.37	8	2
1:A:118:ARG:CD	1:A:162:GLY:O	0.43	2.67	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:ASN:C	1:A:144:THR:HG1	0.43	2.22	2	2
1:A:145:PRO:O	1:A:149:VAL:HG12	0.43	2.13	3	1
1:A:135:THR:OG1	1:A:138:LEU:CD2	0.43	2.67	13	1
1:A:59:GLY:CA	1:A:131:MET:O	0.43	2.67	17	1
1:A:157:ASP:O	1:A:161:ASP:OD1	0.43	2.37	17	1
1:A:20:THR:O	1:A:22:PHE:N	0.43	2.51	15	1
1:A:44:ASP:CG	1:A:45:ALA:N	0.43	2.77	19	2
1:A:21:TYR:CZ	1:A:95:GLY:CA	0.43	3.01	18	1
1:A:49:GLN:OE1	1:A:66:THR:OG1	0.42	2.37	1	1
1:A:107:LEU:C	1:A:107:LEU:CD2	0.42	2.92	12	1
1:A:44:ASP:OD1	1:A:45:ALA:N	0.42	2.50	17	2
1:A:109:ASP:OD1	1:A:110:LEU:N	0.42	2.52	19	1
1:A:51:ILE:O	1:A:55:PHE:CE1	0.42	2.72	20	1
1:A:161:ASP:CG	1:A:162:GLY:N	0.42	2.77	7	1
1:A:101:LEU:O	1:A:101:LEU:HD13	0.42	2.14	13	1
1:A:121:MET:SD	1:A:125:VAL:HG23	0.42	2.54	13	1
1:A:176:ASP:OD1	1:A:176:ASP:C	0.42	2.62	14	1
1:A:24:GLU:OE1	1:A:24:GLU:N	0.42	2.47	17	1
1:A:134:ASN:O	1:A:138:LEU:HD21	0.42	2.13	17	1
1:A:143:ASN:O	1:A:144:THR:CB	0.42	2.68	5	3
1:A:51:ILE:HG13	1:A:52:TYR:N	0.42	2.29	4	2
1:A:132:VAL:HG23	1:A:137:GLU:O	0.42	2.14	12	1
1:A:121:MET:SD	1:A:121:MET:C	0.42	3.02	13	1
1:A:157:ASP:O	1:A:159:ASN:N	0.42	2.52	10	2
1:A:44:ASP:C	1:A:69:PHE:CZ	0.42	2.97	11	1
1:A:45:ALA:CB	1:A:69:PHE:CG	0.42	3.02	13	1
1:A:166:LEU:N	1:A:166:LEU:CD1	0.42	2.81	8	5
1:A:25:LYS:CB	1:A:25:LYS:NZ	0.42	2.82	8	1
1:A:153:PHE:CE2	1:A:164:LEU:HD11	0.42	2.50	11	1
1:A:88:ALA:O	1:A:89:LEU:C	0.42	2.62	12	1
1:A:20:THR:HG21	1:A:27:VAL:HG12	0.42	1.92	19	1
1:A:77:ASP:OD1	1:A:79:ARG:N	0.42	2.50	11	1
1:A:29:GLN:O	1:A:33:GLY:N	0.42	2.53	12	2
1:A:64:PHE:CE2	1:A:107:LEU:HD11	0.42	2.50	4	1
1:A:74:GLU:O	1:A:76:LYS:N	0.42	2.52	9	1
1:A:147:LYS:CG	1:A:148:ARG:N	0.42	2.83	9	1
1:A:105:PHE:CE1	1:A:166:LEU:HD11	0.42	2.49	14	1
1:A:113:ASP:OD1	1:A:113:ASP:N	0.42	2.53	14	1
1:A:157:ASP:OD1	1:A:163:LYS:C	0.42	2.62	15	1
1:A:28:GLN:CD	1:A:28:GLN:C	0.42	2.87	17	1
1:A:67:PHE:CD1	1:A:110:LEU:HD12	0.42	2.50	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:ASP:CG	1:A:163:LYS:O	0.42	2.63	6	1
1:A:58:PHE:O	1:A:60:ASP:OD1	0.42	2.37	8	1
1:A:59:GLY:O	1:A:60:ASP:CB	0.42	2.65	8	1
1:A:16:LEU:C	1:A:16:LEU:CD1	0.42	2.92	9	1
1:A:65:ALA:O	1:A:68:VAL:CG2	0.42	2.68	12	2
1:A:129:TYR:CG	1:A:130:GLN:N	0.41	2.86	2	1
1:A:179:ILE:CG2	1:A:180:VAL:N	0.41	2.83	2	1
1:A:71:VAL:HG22	1:A:110:LEU:O	0.41	2.15	7	1
1:A:48:PHE:O	1:A:49:GLN:C	0.41	2.63	13	1
1:A:34:PHE:C	1:A:36:LYS:N	0.41	2.78	14	1
1:A:184:SER:OG	1:A:184:SER:O	0.41	2.38	14	1
1:A:59:GLY:C	1:A:61:PRO:CD	0.41	2.93	3	1
1:A:35:ILE:O	1:A:36:LYS:C	0.41	2.61	6	1
1:A:164:LEU:CD1	1:A:169:PHE:CE2	0.41	3.03	7	1
1:A:86:ILE:O	1:A:86:ILE:CD1	0.41	2.68	12	1
1:A:48:PHE:CE2	1:A:52:TYR:CE1	0.41	3.07	14	1
1:A:145:PRO:O	1:A:149:VAL:CG2	0.41	2.67	16	2
1:A:101:LEU:CD1	1:A:170:GLN:NE2	0.41	2.83	18	1
1:A:143:ASN:C	1:A:144:THR:CG2	0.41	2.91	3	1
1:A:149:VAL:HG13	1:A:150:ASP:N	0.41	2.31	3	1
1:A:150:ASP:O	1:A:154:ALA:CB	0.41	2.69	7	5
1:A:183:LEU:HD12	1:A:183:LEU:H	0.41	1.76	6	1
1:A:131:MET:O	1:A:136:VAL:HG11	0.41	2.16	9	1
1:A:115:TYR:CD1	1:A:163:LYS:CB	0.41	3.03	12	1
1:A:132:VAL:HG12	1:A:132:VAL:O	0.41	2.16	19	1
1:A:145:PRO:O	1:A:149:VAL:CG1	0.41	2.68	3	1
1:A:73:ASP:OD1	1:A:84:GLU:CD	0.41	2.63	19	1
1:A:145:PRO:O	1:A:146:GLU:C	0.41	2.61	13	2
1:A:157:ASP:OD2	1:A:162:GLY:N	0.41	2.53	4	1
1:A:131:MET:SD	1:A:131:MET:O	0.41	2.78	13	1
1:A:48:PHE:O	1:A:51:ILE:CG1	0.41	2.68	20	2
1:A:170:GLN:OE1	1:A:171:GLU:OE1	0.41	2.38	7	1
1:A:118:ARG:HH12	1:A:157:ASP:CG	0.41	2.22	8	1
1:A:148:ARG:O	1:A:152:ILE:CD1	0.41	2.68	10	1
1:A:20:THR:HG23	1:A:22:PHE:N	0.41	2.29	13	1
1:A:99:GLU:CG	1:A:100:LYS:N	0.41	2.84	19	1
1:A:140:GLU:N	1:A:140:GLU:OE1	0.41	2.54	2	1
1:A:172:GLY:O	1:A:176:ASP:CA	0.41	2.69	6	1
1:A:97:LEU:HD11	1:A:180:VAL:HG21	0.41	1.91	18	1
1:A:24:GLU:OE2	1:A:25:LYS:NZ	0.41	2.50	20	1
1:A:136:VAL:O	1:A:136:VAL:CG2	0.41	2.68	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:MET:HE1	1:A:153:PHE:CD2	0.41	2.50	20	1
1:A:129:TYR:CE2	1:A:144:THR:HG21	0.41	2.50	1	1
1:A:137:GLU:OE1	1:A:137:GLU:N	0.41	2.53	4	1
1:A:142:GLU:OE2	1:A:148:ARG:CD	0.41	2.69	4	1
1:A:44:ASP:CG	1:A:79:ARG:NH1	0.41	2.78	5	1
1:A:107:LEU:O	1:A:107:LEU:CD1	0.41	2.69	7	1
1:A:156:MET:HE1	1:A:168:GLU:HB2	0.41	1.91	15	1
1:A:156:MET:SD	1:A:156:MET:C	0.41	3.04	17	1
1:A:153:PHE:CD2	1:A:164:LEU:HD13	0.41	2.49	20	1
1:A:67:PHE:CD1	1:A:67:PHE:N	0.41	2.88	3	1
1:A:58:PHE:O	1:A:134:ASN:CB	0.41	2.68	7	1
1:A:96:THR:O	1:A:97:LEU:C	0.41	2.62	13	2
1:A:143:ASN:CB	1:A:181:GLN:NE2	0.41	2.84	10	1
1:A:143:ASN:CG	1:A:148:ARG:HH22	0.41	2.24	11	1
1:A:156:MET:CE	1:A:159:ASN:HD21	0.41	2.29	17	1
1:A:48:PHE:CE1	1:A:72:PHE:CE2	0.40	3.09	1	1
1:A:63:LYS:O	1:A:66:THR:OG1	0.40	2.31	11	1
1:A:17:THR:CG2	1:A:24:GLU:CG	0.40	2.99	15	1
1:A:143:ASN:O	1:A:145:PRO:CD	0.40	2.70	15	1
1:A:27:VAL:CG2	1:A:86:ILE:HD11	0.40	2.45	17	1
1:A:118:ARG:NH1	1:A:118:ARG:CG	0.40	2.82	20	1
1:A:146:GLU:H	1:A:146:GLU:CD	0.40	2.25	10	1
1:A:157:ASP:OD1	1:A:162:GLY:N	0.40	2.55	11	1
1:A:166:LEU:CD2	1:A:166:LEU:C	0.40	2.94	12	1
1:A:101:LEU:HD13	1:A:101:LEU:O	0.40	2.17	18	1
1:A:74:GLU:OE2	1:A:103:TRP:CH2	0.40	2.74	1	1
1:A:182:ALA:HB3	1:A:183:LEU:CD2	0.40	2.46	4	1
1:A:128:ILE:O	1:A:129:TYR:C	0.40	2.65	6	1
1:A:101:LEU:HD11	1:A:180:VAL:HG11	0.40	1.92	7	1
1:A:144:THR:N	1:A:145:PRO:HD2	0.40	2.31	7	1
1:A:134:ASN:C	1:A:135:THR:HG23	0.40	2.41	9	2
1:A:49:GLN:HA	1:A:65:ALA:HB1	0.40	1.92	13	1
1:A:171:GLU:O	1:A:175:ALA:N	0.40	2.48	13	1
1:A:11:GLU:H	1:A:11:GLU:CD	0.40	2.23	15	1
1:A:142:GLU:HG3	1:A:143:ASN:N	0.40	2.31	18	1
1:A:61:PRO:C	1:A:62:THR:HG22	0.40	2.41	20	1
1:A:24:GLU:OE1	1:A:25:LYS:CD	0.40	2.70	8	1
1:A:71:VAL:HG11	1:A:106:LYS:O	0.40	2.16	12	1
1:A:58:PHE:CE1	1:A:136:VAL:HG23	0.40	2.51	15	1
1:A:141:GLU:HG3	1:A:142:GLU:N	0.40	2.30	16	1
1:A:71:VAL:CG2	1:A:72:PHE:N	0.40	2.84	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:ASN:H	1:A:159:ASN:HD22	0.40	1.52	5	1
1:A:155:MET:O	1:A:158:LYS:CG	0.40	2.69	6	1
1:A:170:GLN:OE1	1:A:171:GLU:CD	0.40	2.65	7	1
1:A:60:ASP:H	1:A:61:PRO:HD3	0.40	1.76	11	1
1:A:21:TYR:CD2	1:A:90:SER:O	0.40	2.75	19	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	176/190 (93%)	143±33 (81±19%)	17±5 (10±3%)	8±3 (4±2%)	3	28
All	All	3344/3800 (88%)	2856 (85%)	335 (10%)	153 (5%)	3	26

All 40 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	20	THR	15
1	A	159	ASN	13
1	A	62	THR	11
1	A	94	ARG	8
1	A	144	THR	7
1	A	112	ASN	6
1	A	137	GLU	6
1	A	142	GLU	6
1	A	177	PRO	6
1	A	160	ALA	5
1	A	181	GLN	5
1	A	76	LYS	5
1	A	183	LEU	5
1	A	114	GLY	5
1	A	140	GLU	4
1	A	136	VAL	4
1	A	60	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	143	ASN	3
1	A	167	GLN	3
1	A	135	THR	3
1	A	145	PRO	3
1	A	133	GLY	2
1	A	61	PRO	2
1	A	95	GLY	2
1	A	158	LYS	2
1	A	139	PRO	2
1	A	184	SER	2
1	A	73	ASP	2
1	A	182	ALA	2
1	A	134	ASN	1
1	A	9	LYS	1
1	A	31	TYR	1
1	A	157	ASP	1
1	A	178	SER	1
1	A	40	SER	1
1	A	39	PRO	1
1	A	58	PHE	1
1	A	180	VAL	1
1	A	75	ASN	1
1	A	57	PRO	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	156/168 (93%)	139±3 (89±2%)	17±3 (11±2%)	8	51
All	All	3120/3360 (93%)	2771 (89%)	349 (11%)	8	51

All 88 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	183	LEU	20
1	A	80	ILE	18

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Mol	Chain	Res	Type	Models (Total)
1	A	82	PHE	15
1	A	164	LEU	14
1	A	144	THR	13
1	A	86	ILE	11
1	A	96	THR	10
1	A	178	SER	10
1	A	92	THR	9
1	A	153	PHE	9
1	A	27	VAL	8
1	A	166	LEU	8
1	A	69	PHE	7
1	A	108	TYR	7
1	A	60	ASP	6
1	A	159	ASN	6
1	A	20	THR	6
1	A	138	LEU	6
1	A	25	LYS	6
1	A	12	VAL	5
1	A	62	THR	5
1	A	16	LEU	5
1	A	180	VAL	5
1	A	118	ARG	5
1	A	14	GLU	4
1	A	174	LYS	4
1	A	56	PHE	4
1	A	136	VAL	4
1	A	156	MET	4
1	A	24	GLU	4
1	A	115	TYR	4
1	A	170	GLN	4
1	A	75	ASN	4
1	A	89	LEU	4
1	A	30	TRP	3
1	A	129	TYR	3
1	A	176	ASP	3
1	A	184	SER	3
1	A	103	TRP	3
1	A	112	ASN	3
1	A	169	PHE	3
1	A	125	VAL	3
1	A	135	THR	3
1	A	116	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	131	MET	3
1	A	132	VAL	3
1	A	152	ILE	3
1	A	51	ILE	3
1	A	9	LYS	2
1	A	18	ARG	2
1	A	158	LYS	2
1	A	19	LYS	2
1	A	113	ASP	2
1	A	117	THR	2
1	A	149	VAL	2
1	A	163	LYS	2
1	A	21	TYR	2
1	A	54	GLN	2
1	A	55	PHE	2
1	A	101	LEU	2
1	A	49	GLN	2
1	A	106	LYS	1
1	A	143	ASN	1
1	A	72	PHE	1
1	A	31	TYR	1
1	A	63	LYS	1
1	A	76	LYS	1
1	A	107	LEU	1
1	A	161	ASP	1
1	A	52	TYR	1
1	A	109	ASP	1
1	A	122	LEU	1
1	A	146	GLU	1
1	A	64	PHE	1
1	A	119	ASN	1
1	A	74	GLU	1
1	A	151	ARG	1
1	A	34	PHE	1
1	A	148	ARG	1
1	A	35	ILE	1
1	A	97	LEU	1
1	A	17	THR	1
1	A	22	PHE	1
1	A	93	SER	1
1	A	179	ILE	1
1	A	91	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	110	LEU	1
1	A	71	VAL	1

6.3.3 RNA [i](#)

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 58% for the well-defined parts and 56% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1477
Number of shifts mapped to atoms	1477
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	185	-0.80 ± 0.25	Should be checked
$^{13}\text{C}_\beta$	172	0.07 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	183	-0.79 ± 0.14	Should be applied
^{15}N	178	0.14 ± 0.15	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 58%, i.e. 1413 atoms were assigned a chemical shift out of a possible 2438. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	873/876 (100%)	354/355 (100%)	350/352 (99%)	169/169 (100%)
Sidechain	445/1334 (33%)	168/855 (20%)	275/426 (65%)	2/53 (4%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	95/228 (42%)	85/111 (77%)	8/115 (7%)	2/2 (100%)
Overall	1413/2438 (58%)	607/1321 (46%)	633/893 (71%)	173/224 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 56%, i.e. 1477 atoms were assigned a chemical shift out of a possible 2624. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	919/948 (97%)	373/385 (97%)	368/380 (97%)	178/183 (97%)
Sidechain	459/1439 (32%)	171/924 (19%)	286/459 (62%)	2/56 (4%)
Aromatic	99/237 (42%)	89/115 (77%)	8/120 (7%)	2/2 (100%)
Overall	1477/2624 (56%)	633/1424 (44%)	662/959 (69%)	182/241 (76%)

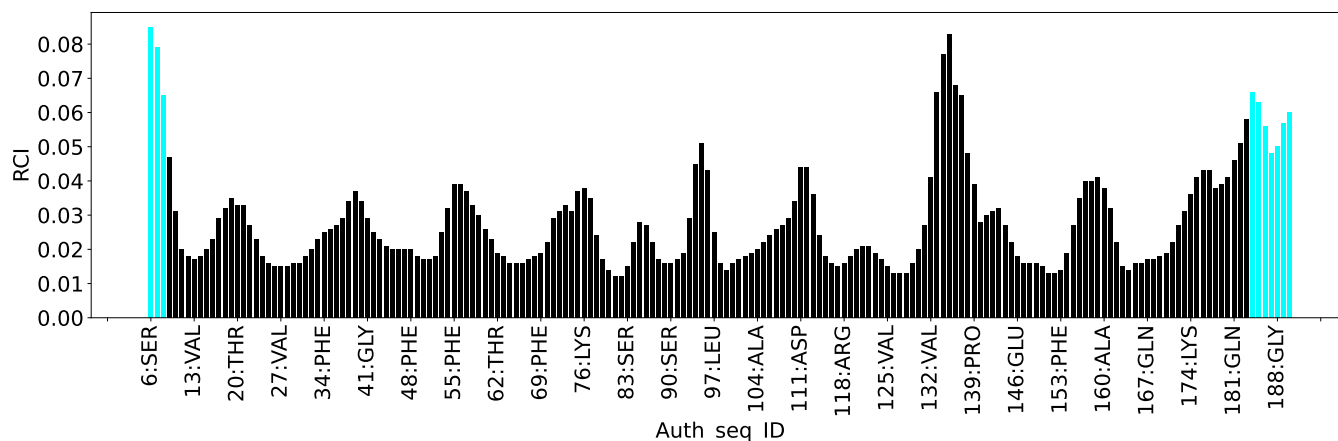
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1441
Intra-residue ($ i-j =0$)	157
Sequential ($ i-j =1$)	428
Medium range ($ i-j >1$ and $ i-j <5$)	371
Long range ($ i-j \geq 5$)	341
Inter-chain	0
Hydrogen bond restraints	126
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	7.5
Number of long range restraints per residue ¹	1.8

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)	57.2	0.2
0.2-0.5 (Medium)	17.8	0.5
>0.5 (Large)	2.7	2.25

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

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

9 Distance violation analysis ⓘ

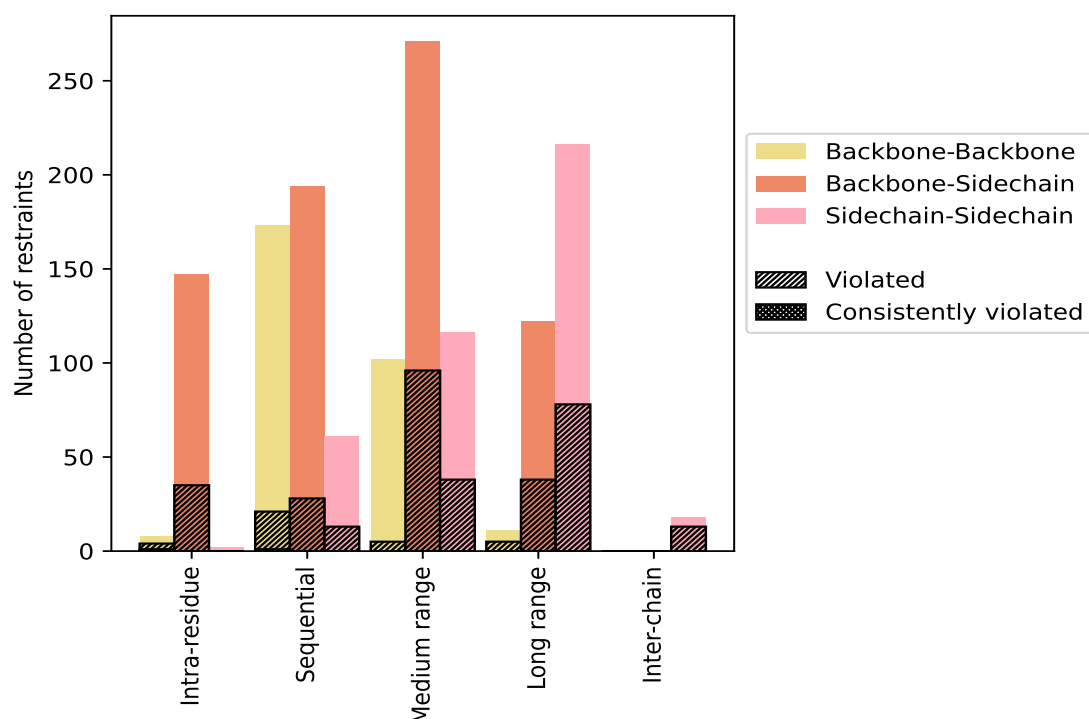
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	157	10.9	39	24.8	2.7	1	0.6	0.1
Backbone-Backbone	8	0.6	4	50.0	0.3	1	12.5	0.1
Backbone-Sidechain	147	10.2	35	23.8	2.4	0	0.0	0.0
Sidechain-Sidechain	2	0.1	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	428	29.7	62	14.5	4.3	1	0.2	0.1
Backbone-Backbone	173	12.0	21	12.1	1.5	1	0.6	0.1
Backbone-Sidechain	194	13.5	28	14.4	1.9	0	0.0	0.0
Sidechain-Sidechain	61	4.2	13	21.3	0.9	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	371	25.7	85	22.9	5.9	0	0.0	0.0
Backbone-Backbone	102	7.1	5	4.9	0.3	0	0.0	0.0
Backbone-Sidechain	153	10.6	42	27.5	2.9	0	0.0	0.0
Sidechain-Sidechain	116	8.0	38	32.8	2.6	0	0.0	0.0
Long range ($i-j \geq 5$)	341	23.7	120	35.2	8.3	0	0.0	0.0
Backbone-Backbone	11	0.8	5	45.5	0.3	0	0.0	0.0
Backbone-Sidechain	114	7.9	37	32.5	2.6	0	0.0	0.0
Sidechain-Sidechain	216	15.0	78	36.1	5.4	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	126	8.7	55	43.7	3.8	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1441	100.0	374	26.0	26.0	2	0.1	0.1
Backbone-Backbone	294	20.4	35	11.9	2.4	2	0.7	0.1
Backbone-Sidechain	734	50.9	197	26.8	13.7	0	0.0	0.0
Sidechain-Sidechain	413	28.7	142	34.4	9.9	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations [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	7	12	23	22	2	66	0.2	1.16	0.16	0.16
2	5	14	27	22	2	70	0.22	1.81	0.22	0.16
3	8	10	27	23	3	71	0.23	2.12	0.29	0.17
4	5	9	33	28	1	76	0.2	2.07	0.23	0.15
5	13	14	31	19	5	82	0.2	1.95	0.24	0.15
6	8	16	36	37	5	102	0.21	1.82	0.23	0.15
7	8	12	33	24	3	80	0.2	1.95	0.21	0.15
8	7	15	36	19	3	80	0.16	0.58	0.07	0.15
9	7	14	28	26	3	78	0.22	1.81	0.27	0.15
10	7	15	30	23	8	83	0.22	1.94	0.27	0.15

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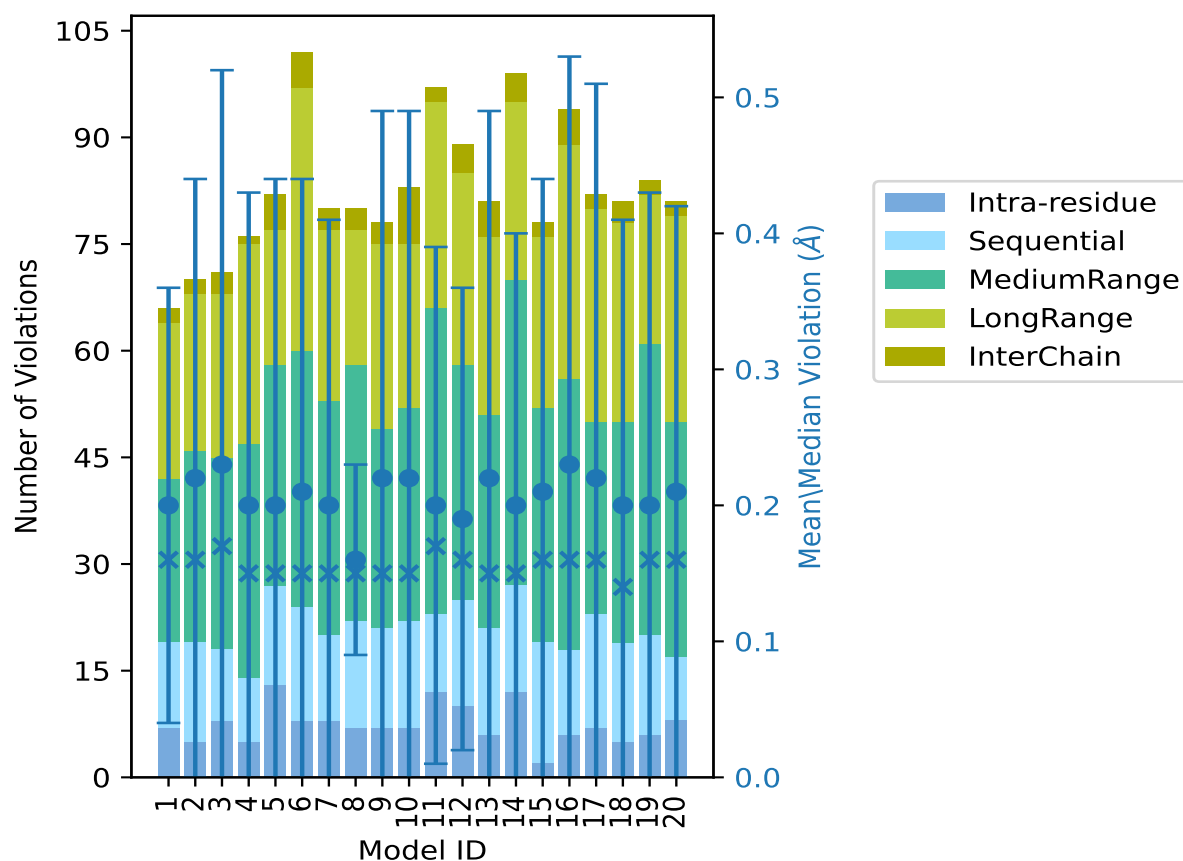
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	12	11	43	29	2	97	0.2	1.83	0.19	0.17
12	10	15	33	27	4	89	0.19	1.63	0.17	0.16
13	6	15	30	25	5	81	0.22	1.74	0.27	0.15
14	12	15	43	25	4	99	0.2	1.54	0.2	0.15
15	2	17	33	24	2	78	0.21	2.07	0.23	0.16
16	6	12	38	33	5	94	0.23	2.18	0.3	0.16
17	7	16	27	30	2	82	0.22	2.25	0.29	0.16
18	5	14	31	28	3	81	0.2	1.82	0.21	0.14
19	6	14	41	21	2	84	0.2	2.13	0.23	0.16
20	8	9	33	29	2	81	0.21	1.92	0.21	0.16

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

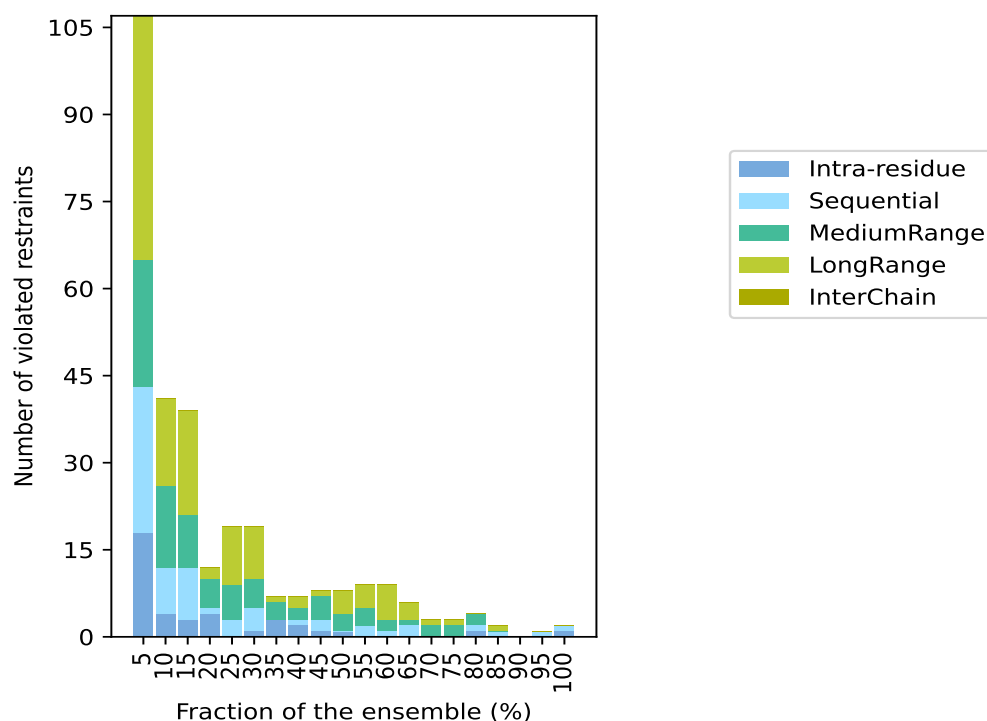
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 991(IR:118, SQ:366, MR:286, LR:221, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
18	25	22	42	0	107	1	5.0
4	8	14	15	0	41	2	10.0
3	9	9	18	0	39	3	15.0
4	1	5	2	0	12	4	20.0
0	3	6	10	0	19	5	25.0
1	4	5	9	0	19	6	30.0
3	0	3	1	0	7	7	35.0
2	1	2	2	0	7	8	40.0
1	2	4	1	0	8	9	45.0
1	0	3	4	0	8	10	50.0
0	2	3	4	0	9	11	55.0
0	1	2	6	0	9	12	60.0
0	2	1	3	0	6	13	65.0
0	0	2	1	0	3	14	70.0
0	0	2	1	0	3	15	75.0
1	1	2	0	0	4	16	80.0
0	1	0	1	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	1	0	0	0	1	19	95.0
1	1	0	0	0	2	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

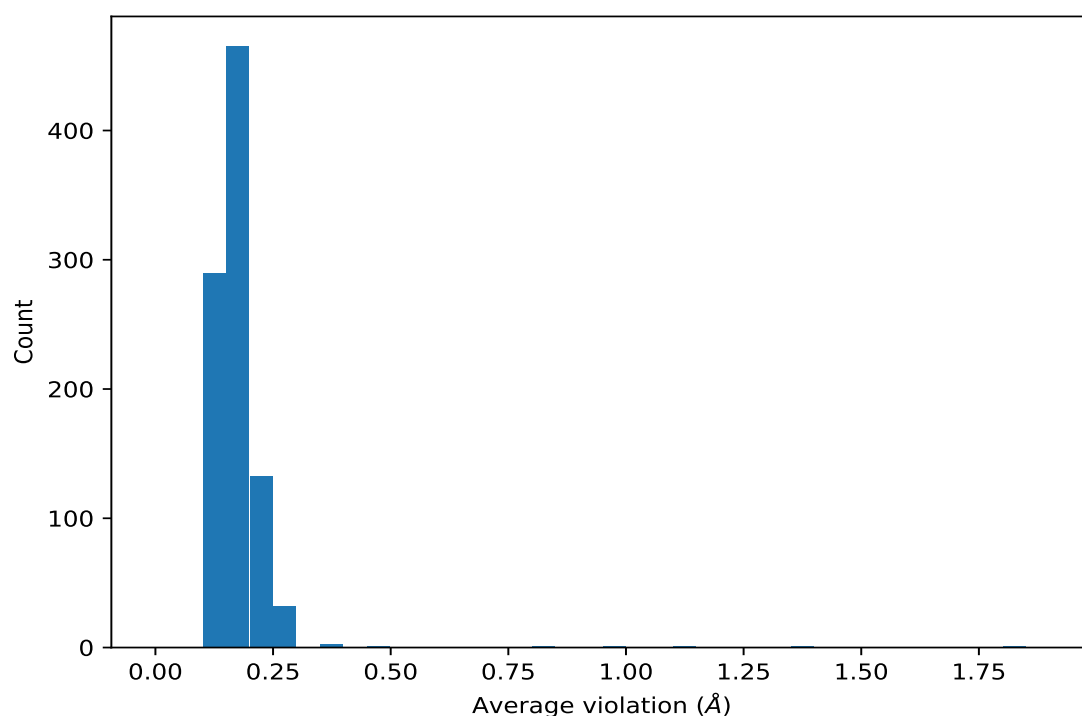
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	20	0.18	0.04	0.18
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	20	0.13	0.01	0.13
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	19	1.82	0.31	1.92
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	19	0.17	0.03	0.17
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	19	0.17	0.03	0.17
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	19	0.17	0.03	0.17
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	18	0.16	0.05	0.16
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	17	0.19	0.07	0.17
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	17	0.19	0.07	0.17
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	17	0.19	0.07	0.17
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	17	0.17	0.03	0.17
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	17	0.17	0.03	0.17
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	17	0.17	0.03	0.17
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	17	0.17	0.03	0.17
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	16	0.98	0.33	0.86
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	16	0.2	0.09	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	16	0.2	0.09	0.16
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	16	0.17	0.05	0.15
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	16	0.17	0.05	0.15
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	16	0.16	0.04	0.15
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	16	0.16	0.04	0.15
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	16	0.16	0.04	0.15
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	16	0.16	0.04	0.15
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	16	0.16	0.04	0.15
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	16	0.16	0.04	0.15
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	16	0.11	0.01	0.11
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	15	0.21	0.09	0.23
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	15	0.21	0.09	0.23
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	15	0.17	0.07	0.15
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	15	0.17	0.07	0.15
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	15	0.17	0.07	0.15
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	15	0.17	0.07	0.15
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	15	0.17	0.07	0.15
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	15	0.17	0.07	0.15
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	15	0.13	0.02	0.13
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	14	0.18	0.07	0.17
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	14	0.17	0.05	0.15
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	14	0.16	0.04	0.16
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	14	0.16	0.04	0.16
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	14	0.16	0.05	0.16
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	14	0.16	0.05	0.16
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	14	0.16	0.05	0.16
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	14	0.16	0.05	0.16
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	14	0.16	0.05	0.15
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	14	0.16	0.05	0.15
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	14	0.16	0.05	0.15
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	14	0.14	0.03	0.13
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	13	0.24	0.07	0.24
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	13	0.24	0.07	0.24
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	13	0.24	0.07	0.24
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	13	0.24	0.07	0.24
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	13	0.24	0.07	0.24
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	13	0.24	0.07	0.24
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	13	0.23	0.11	0.17
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	13	0.23	0.11	0.17
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	13	0.21	0.08	0.2
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	13	0.21	0.08	0.2
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	13	0.21	0.08	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	13	0.2	0.06	0.2
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	13	0.2	0.05	0.18
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	13	0.2	0.05	0.18
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	13	0.19	0.02	0.2
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	13	0.17	0.04	0.15
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	13	0.17	0.04	0.15
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	13	0.17	0.04	0.15
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	13	0.17	0.04	0.15
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	12	0.29	0.13	0.27
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	12	0.29	0.13	0.27
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	12	0.26	0.07	0.28
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	12	0.26	0.07	0.28
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	12	0.26	0.07	0.28
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	12	0.26	0.07	0.28
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	12	0.17	0.03	0.16
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	12	0.16	0.05	0.14
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	12	0.16	0.05	0.14
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	12	0.16	0.05	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	12	0.16	0.05	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	12	0.16	0.05	0.14
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	12	0.15	0.03	0.15
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	12	0.15	0.03	0.15
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	12	0.15	0.03	0.15
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	12	0.15	0.03	0.15
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	12	0.15	0.05	0.13
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	12	0.15	0.05	0.13
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	12	0.14	0.04	0.14
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	11	0.26	0.08	0.25
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	11	0.26	0.08	0.25
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	11	0.22	0.1	0.2
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	11	0.22	0.1	0.2
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	11	0.22	0.1	0.2
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	11	0.22	0.1	0.2
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	11	0.22	0.1	0.2
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	11	0.22	0.1	0.2
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	11	0.21	0.02	0.22
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	11	0.2	0.08	0.18
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	11	0.2	0.08	0.18
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	11	0.2	0.08	0.18
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	11	0.2	0.08	0.18
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	11	0.2	0.08	0.18
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	11	0.2	0.08	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	11	0.19	0.04	0.19
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	11	0.19	0.04	0.19
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	11	0.19	0.04	0.19
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	11	0.19	0.04	0.19
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	11	0.17	0.05	0.16
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	11	0.17	0.03	0.17
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	11	0.17	0.03	0.17
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	11	0.16	0.03	0.17
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	11	0.16	0.03	0.15
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	11	0.15	0.03	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	11	0.15	0.03	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	11	0.15	0.03	0.14
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	10	0.2	0.12	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	10	0.2	0.12	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	10	0.2	0.12	0.16
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	10	0.2	0.06	0.19
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	10	0.2	0.06	0.19
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	10	0.2	0.06	0.19
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	10	0.18	0.06	0.17
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	10	0.18	0.06	0.17
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	10	0.18	0.04	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	10	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	10	0.18	0.05	0.16
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	10	0.16	0.06	0.16
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	10	0.16	0.06	0.16
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	10	0.16	0.06	0.16
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	10	0.16	0.06	0.16
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	10	0.16	0.06	0.16
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	10	0.16	0.06	0.16
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	10	0.16	0.06	0.15
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	10	0.16	0.06	0.15
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	10	0.16	0.02	0.16
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	10	0.15	0.04	0.13
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	10	0.15	0.04	0.13
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	10	0.13	0.02	0.13
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	9	0.27	0.04	0.28
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	9	0.2	0.07	0.19
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	9	0.2	0.07	0.19
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	9	0.18	0.04	0.15
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	9	0.18	0.04	0.15
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	9	0.17	0.04	0.16
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	9	0.16	0.04	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	9	0.16	0.04	0.17
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	9	0.16	0.06	0.14
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	9	0.14	0.01	0.14
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	9	0.14	0.02	0.15
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	9	0.14	0.02	0.15
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	9	0.14	0.02	0.15
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	9	0.14	0.02	0.15
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	9	0.14	0.02	0.15
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	9	0.14	0.02	0.15
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	9	0.12	0.02	0.12
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	8	0.82	0.65	0.47
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	8	0.24	0.04	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	8	0.24	0.04	0.25
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	8	0.24	0.04	0.25
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	8	0.24	0.04	0.25
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	8	0.24	0.04	0.25
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	8	0.24	0.04	0.25
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	8	0.18	0.04	0.18
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	8	0.18	0.04	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	8	0.16	0.05	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	8	0.16	0.05	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	8	0.16	0.05	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	8	0.16	0.05	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	8	0.16	0.05	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	8	0.16	0.05	0.15
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	8	0.16	0.04	0.17
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	8	0.16	0.04	0.17
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	8	0.16	0.04	0.17
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	8	0.16	0.04	0.17
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	8	0.16	0.04	0.17
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	8	0.16	0.04	0.17
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	8	0.16	0.05	0.15
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	8	0.16	0.05	0.15
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	8	0.16	0.05	0.15
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	8	0.16	0.05	0.15
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	8	0.16	0.05	0.15
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	8	0.16	0.05	0.15
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	8	0.16	0.05	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	8	0.16	0.05	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	8	0.16	0.05	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	8	0.16	0.05	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	8	0.16	0.05	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	8	0.16	0.05	0.14
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	8	0.14	0.03	0.13
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	8	0.14	0.03	0.13
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	8	0.14	0.03	0.13
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD2	7	0.35	0.21	0.21
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD3	7	0.35	0.21	0.21
(1,510)	1:66:A:THR:H	1:66:A:THR:HB	7	0.28	0.0	0.28
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD2	7	0.27	0.11	0.32
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD3	7	0.27	0.11	0.32
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG21	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG22	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG23	7	0.22	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG21	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG22	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG23	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG21	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG22	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG23	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG21	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG22	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG23	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG21	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG22	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG23	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG21	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG22	7	0.22	0.05	0.2
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG23	7	0.22	0.05	0.2
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG2	7	0.21	0.07	0.21
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG3	7	0.21	0.07	0.21
(3,27)	1:52:A:TYR:O	1:56:A:PHE:N	7	0.14	0.03	0.13
(3,114)	1:166:A:LEU:O	1:170:A:GLN:H	7	0.13	0.03	0.12
(3,112)	1:169:A:PHE:O	1:173:A:SER:N	7	0.13	0.06	0.11
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG21	7	0.13	0.03	0.12
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG22	7	0.13	0.03	0.12
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG23	7	0.13	0.03	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG21	7	0.13	0.03	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG22	7	0.13	0.03	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG23	7	0.13	0.03	0.12
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD11	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD12	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD13	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD21	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD22	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD23	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD11	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD12	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD13	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD21	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD22	7	0.12	0.02	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD23	7	0.12	0.02	0.11
(3,109)	1:166:A:LEU:O	1:170:A:GLN:N	7	0.12	0.02	0.11
(1,147)	1:20:A:THR:HB	1:21:A:TYR:H	6	0.37	0.09	0.4
(1,50)	1:12:A:VAL:H	1:12:A:VAL:HB	6	0.27	0.02	0.27
(1,1021)	1:142:A:GLU:HG2	1:144:A:THR:H	6	0.25	0.13	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1021)	1:142:A:GLU:HG3	1:144:A:THR:H	6	0.25	0.13	0.23
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD11	6	0.18	0.03	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD12	6	0.18	0.03	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD13	6	0.18	0.03	0.16
(3,102)	1:151:A:ARG:O	1:155:A:MET:N	6	0.18	0.05	0.18
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD11	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD12	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD13	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD21	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD22	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD23	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD11	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD12	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD13	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD21	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD22	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD23	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD11	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD12	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD13	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD21	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD22	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD23	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD11	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD12	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD13	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD21	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD22	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD23	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD11	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD12	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD13	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD21	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD22	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD23	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD11	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD12	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD13	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD21	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD22	6	0.17	0.05	0.16
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD23	6	0.17	0.05	0.16
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB1	6	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB2	6	0.17	0.04	0.16
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB3	6	0.17	0.04	0.16
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG11	6	0.16	0.03	0.16
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG12	6	0.16	0.03	0.16
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG13	6	0.16	0.03	0.16
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG21	6	0.16	0.03	0.16
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG22	6	0.16	0.03	0.16
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG23	6	0.16	0.03	0.16
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD1	6	0.15	0.03	0.15
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD2	6	0.15	0.03	0.15
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD1	6	0.15	0.03	0.15
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD2	6	0.15	0.03	0.15
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB1	6	0.15	0.02	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB2	6	0.15	0.02	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB3	6	0.15	0.02	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB1	6	0.15	0.02	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB2	6	0.15	0.02	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB3	6	0.15	0.02	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB1	6	0.15	0.02	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB2	6	0.15	0.02	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB3	6	0.15	0.02	0.14
(1,1017)	1:142:A:GLU:H	1:143:A:ASN:H	6	0.15	0.05	0.12
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG21	6	0.15	0.02	0.15
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG22	6	0.15	0.02	0.15
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG23	6	0.15	0.02	0.15
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG21	6	0.15	0.02	0.15
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG22	6	0.15	0.02	0.15
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG23	6	0.15	0.02	0.15
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB2	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB3	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB2	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB3	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB2	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB3	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB2	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB3	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB2	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB3	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB2	6	0.14	0.04	0.12
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB3	6	0.14	0.04	0.12
(1,386)	1:48:A:PHE:HE1	1:80:A:ILE:HB	6	0.14	0.02	0.14
(1,386)	1:48:A:PHE:HE2	1:80:A:ILE:HB	6	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1208)	1:169:A:PHE:HA	1:179:A:ILE:HB	6	0.13	0.03	0.12
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB2	6	0.13	0.02	0.12
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB3	6	0.13	0.02	0.12
(1,988)	1:135:A:THR:HB	1:138:A:LEU:H	6	0.13	0.01	0.13
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD11	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD12	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD13	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD21	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD22	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD23	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD11	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD12	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD13	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD21	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD22	6	0.13	0.02	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD23	6	0.13	0.02	0.12
(1,715)	1:96:A:THR:HB	1:98:A:ASP:H	6	0.12	0.02	0.13
(3,118)	1:170:A:GLN:O	1:174:A:LYS:H	6	0.12	0.04	0.11
(1,773)	1:107:A:LEU:HD11	1:108:A:TYR:H	6	0.12	0.01	0.12
(1,773)	1:107:A:LEU:HD12	1:108:A:TYR:H	6	0.12	0.01	0.12
(1,773)	1:107:A:LEU:HD13	1:108:A:TYR:H	6	0.12	0.01	0.12
(1,773)	1:107:A:LEU:HD21	1:108:A:TYR:H	6	0.12	0.01	0.12
(1,773)	1:107:A:LEU:HD22	1:108:A:TYR:H	6	0.12	0.01	0.12
(1,773)	1:107:A:LEU:HD23	1:108:A:TYR:H	6	0.12	0.01	0.12
(3,4)	1:11:A:GLU:O	1:15:A:GLU:H	6	0.12	0.01	0.12
(2,9)	1:113:A:ASP:OD1	2:601:A:CA:CA	5	1.14	0.67	0.62
(1,953)	1:125:A:VAL:HG11	1:129:A:TYR:H	5	0.25	0.09	0.27
(1,953)	1:125:A:VAL:HG12	1:129:A:TYR:H	5	0.25	0.09	0.27
(1,953)	1:125:A:VAL:HG13	1:129:A:TYR:H	5	0.25	0.09	0.27
(1,953)	1:125:A:VAL:HG21	1:129:A:TYR:H	5	0.25	0.09	0.27
(1,953)	1:125:A:VAL:HG22	1:129:A:TYR:H	5	0.25	0.09	0.27
(1,953)	1:125:A:VAL:HG23	1:129:A:TYR:H	5	0.25	0.09	0.27
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD1	5	0.22	0.16	0.16
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD2	5	0.22	0.16	0.16
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB2	5	0.21	0.1	0.2
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB3	5	0.21	0.1	0.2
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB2	5	0.21	0.1	0.2
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB3	5	0.21	0.1	0.2
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD1	5	0.2	0.12	0.14
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD2	5	0.2	0.12	0.14
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD2	5	0.19	0.05	0.19
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD3	5	0.19	0.05	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD2	5	0.19	0.05	0.19
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD3	5	0.19	0.05	0.19
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG11	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG12	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG13	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG21	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG22	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG23	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG11	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG12	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG13	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG21	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG22	5	0.19	0.06	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG23	5	0.19	0.06	0.18
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE1	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE2	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE1	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE2	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE1	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE2	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE1	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE2	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE1	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE2	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE1	5	0.19	0.03	0.18
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE2	5	0.19	0.03	0.18
(1,117)	1:16:A:LEU:HD11	1:19:A:LYS:HA	5	0.19	0.09	0.16
(1,117)	1:16:A:LEU:HD12	1:19:A:LYS:HA	5	0.19	0.09	0.16
(1,117)	1:16:A:LEU:HD13	1:19:A:LYS:HA	5	0.19	0.09	0.16
(1,117)	1:16:A:LEU:HD21	1:19:A:LYS:HA	5	0.19	0.09	0.16
(1,117)	1:16:A:LEU:HD22	1:19:A:LYS:HA	5	0.19	0.09	0.16
(1,117)	1:16:A:LEU:HD23	1:19:A:LYS:HA	5	0.19	0.09	0.16
(1,468)	1:58:A:PHE:HA	1:59:A:GLY:H	5	0.18	0.02	0.18
(1,800)	1:109:A:ASP:HA	1:116:A:ILE:HA	5	0.18	0.04	0.19
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG2	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG3	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG2	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG3	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG2	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG3	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG2	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG3	5	0.17	0.04	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG2	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG3	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG2	5	0.17	0.04	0.19
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG3	5	0.17	0.04	0.19
(1,1241)	1:174:A:LYS:HA	1:175:A:ALA:H	5	0.17	0.05	0.18
(1,399)	1:49:A:GLN:HB2	1:65:A:ALA:HA	5	0.17	0.03	0.17
(1,399)	1:49:A:GLN:HB3	1:65:A:ALA:HA	5	0.17	0.03	0.17
(1,1167)	1:164:A:LEU:H	1:165:A:THR:HA	5	0.16	0.05	0.13
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB1	5	0.16	0.02	0.16
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB2	5	0.16	0.02	0.16
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB3	5	0.16	0.02	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB1	5	0.16	0.02	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB2	5	0.16	0.02	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB3	5	0.16	0.02	0.16
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD11	5	0.16	0.03	0.15
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD12	5	0.16	0.03	0.15
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD13	5	0.16	0.03	0.15
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD11	5	0.16	0.03	0.15
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD12	5	0.16	0.03	0.15
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD13	5	0.16	0.03	0.15
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG11	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG12	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG13	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG21	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG22	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG23	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG11	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG12	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG13	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG21	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG22	5	0.16	0.03	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG23	5	0.16	0.03	0.17
(3,94)	1:127:A:ALA:O	1:131:A:MET:H	5	0.16	0.05	0.14
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD11	5	0.14	0.03	0.13
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD12	5	0.14	0.03	0.13
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD13	5	0.14	0.03	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD11	5	0.14	0.03	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD12	5	0.14	0.03	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD13	5	0.14	0.03	0.13
(3,45)	1:67:A:PHE:O	1:71:A:VAL:H	5	0.14	0.01	0.13
(1,311)	1:42:A:GLN:HG2	1:79:A:ARG:HA	5	0.13	0.03	0.11
(1,311)	1:42:A:GLN:HG3	1:79:A:ARG:HA	5	0.13	0.03	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,563)	1:71:A:VAL:H	1:71:A:VAL:HB	4	0.29	0.06	0.29
(1,531)	1:68:A:VAL:H	1:68:A:VAL:HB	4	0.29	0.0	0.29
(1,945)	1:125:A:VAL:H	1:125:A:VAL:HB	4	0.26	0.03	0.26
(1,508)	1:65:A:ALA:HB1	1:68:A:VAL:HB	4	0.25	0.04	0.24
(1,508)	1:65:A:ALA:HB2	1:68:A:VAL:HB	4	0.25	0.04	0.24
(1,508)	1:65:A:ALA:HB3	1:68:A:VAL:HB	4	0.25	0.04	0.24
(1,595)	1:75:A:ASN:HA	1:76:A:LYS:H	4	0.18	0.01	0.18
(1,229)	1:30:A:TRP:H	1:30:A:TRP:HD1	4	0.17	0.04	0.16
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD11	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD12	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD13	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD21	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD22	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD23	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD11	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD12	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD13	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD21	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD22	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD23	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD11	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD12	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD13	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD21	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD22	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD23	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD11	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD12	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD13	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD21	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD22	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD23	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD11	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD12	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD13	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD21	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD22	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD23	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD11	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD12	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD13	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD21	4	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD22	4	0.16	0.03	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD23	4	0.16	0.03	0.15
(1,66)	1:12:A:VAL:HG21	1:16:A:LEU:HG	4	0.16	0.02	0.15
(1,66)	1:12:A:VAL:HG22	1:16:A:LEU:HG	4	0.16	0.02	0.15
(1,66)	1:12:A:VAL:HG23	1:16:A:LEU:HG	4	0.16	0.02	0.15
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG12	4	0.13	0.02	0.13
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG13	4	0.13	0.02	0.13
(1,1283)	1:184:A:SER:HB2	1:186:A:TYR:H	4	0.13	0.03	0.12
(1,1283)	1:184:A:SER:HB3	1:186:A:TYR:H	4	0.13	0.03	0.12
(3,115)	1:167:A:GLN:O	1:171:A:GLU:H	4	0.13	0.02	0.12
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG21	4	0.12	0.01	0.12
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG22	4	0.12	0.01	0.12
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG23	4	0.12	0.01	0.12
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB2	4	0.11	0.0	0.11
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB3	4	0.11	0.0	0.11
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB2	4	0.11	0.0	0.11
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB3	4	0.11	0.0	0.11
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB2	4	0.11	0.0	0.11
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB3	4	0.11	0.0	0.11
(2,15)	1:161:A:ASP:OD2	2:602:A:CA:CA	3	0.46	0.25	0.55
(1,825)	1:112:A:ASN:HA	1:113:A:ASP:H	3	0.25	0.0	0.25
(1,424)	1:52:A:TYR:HA	1:55:A:PHE:HD1	3	0.22	0.0	0.22
(1,424)	1:52:A:TYR:HA	1:55:A:PHE:HD2	3	0.22	0.0	0.22
(1,150)	1:20:A:THR:HG21	1:22:A:PHE:H	3	0.21	0.05	0.23
(1,150)	1:20:A:THR:HG22	1:22:A:PHE:H	3	0.21	0.05	0.23
(1,150)	1:20:A:THR:HG23	1:22:A:PHE:H	3	0.21	0.05	0.23
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG11	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG12	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG13	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG21	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG22	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG23	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG11	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG12	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG13	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG21	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG22	3	0.21	0.05	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG23	3	0.21	0.05	0.22
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD11	3	0.21	0.06	0.24
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD12	3	0.21	0.06	0.24
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD13	3	0.21	0.06	0.24
(1,895)	1:118:A:ARG:H	1:118:A:ARG:HD2	3	0.19	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,895)	1:118:A:ARG:H	1:118:A:ARG:HD3	3	0.19	0.04	0.2
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD11	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD12	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD13	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD21	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD22	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD23	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD11	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD12	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD13	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD21	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD22	3	0.18	0.07	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD23	3	0.18	0.07	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD11	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD12	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD13	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD21	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD22	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD23	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD11	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD12	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD13	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD21	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD22	3	0.18	0.06	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD23	3	0.18	0.06	0.16
(1,387)	1:48:A:PHE:HE1	1:80:A:ILE:HG12	3	0.17	0.02	0.17
(1,387)	1:48:A:PHE:HE1	1:80:A:ILE:HG13	3	0.17	0.02	0.17
(1,387)	1:48:A:PHE:HE2	1:80:A:ILE:HG12	3	0.17	0.02	0.17
(1,387)	1:48:A:PHE:HE2	1:80:A:ILE:HG13	3	0.17	0.02	0.17
(1,444)	1:53:A:LYS:HB2	1:57:A:PRO:HG2	3	0.17	0.03	0.18
(1,444)	1:53:A:LYS:HB2	1:57:A:PRO:HG3	3	0.17	0.03	0.18
(1,444)	1:53:A:LYS:HB3	1:57:A:PRO:HG2	3	0.17	0.03	0.18
(1,444)	1:53:A:LYS:HB3	1:57:A:PRO:HG3	3	0.17	0.03	0.18
(1,605)	1:77:A:ASP:HA	1:78:A:GLY:H	3	0.17	0.05	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG21	3	0.17	0.03	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG22	3	0.17	0.03	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG23	3	0.17	0.03	0.19
(1,1024)	1:143:A:ASN:H	1:183:A:LEU:HB2	3	0.17	0.03	0.15
(1,1024)	1:143:A:ASN:H	1:183:A:LEU:HB3	3	0.17	0.03	0.15
(1,900)	1:118:A:ARG:HB2	1:150:A:ASP:HA	3	0.16	0.02	0.16
(1,900)	1:118:A:ARG:HB3	1:150:A:ASP:HA	3	0.16	0.02	0.16
(1,476)	1:60:A:ASP:HB2	1:130:A:GLN:HB2	3	0.16	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,476)	1:60:A:ASP:HB2	1:130:A:GLN:HB3	3	0.16	0.02	0.15
(1,476)	1:60:A:ASP:HB3	1:130:A:GLN:HB2	3	0.16	0.02	0.15
(1,476)	1:60:A:ASP:HB3	1:130:A:GLN:HB3	3	0.16	0.02	0.15
(1,70)	1:13:A:VAL:H	1:14:A:GLU:HG2	3	0.16	0.04	0.15
(1,70)	1:13:A:VAL:H	1:14:A:GLU:HG3	3	0.16	0.04	0.15
(1,1073)	1:152:A:ILE:H	1:152:A:ILE:HG12	3	0.16	0.03	0.15
(1,1073)	1:152:A:ILE:H	1:152:A:ILE:HG13	3	0.16	0.03	0.15
(1,406)	1:49:A:GLN:HG2	1:66:A:THR:HA	3	0.15	0.02	0.16
(1,406)	1:49:A:GLN:HG3	1:66:A:THR:HA	3	0.15	0.02	0.16
(1,463)	1:57:A:PRO:HD2	1:58:A:PHE:HA	3	0.15	0.03	0.14
(1,463)	1:57:A:PRO:HD3	1:58:A:PHE:HA	3	0.15	0.03	0.14
(1,1065)	1:149:A:VAL:HG11	1:153:A:PHE:HZ	3	0.15	0.03	0.16
(1,1065)	1:149:A:VAL:HG12	1:153:A:PHE:HZ	3	0.15	0.03	0.16
(1,1065)	1:149:A:VAL:HG13	1:153:A:PHE:HZ	3	0.15	0.03	0.16
(1,1065)	1:149:A:VAL:HG21	1:153:A:PHE:HZ	3	0.15	0.03	0.16
(1,1065)	1:149:A:VAL:HG22	1:153:A:PHE:HZ	3	0.15	0.03	0.16
(1,1065)	1:149:A:VAL:HG23	1:153:A:PHE:HZ	3	0.15	0.03	0.16
(1,1172)	1:164:A:LEU:HG	1:165:A:THR:H	3	0.15	0.05	0.13
(3,13)	1:29:A:GLN:O	1:33:A:GLY:N	3	0.15	0.03	0.17
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG21	3	0.15	0.02	0.14
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG22	3	0.15	0.02	0.14
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG23	3	0.15	0.02	0.14
(1,924)	1:122:A:LEU:HD11	1:126:A:ASP:HA	3	0.15	0.04	0.15
(1,924)	1:122:A:LEU:HD12	1:126:A:ASP:HA	3	0.15	0.04	0.15
(1,924)	1:122:A:LEU:HD13	1:126:A:ASP:HA	3	0.15	0.04	0.15
(1,924)	1:122:A:LEU:HD21	1:126:A:ASP:HA	3	0.15	0.04	0.15
(1,924)	1:122:A:LEU:HD22	1:126:A:ASP:HA	3	0.15	0.04	0.15
(1,924)	1:122:A:LEU:HD23	1:126:A:ASP:HA	3	0.15	0.04	0.15
(3,2)	1:12:A:VAL:O	1:16:A:LEU:N	3	0.15	0.04	0.13
(1,1136)	1:157:A:ASP:HA	1:158:A:LYS:HG2	3	0.14	0.03	0.16
(1,1136)	1:157:A:ASP:HA	1:158:A:LYS:HG3	3	0.14	0.03	0.16
(3,9)	1:25:A:LYS:O	1:29:A:GLN:N	3	0.14	0.0	0.14
(3,100)	1:149:A:VAL:O	1:153:A:PHE:N	3	0.14	0.04	0.12
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD11	3	0.14	0.02	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD12	3	0.14	0.02	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD13	3	0.14	0.02	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD21	3	0.14	0.02	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD22	3	0.14	0.02	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD23	3	0.14	0.02	0.15
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD11	3	0.14	0.03	0.14
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD12	3	0.14	0.03	0.14
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD13	3	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD11	3	0.14	0.03	0.14
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD12	3	0.14	0.03	0.14
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD13	3	0.14	0.03	0.14
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD11	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD12	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD13	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD21	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD22	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD23	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD11	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD12	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD13	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD21	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD22	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD23	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD11	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD12	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD13	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD21	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD22	3	0.14	0.03	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD23	3	0.14	0.03	0.13
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD11	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD12	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD13	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD21	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD22	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD23	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD11	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD12	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD13	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD21	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD22	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD23	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD11	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD12	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD13	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD21	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD22	3	0.14	0.03	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD23	3	0.14	0.03	0.14
(1,258)	1:32:A:LYS:HA	1:35:A:ILE:HG12	3	0.14	0.04	0.11
(1,258)	1:32:A:LYS:HA	1:35:A:ILE:HG13	3	0.14	0.04	0.11
(1,54)	1:12:A:VAL:HA	1:14:A:GLU:HB2	3	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,54)	1:12:A:VAL:HA	1:14:A:GLU:HB3	3	0.13	0.02	0.13
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD11	3	0.13	0.01	0.14
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD12	3	0.13	0.01	0.14
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD13	3	0.13	0.01	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD11	3	0.13	0.01	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD12	3	0.13	0.01	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD13	3	0.13	0.01	0.14
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD11	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD12	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD13	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD21	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD22	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD23	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD11	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD12	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD13	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD21	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD22	3	0.13	0.01	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD23	3	0.13	0.01	0.13
(1,580)	1:72:A:PHE:HZ	1:80:A:ILE:HG12	3	0.13	0.03	0.11
(1,580)	1:72:A:PHE:HZ	1:80:A:ILE:HG13	3	0.13	0.03	0.11
(3,92)	1:125:A:VAL:O	1:129:A:TYR:H	3	0.13	0.02	0.14
(1,775)	1:107:A:LEU:HD11	1:110:A:LEU:HB2	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD11	1:110:A:LEU:HB3	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD12	1:110:A:LEU:HB2	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD12	1:110:A:LEU:HB3	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD13	1:110:A:LEU:HB2	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD13	1:110:A:LEU:HB3	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD21	1:110:A:LEU:HB2	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD21	1:110:A:LEU:HB3	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD22	1:110:A:LEU:HB2	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD22	1:110:A:LEU:HB3	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD23	1:110:A:LEU:HB2	3	0.12	0.01	0.12
(1,775)	1:107:A:LEU:HD23	1:110:A:LEU:HB3	3	0.12	0.01	0.12
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD11	3	0.12	0.01	0.13
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD12	3	0.12	0.01	0.13
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD13	3	0.12	0.01	0.13
(3,14)	1:30:A:TRP:O	1:34:A:PHE:N	3	0.12	0.02	0.13
(3,59)	1:87:A:GLN:O	1:91:A:VAL:H	3	0.11	0.01	0.11
(1,4)	1:7:A:LYS:HA	1:32:A:LYS:HG2	3	0.11	0.0	0.11
(1,4)	1:7:A:LYS:HA	1:32:A:LYS:HG3	3	0.11	0.0	0.11
(3,124)	1:164:A:LEU:O	1:116:A:ILE:H	3	0.11	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD11	3	0.11	0.0	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD12	3	0.11	0.0	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD13	3	0.11	0.0	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD21	3	0.11	0.0	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD22	3	0.11	0.0	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD23	3	0.11	0.0	0.11
(2,17)	1:168:A:GLU:OE1	2:602:A:CA:CA	3	0.11	0.01	0.11
(3,6)	1:13:A:VAL:O	1:17:A:THR:H	3	0.11	0.0	0.11
(1,273)	1:34:A:PHE:HE1	1:35:A:ILE:HB	3	0.1	0.0	0.1
(1,273)	1:34:A:PHE:HE2	1:35:A:ILE:HB	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE1	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE2	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE3	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE1	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE2	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE3	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE1	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE2	3	0.1	0.0	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE3	3	0.1	0.0	0.1
(2,7)	1:109:A:ASP:OD2	2:601:A:CA:CA	2	1.39	0.04	1.39
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD11	2	0.28	0.14	0.28
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD12	2	0.28	0.14	0.28
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD13	2	0.28	0.14	0.28
(1,992)	1:136:A:VAL:H	1:136:A:VAL:HB	2	0.26	0.1	0.26
(2,10)	1:115:A:TYR:O	2:601:A:CA:CA	2	0.24	0.13	0.24
(1,477)	1:62:A:THR:H	1:62:A:THR:HB	2	0.23	0.06	0.23
(1,195)	1:24:A:GLU:H	1:25:A:LYS:HD2	2	0.22	0.01	0.22
(1,195)	1:24:A:GLU:H	1:25:A:LYS:HD3	2	0.22	0.01	0.22
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD11	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD12	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD13	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD21	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD22	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD23	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD11	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD12	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD13	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD21	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD22	2	0.2	0.1	0.2
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD23	2	0.2	0.1	0.2
(1,820)	1:110:A:LEU:HD11	1:112:A:ASN:HB2	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD11	1:112:A:ASN:HB3	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)
(1,820)	1:110:A:LEU:HD12	1:112:A:ASN:HB2	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD12	1:112:A:ASN:HB3	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD13	1:112:A:ASN:HB2	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD13	1:112:A:ASN:HB3	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD21	1:112:A:ASN:HB2	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD21	1:112:A:ASN:HB3	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD22	1:112:A:ASN:HB2	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD22	1:112:A:ASN:HB3	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD23	1:112:A:ASN:HB2	2	0.2	0.02	0.2
(1,820)	1:110:A:LEU:HD23	1:112:A:ASN:HB3	2	0.2	0.02	0.2
(1,123)	1:17:A:THR:HA	1:24:A:GLU:HA	2	0.2	0.02	0.2
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG21	2	0.2	0.01	0.2
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG22	2	0.2	0.01	0.2
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG23	2	0.2	0.01	0.2
(1,322)	1:43:A:LEU:HD11	1:44:A:ASP:H	2	0.2	0.02	0.2
(1,322)	1:43:A:LEU:HD12	1:44:A:ASP:H	2	0.2	0.02	0.2
(1,322)	1:43:A:LEU:HD13	1:44:A:ASP:H	2	0.2	0.02	0.2
(1,322)	1:43:A:LEU:HD21	1:44:A:ASP:H	2	0.2	0.02	0.2
(1,322)	1:43:A:LEU:HD22	1:44:A:ASP:H	2	0.2	0.02	0.2
(1,322)	1:43:A:LEU:HD23	1:44:A:ASP:H	2	0.2	0.02	0.2
(1,706)	1:94:A:ARG:H	1:95:A:GLY:H	2	0.2	0.01	0.2
(3,96)	1:129:A:TYR:O	1:133:A:GLY:H	2	0.2	0.05	0.2
(1,1220)	1:172:A:GLY:HA2	1:175:A:ALA:HA	2	0.19	0.09	0.19
(1,1220)	1:172:A:GLY:HA3	1:175:A:ALA:HA	2	0.19	0.09	0.19
(1,126)	1:17:A:THR:HB	1:24:A:GLU:HG2	2	0.18	0.04	0.18
(1,126)	1:17:A:THR:HB	1:24:A:GLU:HG3	2	0.18	0.04	0.18
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD11	2	0.18	0.04	0.18
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD12	2	0.18	0.04	0.18
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD13	2	0.18	0.04	0.18
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD21	2	0.18	0.04	0.18
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD22	2	0.18	0.04	0.18
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD23	2	0.18	0.04	0.18
(1,102)	1:15:A:GLU:HG2	1:18:A:ARG:HD2	2	0.18	0.03	0.18
(1,102)	1:15:A:GLU:HG2	1:18:A:ARG:HD3	2	0.18	0.03	0.18
(1,102)	1:15:A:GLU:HG3	1:18:A:ARG:HD2	2	0.18	0.03	0.18
(1,102)	1:15:A:GLU:HG3	1:18:A:ARG:HD3	2	0.18	0.03	0.18
(1,1139)	1:157:A:ASP:HB2	1:164:A:LEU:HB2	2	0.18	0.06	0.18
(1,1139)	1:157:A:ASP:HB2	1:164:A:LEU:HB3	2	0.18	0.06	0.18
(1,1139)	1:157:A:ASP:HB3	1:164:A:LEU:HB2	2	0.18	0.06	0.18
(1,1139)	1:157:A:ASP:HB3	1:164:A:LEU:HB3	2	0.18	0.06	0.18
(1,1100)	1:153:A:PHE:HD1	1:157:A:ASP:HB2	2	0.17	0.01	0.17
(1,1100)	1:153:A:PHE:HD1	1:157:A:ASP:HB3	2	0.17	0.01	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1100)	1:153:A:PHE:HD2	1:157:A:ASP:HB2	2	0.17	0.01	0.17
(1,1100)	1:153:A:PHE:HD2	1:157:A:ASP:HB3	2	0.17	0.01	0.17
(1,64)	1:12:A:VAL:HG21	1:15:A:GLU:HG2	2	0.16	0.04	0.16
(1,64)	1:12:A:VAL:HG21	1:15:A:GLU:HG3	2	0.16	0.04	0.16
(1,64)	1:12:A:VAL:HG22	1:15:A:GLU:HG2	2	0.16	0.04	0.16
(1,64)	1:12:A:VAL:HG22	1:15:A:GLU:HG3	2	0.16	0.04	0.16
(1,64)	1:12:A:VAL:HG23	1:15:A:GLU:HG2	2	0.16	0.04	0.16
(1,64)	1:12:A:VAL:HG23	1:15:A:GLU:HG3	2	0.16	0.04	0.16
(1,491)	1:63:A:LYS:HB2	1:67:A:PHE:H	2	0.16	0.06	0.16
(1,491)	1:63:A:LYS:HB3	1:67:A:PHE:H	2	0.16	0.06	0.16
(1,1034)	1:144:A:THR:HG21	1:146:A:GLU:H	2	0.16	0.02	0.16
(1,1034)	1:144:A:THR:HG22	1:146:A:GLU:H	2	0.16	0.02	0.16
(1,1034)	1:144:A:THR:HG23	1:146:A:GLU:H	2	0.16	0.02	0.16
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG11	2	0.16	0.04	0.16
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG12	2	0.16	0.04	0.16
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG13	2	0.16	0.04	0.16
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG21	2	0.16	0.04	0.16
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG22	2	0.16	0.04	0.16
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG23	2	0.16	0.04	0.16
(1,420)	1:51:A:ILE:HD11	1:85:A:PHE:HB2	2	0.16	0.02	0.16
(1,420)	1:51:A:ILE:HD11	1:85:A:PHE:HB3	2	0.16	0.02	0.16
(1,420)	1:51:A:ILE:HD12	1:85:A:PHE:HB2	2	0.16	0.02	0.16
(1,420)	1:51:A:ILE:HD12	1:85:A:PHE:HB3	2	0.16	0.02	0.16
(1,420)	1:51:A:ILE:HD13	1:85:A:PHE:HB2	2	0.16	0.02	0.16
(1,420)	1:51:A:ILE:HD13	1:85:A:PHE:HB3	2	0.16	0.02	0.16
(2,4)	1:79:A:ARG:O	2:600:A:CA:CA	2	0.16	0.02	0.16
(1,853)	1:115:A:TYR:HD1	1:165:A:THR:HB	2	0.16	0.04	0.16
(1,853)	1:115:A:TYR:HD2	1:165:A:THR:HB	2	0.16	0.04	0.16
(1,816)	1:110:A:LEU:HB2	1:111:A:ASP:H	2	0.15	0.0	0.15
(1,816)	1:110:A:LEU:HB3	1:111:A:ASP:H	2	0.15	0.0	0.15
(1,927)	1:122:A:LEU:HD11	1:146:A:GLU:HG2	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD11	1:146:A:GLU:HG3	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD12	1:146:A:GLU:HG2	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD12	1:146:A:GLU:HG3	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD13	1:146:A:GLU:HG2	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD13	1:146:A:GLU:HG3	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD21	1:146:A:GLU:HG2	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD21	1:146:A:GLU:HG3	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD22	1:146:A:GLU:HG2	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD22	1:146:A:GLU:HG3	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD23	1:146:A:GLU:HG2	2	0.15	0.02	0.15
(1,927)	1:122:A:LEU:HD23	1:146:A:GLU:HG3	2	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,145)	1:20:A:THR:H	1:21:A:TYR:H	2	0.14	0.03	0.14
(1,160)	1:21:A:TYR:HA	1:22:A:PHE:H	2	0.14	0.01	0.14
(1,199)	1:24:A:GLU:HB2	1:27:A:VAL:H	2	0.14	0.0	0.14
(1,199)	1:24:A:GLU:HB3	1:27:A:VAL:H	2	0.14	0.0	0.14
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG21	2	0.14	0.01	0.14
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG22	2	0.14	0.01	0.14
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG23	2	0.14	0.01	0.14
(3,57)	1:85:A:PHE:O	1:89:A:LEU:H	2	0.14	0.03	0.14
(3,95)	1:128:A:ILE:O	1:132:A:VAL:H	2	0.14	0.03	0.14
(3,103)	1:152:A:ILE:O	1:156:A:MET:N	2	0.14	0.03	0.14
(1,367)	1:47:A:GLY:HA2	1:51:A:ILE:HG12	2	0.14	0.01	0.14
(1,367)	1:47:A:GLY:HA2	1:51:A:ILE:HG13	2	0.14	0.01	0.14
(1,367)	1:47:A:GLY:HA3	1:51:A:ILE:HG12	2	0.14	0.01	0.14
(1,367)	1:47:A:GLY:HA3	1:51:A:ILE:HG13	2	0.14	0.01	0.14
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD11	2	0.14	0.02	0.14
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD12	2	0.14	0.02	0.14
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD13	2	0.14	0.02	0.14
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD21	2	0.14	0.02	0.14
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD22	2	0.14	0.02	0.14
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD23	2	0.14	0.02	0.14
(3,50)	1:85:A:PHE:O	1:89:A:LEU:N	2	0.14	0.02	0.14
(3,83)	1:125:A:VAL:O	1:129:A:TYR:N	2	0.14	0.02	0.14
(1,192)	1:23:A:THR:HG21	1:24:A:GLU:HB2	2	0.13	0.01	0.13
(1,192)	1:23:A:THR:HG21	1:24:A:GLU:HB3	2	0.13	0.01	0.13
(1,192)	1:23:A:THR:HG22	1:24:A:GLU:HB2	2	0.13	0.01	0.13
(1,192)	1:23:A:THR:HG22	1:24:A:GLU:HB3	2	0.13	0.01	0.13
(1,192)	1:23:A:THR:HG23	1:24:A:GLU:HB2	2	0.13	0.01	0.13
(1,192)	1:23:A:THR:HG23	1:24:A:GLU:HB3	2	0.13	0.01	0.13
(1,306)	1:42:A:GLN:HA	1:81:A:GLU:H	2	0.13	0.01	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG11	2	0.13	0.0	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG12	2	0.13	0.0	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG13	2	0.13	0.0	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG21	2	0.13	0.0	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG22	2	0.13	0.0	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG23	2	0.13	0.0	0.13
(3,43)	1:65:A:ALA:O	1:69:A:PHE:H	2	0.13	0.03	0.13
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG21	2	0.12	0.01	0.12
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG22	2	0.12	0.01	0.12
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG23	2	0.12	0.01	0.12
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG21	2	0.12	0.01	0.12
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG22	2	0.12	0.01	0.12
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG23	2	0.12	0.01	0.12

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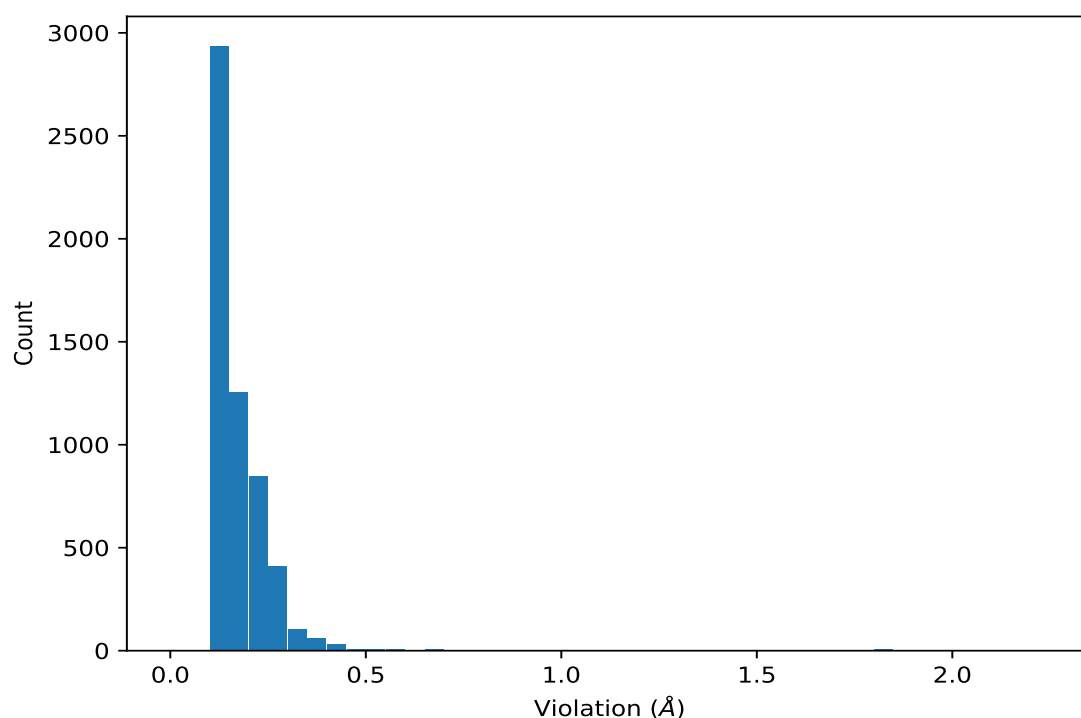
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG21	2	0.12	0.01	0.12
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG22	2	0.12	0.01	0.12
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG23	2	0.12	0.01	0.12
(1,193)	1:24:A:GLU:H	1:24:A:GLU:HG2	2	0.12	0.02	0.12
(1,193)	1:24:A:GLU:H	1:24:A:GLU:HG3	2	0.12	0.02	0.12
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD11	2	0.12	0.01	0.12
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD12	2	0.12	0.01	0.12
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD13	2	0.12	0.01	0.12
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD11	2	0.12	0.01	0.12
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD12	2	0.12	0.01	0.12
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD13	2	0.12	0.01	0.12
(3,25)	1:50:A:LYS:O	1:54:A:GLN:N	2	0.12	0.02	0.12
(1,865)	1:116:A:ILE:HB	1:164:A:LEU:HA	2	0.12	0.01	0.12
(2,2)	1:75:A:ASN:OD1	2:600:A:CA:CA	2	0.12	0.01	0.12
(3,23)	1:48:A:PHE:O	1:52:A:TYR:N	2	0.12	0.01	0.12
(1,65)	1:12:A:VAL:HG21	1:16:A:LEU:H	2	0.12	0.02	0.12
(1,65)	1:12:A:VAL:HG22	1:16:A:LEU:H	2	0.12	0.02	0.12
(1,65)	1:12:A:VAL:HG23	1:16:A:LEU:H	2	0.12	0.02	0.12
(1,83)	1:13:A:VAL:HG11	1:24:A:GLU:HA	2	0.12	0.02	0.12
(1,83)	1:13:A:VAL:HG12	1:24:A:GLU:HA	2	0.12	0.02	0.12
(1,83)	1:13:A:VAL:HG13	1:24:A:GLU:HA	2	0.12	0.02	0.12
(1,83)	1:13:A:VAL:HG21	1:24:A:GLU:HA	2	0.12	0.02	0.12
(1,83)	1:13:A:VAL:HG22	1:24:A:GLU:HA	2	0.12	0.02	0.12
(1,83)	1:13:A:VAL:HG23	1:24:A:GLU:HA	2	0.12	0.02	0.12
(1,557)	1:69:A:PHE:HD1	1:80:A:ILE:HA	2	0.12	0.02	0.12
(1,557)	1:69:A:PHE:HD2	1:80:A:ILE:HA	2	0.12	0.02	0.12
(2,14)	1:159:A:ASN:OD1	2:602:A:CA:CA	2	0.12	0.02	0.12
(3,74)	1:103:A:TRP:O	1:107:A:LEU:H	2	0.12	0.0	0.12
(1,1056)	1:149:A:VAL:HB	1:153:A:PHE:H	2	0.11	0.0	0.11
(3,5)	1:12:A:VAL:O	1:16:A:LEU:H	2	0.11	0.01	0.11
(3,58)	1:86:A:ILE:O	1:90:A:SER:H	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)
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	17	2.25
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	16	2.18
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	19	2.13
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	3	2.12
(2,9)	1:113:A:ASP:OD1	2:601:A:CA:CA	16	2.09
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	4	2.07
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	15	2.07
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	5	1.95
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	7	1.95
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	10	1.94
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	20	1.92
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	11	1.83
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	18	1.82
(2,9)	1:113:A:ASP:OD1	2:601:A:CA:CA	6	1.82
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	2	1.81
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	9	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	13	1.74
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	17	1.69
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	12	1.63
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	9	1.6
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	13	1.59
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	3	1.57
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	14	1.54
(2,7)	1:109:A:ASP:OD2	2:601:A:CA:CA	14	1.43
(2,7)	1:109:A:ASP:OD2	2:601:A:CA:CA	10	1.35
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	5	1.32
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	13	1.29
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	10	1.26
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	9	1.2
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	1	1.16
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	6	1.14
(2,13)	1:157:A:ASP:OD2	2:602:A:CA:CA	6	1.09
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	11	1.0
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	2	0.87
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	1	0.84
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	15	0.77
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	14	0.75
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	19	0.71
(2,15)	1:161:A:ASP:OD2	2:602:A:CA:CA	6	0.7
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD2	16	0.69
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD3	16	0.69
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	16	0.67
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	18	0.66
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	20	0.64
(2,9)	1:113:A:ASP:OD1	2:601:A:CA:CA	18	0.62
(2,9)	1:113:A:ASP:OD1	2:601:A:CA:CA	10	0.61
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	6	0.61
(2,9)	1:113:A:ASP:OD1	2:601:A:CA:CA	3	0.58
(2,1)	1:73:A:ASP:OD2	2:600:A:CA:CA	8	0.58
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	2	0.56
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	2	0.56
(2,15)	1:161:A:ASP:OD2	2:602:A:CA:CA	7	0.55
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD2	10	0.55
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD3	10	0.55
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD2	17	0.54
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD3	17	0.54
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD1	17	0.53
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD2	17	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:29:A:GLN:H	1:29:A:GLN:HG2	17	0.53
(1,225)	1:29:A:GLN:H	1:29:A:GLN:HG3	17	0.53
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	16	0.5
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	16	0.5
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	16	0.5
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	18	0.49
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	18	0.49
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	5	0.47
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	5	0.47
(1,147)	1:20:A:THR:HB	1:21:A:TYR:H	16	0.47
(1,45)	1:11:A:GLU:HA	1:12:A:VAL:HG21	1	0.45
(1,45)	1:11:A:GLU:HA	1:12:A:VAL:HG22	1	0.45
(1,45)	1:11:A:GLU:HA	1:12:A:VAL:HG23	1	0.45
(1,1021)	1:142:A:GLU:HG2	1:144:A:THR:H	19	0.44
(1,1021)	1:142:A:GLU:HG3	1:144:A:THR:H	19	0.44
(1,147)	1:20:A:THR:HB	1:21:A:TYR:H	7	0.44
(1,58)	1:12:A:VAL:HB	1:13:A:VAL:HA	1	0.44
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD1	4	0.43
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD2	4	0.43
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	17	0.43
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	17	0.43
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD11	15	0.42
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD12	15	0.42
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD13	15	0.42
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	13	0.42
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	13	0.42
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	13	0.41
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	13	0.41
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	13	0.41
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	13	0.41
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	13	0.41
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	13	0.41
(1,147)	1:20:A:THR:HB	1:21:A:TYR:H	13	0.41
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD2	6	0.4
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD3	6	0.4
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD2	18	0.4
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD3	18	0.4
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	12	0.4
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	12	0.4
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	19	0.4
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	19	0.4
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	1	0.4
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	1	0.4
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	1	0.4
(1,147)	1:20:A:THR:HB	1:21:A:TYR:H	12	0.4
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	4	0.39
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	4	0.39
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB2	11	0.39
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB3	11	0.39
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB2	11	0.39
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB3	11	0.39
(1,953)	1:125:A:VAL:HG11	1:129:A:TYR:H	14	0.38
(1,953)	1:125:A:VAL:HG12	1:129:A:TYR:H	14	0.38
(1,953)	1:125:A:VAL:HG13	1:129:A:TYR:H	14	0.38
(1,953)	1:125:A:VAL:HG21	1:129:A:TYR:H	14	0.38
(1,953)	1:125:A:VAL:HG22	1:129:A:TYR:H	14	0.38
(1,953)	1:125:A:VAL:HG23	1:129:A:TYR:H	14	0.38
(2,10)	1:115:A:TYR:O	2:601:A:CA:CA	10	0.37
(1,1021)	1:142:A:GLU:HG2	1:144:A:THR:H	20	0.37
(1,1021)	1:142:A:GLU:HG3	1:144:A:THR:H	20	0.37
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	20	0.37
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	20	0.37
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	20	0.37
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	2	0.37
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	2	0.37
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	2	0.37
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	14	0.37
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	14	0.37
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	14	0.37
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	14	0.37
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	14	0.37
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	14	0.37
(1,563)	1:71:A:VAL:H	1:71:A:VAL:HB	1	0.37
(1,283)	1:35:A:ILE:HA	1:35:A:ILE:HD11	14	0.37
(1,283)	1:35:A:ILE:HA	1:35:A:ILE:HD12	14	0.37
(1,283)	1:35:A:ILE:HA	1:35:A:ILE:HD13	14	0.37
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	1	0.36
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	16	0.36
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	16	0.36
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	4	0.36
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	4	0.36
(1,992)	1:136:A:VAL:H	1:136:A:VAL:HB	9	0.36
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	9	0.36
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	9	0.36
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	9	0.36
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	9	0.36
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	9	0.36
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	17	0.36
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	17	0.36
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	17	0.36
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	17	0.36
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	17	0.36
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	17	0.36
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	18	0.36
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	18	0.36
(1,117)	1:16:A:LEU:HD11	1:19:A:LYS:HA	17	0.36
(1,117)	1:16:A:LEU:HD12	1:19:A:LYS:HA	17	0.36
(1,117)	1:16:A:LEU:HD13	1:19:A:LYS:HA	17	0.36
(1,117)	1:16:A:LEU:HD21	1:19:A:LYS:HA	17	0.36
(1,117)	1:16:A:LEU:HD22	1:19:A:LYS:HA	17	0.36
(1,117)	1:16:A:LEU:HD23	1:19:A:LYS:HA	17	0.36
(1,15)	1:8:A:LEU:HG	1:31:A:TYR:HE1	12	0.36
(1,15)	1:8:A:LEU:HG	1:31:A:TYR:HE2	12	0.36
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	2	0.35
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	2	0.35
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	2	0.35
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	15	0.34
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD2	3	0.34
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD3	3	0.34
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	4	0.34
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	4	0.34
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	20	0.34
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	20	0.34
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	14	0.33
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	16	0.33
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	16	0.33
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	16	0.33
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	20	0.33
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	20	0.33
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	20	0.33
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	7	0.33
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	7	0.33
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	12	0.33
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	12	0.33
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	12	0.33
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	12	0.33
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	12	0.33
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	16	0.33
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	16	0.33
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	16	0.33
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	16	0.33
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	16	0.33
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	16	0.33
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	13	0.32
(1,1255)	1:176:A:ASP:HB2	1:179:A:ILE:HD11	6	0.32
(1,1255)	1:176:A:ASP:HB2	1:179:A:ILE:HD12	6	0.32
(1,1255)	1:176:A:ASP:HB2	1:179:A:ILE:HD13	6	0.32
(1,1255)	1:176:A:ASP:HB3	1:179:A:ILE:HD11	6	0.32
(1,1255)	1:176:A:ASP:HB3	1:179:A:ILE:HD12	6	0.32
(1,1255)	1:176:A:ASP:HB3	1:179:A:ILE:HD13	6	0.32
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD2	5	0.32
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD3	5	0.32
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	11	0.32
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	11	0.32
(1,953)	1:125:A:VAL:HG11	1:129:A:TYR:H	12	0.32
(1,953)	1:125:A:VAL:HG12	1:129:A:TYR:H	12	0.32
(1,953)	1:125:A:VAL:HG13	1:129:A:TYR:H	12	0.32
(1,953)	1:125:A:VAL:HG21	1:129:A:TYR:H	12	0.32
(1,953)	1:125:A:VAL:HG22	1:129:A:TYR:H	12	0.32
(1,953)	1:125:A:VAL:HG23	1:129:A:TYR:H	12	0.32
(1,822)	1:111:A:ASP:H	1:112:A:ASN:HA	10	0.32
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	15	0.32
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	15	0.32
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	15	0.32
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	3	0.32
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	3	0.32
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	3	0.32
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	3	0.32
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	3	0.32
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	3	0.32
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG2	14	0.32
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG3	14	0.32
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	10	0.31
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	11	0.31
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	2	0.31
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD11	8	0.31
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD12	8	0.31
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD13	8	0.31
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD21	8	0.31
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD22	8	0.31
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD23	8	0.31
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD11	8	0.31
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD12	8	0.31
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD13	8	0.31
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD21	8	0.31
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD22	8	0.31
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD23	8	0.31
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	6	0.31
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	6	0.31
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	6	0.31
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	6	0.31
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	18	0.31
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	18	0.31
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	18	0.31
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	18	0.31
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	11	0.31
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	11	0.31
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	11	0.31
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	11	0.31
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	11	0.31
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	11	0.31
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	15	0.31
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	15	0.31
(1,508)	1:65:A:ALA:HB1	1:68:A:VAL:HB	12	0.31
(1,508)	1:65:A:ALA:HB2	1:68:A:VAL:HB	12	0.31
(1,508)	1:65:A:ALA:HB3	1:68:A:VAL:HB	12	0.31
(1,164)	1:21:A:TYR:HD1	1:94:A:ARG:HG2	18	0.31
(1,164)	1:21:A:TYR:HD1	1:94:A:ARG:HG3	18	0.31
(1,164)	1:21:A:TYR:HD2	1:94:A:ARG:HG2	18	0.31
(1,164)	1:21:A:TYR:HD2	1:94:A:ARG:HG3	18	0.31
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	7	0.31
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	7	0.31
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	7	0.31
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	7	0.31
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	7	0.31
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	9	0.3
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	12	0.3
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	7	0.3
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	9	0.3
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	9	0.3
(1,1021)	1:142:A:GLU:HG2	1:144:A:THR:H	18	0.3
(1,1021)	1:142:A:GLU:HG3	1:144:A:THR:H	18	0.3
(1,945)	1:125:A:VAL:H	1:125:A:VAL:HB	14	0.3
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	19	0.3
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	19	0.3
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	19	0.3
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	19	0.3
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	20	0.3
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	20	0.3
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	20	0.3
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	20	0.3
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	20	0.3
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	20	0.3
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	16	0.3
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	16	0.3
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	16	0.3
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	16	0.3
(1,563)	1:71:A:VAL:H	1:71:A:VAL:HB	2	0.3
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	4	0.3
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	4	0.3
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	4	0.3
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	4	0.3
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	4	0.3
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	4	0.3
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	4	0.3
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	4	0.3
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	4	0.3
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	4	0.3
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	4	0.3
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	4	0.3
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	15	0.3
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	15	0.3
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	15	0.3
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	15	0.3
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	15	0.3
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	15	0.3
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG2	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG3	8	0.3
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	12	0.29
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	1	0.29
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	1	0.29
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	1	0.29
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	1	0.29
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	1	0.29
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	1	0.29
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	3	0.29
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	20	0.29
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	20	0.29
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG21	2	0.29
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG22	2	0.29
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG23	2	0.29
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG21	2	0.29
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG22	2	0.29
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG23	2	0.29
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG21	2	0.29
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG22	2	0.29
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG23	2	0.29
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG21	2	0.29
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG22	2	0.29
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG23	2	0.29
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG21	2	0.29
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG22	2	0.29
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG23	2	0.29
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG21	2	0.29
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG22	2	0.29
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG23	2	0.29
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	4	0.29
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	4	0.29
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	20	0.29
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	20	0.29
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	20	0.29
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	20	0.29
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	20	0.29
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	20	0.29
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	12	0.29
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	12	0.29
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	12	0.29
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	12	0.29
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	12	0.29
(1,531)	1:68:A:VAL:H	1:68:A:VAL:HB	11	0.29
(1,531)	1:68:A:VAL:H	1:68:A:VAL:HB	20	0.29
(1,50)	1:12:A:VAL:H	1:12:A:VAL:HB	9	0.29
(1,50)	1:12:A:VAL:H	1:12:A:VAL:HB	11	0.29
(3,112)	1:169:A:PHE:O	1:173:A:SER:N	6	0.28
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	20	0.28
(1,1292)	1:187:A:ASP:H	1:187:A:ASP:HB2	12	0.28
(1,1292)	1:187:A:ASP:H	1:187:A:ASP:HB3	12	0.28
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	19	0.28
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	19	0.28
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	19	0.28
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	19	0.28
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	19	0.28
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	19	0.28
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	20	0.28
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG11	6	0.28
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG12	6	0.28
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG13	6	0.28
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG21	6	0.28
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG22	6	0.28
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG23	6	0.28
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG11	6	0.28
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG12	6	0.28
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG13	6	0.28
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG21	6	0.28
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG22	6	0.28
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG23	6	0.28
(1,1222)	1:172:A:GLY:HA2	1:176:A:ASP:HB2	6	0.28
(1,1222)	1:172:A:GLY:HA2	1:176:A:ASP:HB3	6	0.28
(1,1222)	1:172:A:GLY:HA3	1:176:A:ASP:HB2	6	0.28
(1,1222)	1:172:A:GLY:HA3	1:176:A:ASP:HB3	6	0.28
(1,1220)	1:172:A:GLY:HA2	1:175:A:ALA:HA	6	0.28
(1,1220)	1:172:A:GLY:HA3	1:175:A:ALA:HA	6	0.28
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	18	0.28
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	18	0.28
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG21	3	0.28
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG22	3	0.28
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG23	3	0.28
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG21	3	0.28
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG22	3	0.28
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG23	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG21	3	0.28
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG22	3	0.28
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG23	3	0.28
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG21	3	0.28
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG22	3	0.28
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG23	3	0.28
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG21	3	0.28
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG22	3	0.28
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG23	3	0.28
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG21	3	0.28
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG22	3	0.28
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG23	3	0.28
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	12	0.28
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	6	0.28
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	3	0.28
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	3	0.28
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	3	0.28
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	3	0.28
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	13	0.28
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	13	0.28
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	13	0.28
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	13	0.28
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	1	0.28
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	1	0.28
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	1	0.28
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	1	0.28
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	1	0.28
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	1	0.28
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	15	0.28
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	15	0.28
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	15	0.28
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	15	0.28
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	15	0.28
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	15	0.28
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	7	0.28
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	7	0.28
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	7	0.28
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	7	0.28
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	7	0.28
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	7	0.28
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	16	0.28
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	20	0.28
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	20	0.28
(1,563)	1:71:A:VAL:H	1:71:A:VAL:HB	3	0.28
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	7	0.28
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	7	0.28
(1,531)	1:68:A:VAL:H	1:68:A:VAL:HB	12	0.28
(1,531)	1:68:A:VAL:H	1:68:A:VAL:HB	18	0.28
(1,510)	1:66:A:THR:H	1:66:A:THR:HB	3	0.28
(1,510)	1:66:A:THR:H	1:66:A:THR:HB	6	0.28
(1,510)	1:66:A:THR:H	1:66:A:THR:HB	7	0.28
(1,510)	1:66:A:THR:H	1:66:A:THR:HB	9	0.28
(1,510)	1:66:A:THR:H	1:66:A:THR:HB	11	0.28
(1,510)	1:66:A:THR:H	1:66:A:THR:HB	14	0.28
(1,510)	1:66:A:THR:H	1:66:A:THR:HB	18	0.28
(1,477)	1:62:A:THR:H	1:62:A:THR:HB	11	0.28
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	15	0.28
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	15	0.28
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	15	0.28
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	15	0.28
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	15	0.28
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	15	0.28
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	16	0.28
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	16	0.28
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	16	0.28
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	16	0.28
(1,50)	1:12:A:VAL:H	1:12:A:VAL:HB	5	0.28
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	19	0.27
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	5	0.27
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	5	0.27
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	5	0.27
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	5	0.27
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	5	0.27
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	5	0.27
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	13	0.27
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	13	0.27
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	13	0.27
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	13	0.27
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	13	0.27
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	13	0.27
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	19	0.27
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	19	0.27
(1,1104)	1:153:A:PHE:HE1	1:164:A:LEU:HG	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:153:A:PHE:HE2	1:164:A:LEU:HG	20	0.27
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD11	4	0.27
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD12	4	0.27
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD13	4	0.27
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD21	4	0.27
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD22	4	0.27
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD23	4	0.27
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD11	4	0.27
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD12	4	0.27
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD13	4	0.27
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD21	4	0.27
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD22	4	0.27
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD23	4	0.27
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	3	0.27
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	3	0.27
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	20	0.27
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	20	0.27
(1,953)	1:125:A:VAL:HG11	1:129:A:TYR:H	5	0.27
(1,953)	1:125:A:VAL:HG12	1:129:A:TYR:H	5	0.27
(1,953)	1:125:A:VAL:HG13	1:129:A:TYR:H	5	0.27
(1,953)	1:125:A:VAL:HG21	1:129:A:TYR:H	5	0.27
(1,953)	1:125:A:VAL:HG22	1:129:A:TYR:H	5	0.27
(1,953)	1:125:A:VAL:HG23	1:129:A:TYR:H	5	0.27
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	19	0.27
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	19	0.27
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	8	0.27
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	8	0.27
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	15	0.27
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	15	0.27
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	15	0.27
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	15	0.27
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	11	0.27
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	11	0.27
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG11	15	0.27
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG12	15	0.27
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG13	15	0.27
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG21	15	0.27
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG22	15	0.27
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG23	15	0.27
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG11	15	0.27
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG12	15	0.27
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG13	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG21	15	0.27
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG22	15	0.27
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG23	15	0.27
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	20	0.26
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	14	0.26
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	14	0.26
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	14	0.26
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	14	0.26
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	14	0.26
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	14	0.26
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	6	0.26
(1,1167)	1:164:A:LEU:H	1:165:A:THR:HA	17	0.26
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	15	0.26
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	15	0.26
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	14	0.26
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	14	0.26
(1,945)	1:125:A:VAL:H	1:125:A:VAL:HB	12	0.26
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	14	0.26
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	14	0.26
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	14	0.26
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	9	0.26
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	9	0.26
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	4	0.26
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	4	0.26
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	4	0.26
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD2	1	0.26
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD3	1	0.26
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD2	1	0.26
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD3	1	0.26
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD11	1	0.26
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD12	1	0.26
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD13	1	0.26
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD21	1	0.26
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD22	1	0.26
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD23	1	0.26
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD11	1	0.26
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD12	1	0.26
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD13	1	0.26
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD21	1	0.26
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD22	1	0.26
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD23	1	0.26
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	8	0.26
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	8	0.26
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	8	0.26
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	8	0.26
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	8	0.26
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	8	0.26
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	8	0.26
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	8	0.26
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	8	0.26
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	8	0.26
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	8	0.26
(1,684)	1:91:A:VAL:H	1:91:A:VAL:HB	19	0.26
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	19	0.26
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	19	0.26
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD11	10	0.26
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD12	10	0.26
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD13	10	0.26
(1,508)	1:65:A:ALA:HB1	1:68:A:VAL:HB	18	0.26
(1,508)	1:65:A:ALA:HB2	1:68:A:VAL:HB	18	0.26
(1,508)	1:65:A:ALA:HB3	1:68:A:VAL:HB	18	0.26
(1,447)	1:54:A:GLN:HA	1:55:A:PHE:HD1	14	0.26
(1,447)	1:54:A:GLN:HA	1:55:A:PHE:HD2	14	0.26
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	17	0.26
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	2	0.26
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	11	0.26
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	11	0.26
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	11	0.26
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	11	0.26
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	11	0.26
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	11	0.26
(1,150)	1:20:A:THR:HG21	1:22:A:PHE:H	6	0.26
(1,150)	1:20:A:THR:HG22	1:22:A:PHE:H	6	0.26
(1,150)	1:20:A:THR:HG23	1:22:A:PHE:H	6	0.26
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	15	0.26
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	15	0.26
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	15	0.26
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	15	0.26
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	15	0.26
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	15	0.26
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	7	0.26
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	7	0.26
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:12:A:VAL:H	1:12:A:VAL:HB	2	0.26
(1,32)	1:9:A:LYS:H	1:9:A:LYS:HB2	5	0.26
(1,32)	1:9:A:LYS:H	1:9:A:LYS:HB3	5	0.26
(3,96)	1:129:A:TYR:O	1:133:A:GLY:H	18	0.25
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	16	0.25
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	14	0.25
(1,1241)	1:174:A:LYS:HA	1:175:A:ALA:H	6	0.25
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE1	9	0.25
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE2	9	0.25
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE1	9	0.25
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE2	9	0.25
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE1	9	0.25
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE2	9	0.25
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE1	9	0.25
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE2	9	0.25
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE1	9	0.25
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE2	9	0.25
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE1	9	0.25
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE2	9	0.25
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	9	0.25
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	9	0.25
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	9	0.25
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	9	0.25
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	9	0.25
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	9	0.25
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	8	0.25
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	8	0.25
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	3	0.25
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	3	0.25
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	6	0.25
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	6	0.25
(1,1017)	1:142:A:GLU:H	1:143:A:ASN:H	16	0.25
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	8	0.25
(1,987)	1:135:A:THR:HB	1:136:A:VAL:HG11	15	0.25
(1,987)	1:135:A:THR:HB	1:136:A:VAL:HG12	15	0.25
(1,987)	1:135:A:THR:HB	1:136:A:VAL:HG13	15	0.25
(1,987)	1:135:A:THR:HB	1:136:A:VAL:HG21	15	0.25
(1,987)	1:135:A:THR:HB	1:136:A:VAL:HG22	15	0.25
(1,987)	1:135:A:THR:HB	1:136:A:VAL:HG23	15	0.25
(1,945)	1:125:A:VAL:H	1:125:A:VAL:HB	5	0.25
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	8	0.25
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	8	0.25
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	2	0.25
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	2	0.25
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	2	0.25
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	2	0.25
(1,825)	1:112:A:ASN:HA	1:113:A:ASP:H	8	0.25
(1,825)	1:112:A:ASN:HA	1:113:A:ASP:H	10	0.25
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	20	0.25
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	20	0.25
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	6	0.25
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	6	0.25
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	6	0.25
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	2	0.25
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	2	0.25
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	7	0.25
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	7	0.25
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	7	0.25
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	7	0.25
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	7	0.25
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	7	0.25
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	7	0.25
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	7	0.25
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	7	0.25
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	7	0.25
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	7	0.25
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	7	0.25
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	19	0.25
(1,147)	1:20:A:THR:HB	1:21:A:TYR:H	17	0.25
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	1	0.25
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	1	0.25
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	1	0.25
(1,50)	1:12:A:VAL:H	1:12:A:VAL:HB	4	0.25
(1,50)	1:12:A:VAL:H	1:12:A:VAL:HB	20	0.25
(3,102)	1:151:A:ARG:O	1:155:A:MET:N	11	0.24
(3,94)	1:127:A:ALA:O	1:131:A:MET:H	3	0.24
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	9	0.24
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	9	0.24
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	9	0.24
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	9	0.24
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	9	0.24
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	9	0.24
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG11	2	0.24
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG12	2	0.24
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG13	2	0.24
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG21	2	0.24
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG22	2	0.24
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG23	2	0.24
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG11	2	0.24
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG12	2	0.24
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG13	2	0.24
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG21	2	0.24
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG22	2	0.24
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG23	2	0.24
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	15	0.24
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	2	0.24
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	2	0.24
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	3	0.24
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	3	0.24
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	6	0.24
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	6	0.24
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	10	0.24
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	10	0.24
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG21	11	0.24
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG22	11	0.24
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG23	11	0.24
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG21	11	0.24
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG22	11	0.24
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG23	11	0.24
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG21	11	0.24
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG22	11	0.24
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG23	11	0.24
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG21	11	0.24
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG22	11	0.24
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG23	11	0.24
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG21	11	0.24
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG22	11	0.24
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG23	11	0.24
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG21	11	0.24
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG22	11	0.24
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG23	11	0.24
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	14	0.24
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	14	0.24
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	17	0.24
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	17	0.24
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	16	0.24
(1,895)	1:118:A:ARG:H	1:118:A:ARG:HD2	11	0.24
(1,895)	1:118:A:ARG:H	1:118:A:ARG:HD3	11	0.24
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	19	0.24
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	19	0.24
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	11	0.24
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	11	0.24
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	11	0.24
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	4	0.24
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	4	0.24
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	4	0.24
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	4	0.24
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	14	0.24
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	14	0.24
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	14	0.24
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	14	0.24
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	14	0.24
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	14	0.24
(1,825)	1:112:A:ASN:HA	1:113:A:ASP:H	13	0.24
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB1	6	0.24
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB2	6	0.24
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB3	6	0.24
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD11	15	0.24
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD12	15	0.24
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD13	15	0.24
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	15	0.24
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	15	0.24
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	15	0.24
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	15	0.24
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	15	0.24
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	15	0.24
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	15	0.24
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	15	0.24
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	15	0.24
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	15	0.24
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	15	0.24
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	15	0.24
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	9	0.24
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD11	5	0.24
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD12	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD13	5	0.24
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD11	12	0.24
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD12	12	0.24
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD13	12	0.24
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD21	12	0.24
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD22	12	0.24
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD23	12	0.24
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD11	12	0.24
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD12	12	0.24
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD13	12	0.24
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD21	12	0.24
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD22	12	0.24
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD23	12	0.24
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD11	12	0.24
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD12	12	0.24
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD13	12	0.24
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD21	12	0.24
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD22	12	0.24
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD23	12	0.24
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD11	12	0.24
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD12	12	0.24
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD13	12	0.24
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD21	12	0.24
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD22	12	0.24
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD23	12	0.24
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD11	12	0.24
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD12	12	0.24
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD13	12	0.24
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD21	12	0.24
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD22	12	0.24
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD23	12	0.24
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD11	12	0.24
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD12	12	0.24
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD13	12	0.24
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD21	12	0.24
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD22	12	0.24
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD23	12	0.24
(1,14)	1:8:A:LEU:HG	1:31:A:TYR:HB2	12	0.24
(1,14)	1:8:A:LEU:HG	1:31:A:TYR:HB3	12	0.24
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	5	0.23
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	12	0.23
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	13	0.23
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	2	0.23
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	2	0.23
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	2	0.23
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	2	0.23
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	2	0.23
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	2	0.23
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	3	0.23
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	3	0.23
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	12	0.23
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	12	0.23
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	12	0.23
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	12	0.23
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	12	0.23
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	12	0.23
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	12	0.23
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	12	0.23
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	17	0.23
(1,1139)	1:157:A:ASP:HB2	1:164:A:LEU:HB2	11	0.23
(1,1139)	1:157:A:ASP:HB2	1:164:A:LEU:HB3	11	0.23
(1,1139)	1:157:A:ASP:HB3	1:164:A:LEU:HB2	11	0.23
(1,1139)	1:157:A:ASP:HB3	1:164:A:LEU:HB3	11	0.23
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	20	0.23
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	20	0.23
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	16	0.23
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	16	0.23
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	2	0.23
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	2	0.23
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	6	0.23
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	6	0.23
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	1	0.23
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	2	0.23
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	3	0.23
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	15	0.23
(1,922)	1:122:A:LEU:HB2	1:149:A:VAL:HG11	10	0.23
(1,922)	1:122:A:LEU:HB2	1:149:A:VAL:HG12	10	0.23
(1,922)	1:122:A:LEU:HB2	1:149:A:VAL:HG13	10	0.23
(1,922)	1:122:A:LEU:HB2	1:149:A:VAL:HG21	10	0.23
(1,922)	1:122:A:LEU:HB2	1:149:A:VAL:HG22	10	0.23
(1,922)	1:122:A:LEU:HB2	1:149:A:VAL:HG23	10	0.23
(1,922)	1:122:A:LEU:HB3	1:149:A:VAL:HG11	10	0.23
(1,922)	1:122:A:LEU:HB3	1:149:A:VAL:HG12	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:122:A:LEU:HB3	1:149:A:VAL:HG13	10	0.23
(1,922)	1:122:A:LEU:HB3	1:149:A:VAL:HG21	10	0.23
(1,922)	1:122:A:LEU:HB3	1:149:A:VAL:HG22	10	0.23
(1,922)	1:122:A:LEU:HB3	1:149:A:VAL:HG23	10	0.23
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	20	0.23
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	20	0.23
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	3	0.23
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	3	0.23
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	3	0.23
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	14	0.23
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	14	0.23
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	14	0.23
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	14	0.23
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	14	0.23
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	14	0.23
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB2	19	0.23
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB3	19	0.23
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB2	19	0.23
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB3	19	0.23
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	11	0.23
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	11	0.23
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	11	0.23
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	11	0.23
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	11	0.23
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	9	0.23
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	9	0.23
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	14	0.23
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	14	0.23
(1,491)	1:63:A:LYS:HB2	1:67:A:PHE:H	16	0.23
(1,491)	1:63:A:LYS:HB3	1:67:A:PHE:H	16	0.23
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	11	0.23
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	11	0.23
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	11	0.23
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	11	0.23
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	11	0.23
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	11	0.23
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	19	0.23
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	19	0.23
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	19	0.23
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	19	0.23
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	19	0.23
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	19	0.23
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	19	0.23
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	19	0.23
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	19	0.23
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	19	0.23
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	19	0.23
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	13	0.23
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	13	0.23
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	13	0.23
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	13	0.23
(1,229)	1:30:A:TRP:H	1:30:A:TRP:HD1	12	0.23
(1,195)	1:24:A:GLU:H	1:25:A:LYS:HD2	10	0.23
(1,195)	1:24:A:GLU:H	1:25:A:LYS:HD3	10	0.23
(1,150)	1:20:A:THR:HG21	1:22:A:PHE:H	7	0.23
(1,150)	1:20:A:THR:HG22	1:22:A:PHE:H	7	0.23
(1,150)	1:20:A:THR:HG23	1:22:A:PHE:H	7	0.23
(1,147)	1:20:A:THR:HB	1:21:A:TYR:H	6	0.23
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG2	10	0.23
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG3	10	0.23
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG2	10	0.23
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG3	10	0.23
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG2	10	0.23
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG3	10	0.23
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG2	10	0.23
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG3	10	0.23
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG2	10	0.23
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG3	10	0.23
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG2	10	0.23
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG3	10	0.23
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	14	0.23
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	14	0.23
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	14	0.23
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG2	2	0.23
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG3	2	0.23
(3,102)	1:151:A:ARG:O	1:155:A:MET:N	16	0.22
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	12	0.22
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	17	0.22
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	17	0.22
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	17	0.22
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	17	0.22
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	17	0.22
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	14	0.22
(1,1172)	1:164:A:LEU:HG	1:165:A:THR:H	8	0.22
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	3	0.22
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	7	0.22
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	19	0.22
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	15	0.22
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	15	0.22
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD11	19	0.22
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD12	19	0.22
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD13	19	0.22
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD21	19	0.22
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD22	19	0.22
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD23	19	0.22
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	19	0.22
(1,945)	1:125:A:VAL:H	1:125:A:VAL:HB	8	0.22
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	3	0.22
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	3	0.22
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	3	0.22
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD2	12	0.22
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD3	12	0.22
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD2	12	0.22
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD3	12	0.22
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	19	0.22
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	19	0.22
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	19	0.22
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	19	0.22
(1,820)	1:110:A:LEU:HD11	1:112:A:ASN:HB2	9	0.22
(1,820)	1:110:A:LEU:HD11	1:112:A:ASN:HB3	9	0.22
(1,820)	1:110:A:LEU:HD12	1:112:A:ASN:HB2	9	0.22
(1,820)	1:110:A:LEU:HD12	1:112:A:ASN:HB3	9	0.22
(1,820)	1:110:A:LEU:HD13	1:112:A:ASN:HB2	9	0.22
(1,820)	1:110:A:LEU:HD13	1:112:A:ASN:HB3	9	0.22
(1,820)	1:110:A:LEU:HD21	1:112:A:ASN:HB2	9	0.22
(1,820)	1:110:A:LEU:HD21	1:112:A:ASN:HB3	9	0.22
(1,820)	1:110:A:LEU:HD22	1:112:A:ASN:HB2	9	0.22
(1,820)	1:110:A:LEU:HD22	1:112:A:ASN:HB3	9	0.22
(1,820)	1:110:A:LEU:HD23	1:112:A:ASN:HB2	9	0.22
(1,820)	1:110:A:LEU:HD23	1:112:A:ASN:HB3	9	0.22
(1,800)	1:109:A:ASP:HA	1:116:A:ILE:HA	3	0.22
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	10	0.22
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	10	0.22
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	10	0.22
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	11	0.22
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	11	0.22
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	11	0.22
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	11	0.22
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	18	0.22
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	18	0.22
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	18	0.22
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	18	0.22
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	3	0.22
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	3	0.22
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	3	0.22
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	3	0.22
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	3	0.22
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	3	0.22
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	3	0.22
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	3	0.22
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	3	0.22
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	3	0.22
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	3	0.22
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	3	0.22
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	2	0.22
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	2	0.22
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	2	0.22
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	2	0.22
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	2	0.22
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	20	0.22
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	20	0.22
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	20	0.22
(1,605)	1:77:A:ASP:HA	1:78:A:GLY:H	9	0.22
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	20	0.22
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	20	0.22
(1,508)	1:65:A:ALA:HB1	1:68:A:VAL:HB	11	0.22
(1,508)	1:65:A:ALA:HB2	1:68:A:VAL:HB	11	0.22
(1,508)	1:65:A:ALA:HB3	1:68:A:VAL:HB	11	0.22
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	4	0.22
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	4	0.22
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	4	0.22
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	4	0.22
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	7	0.22
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	7	0.22
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	7	0.22
(1,424)	1:52:A:TYR:HA	1:55:A:PHE:HD1	12	0.22
(1,424)	1:52:A:TYR:HA	1:55:A:PHE:HD2	12	0.22
(1,424)	1:52:A:TYR:HA	1:55:A:PHE:HD1	15	0.22
(1,424)	1:52:A:TYR:HA	1:55:A:PHE:HD2	15	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG11	3	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG12	3	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG13	3	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG21	3	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG22	3	0.22
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG23	3	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG11	3	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG12	3	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG13	3	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG21	3	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG22	3	0.22
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG23	3	0.22
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	13	0.22
(1,322)	1:43:A:LEU:HD11	1:44:A:ASP:H	14	0.22
(1,322)	1:43:A:LEU:HD12	1:44:A:ASP:H	14	0.22
(1,322)	1:43:A:LEU:HD13	1:44:A:ASP:H	14	0.22
(1,322)	1:43:A:LEU:HD21	1:44:A:ASP:H	14	0.22
(1,322)	1:43:A:LEU:HD22	1:44:A:ASP:H	14	0.22
(1,322)	1:43:A:LEU:HD23	1:44:A:ASP:H	14	0.22
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	6	0.22
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG11	10	0.22
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG12	10	0.22
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG13	10	0.22
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG21	10	0.22
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG22	10	0.22
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG23	10	0.22
(1,126)	1:17:A:THR:HB	1:24:A:GLU:HG2	18	0.22
(1,126)	1:17:A:THR:HB	1:24:A:GLU:HG3	18	0.22
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD11	17	0.22
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD12	17	0.22
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD13	17	0.22
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD21	17	0.22
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD22	17	0.22
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD23	17	0.22
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD11	17	0.22
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD12	17	0.22
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD13	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD21	17	0.22
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD22	17	0.22
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD23	17	0.22
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD11	17	0.22
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD12	17	0.22
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD13	17	0.22
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD21	17	0.22
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD22	17	0.22
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD23	17	0.22
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD11	17	0.22
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD12	17	0.22
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD13	17	0.22
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD21	17	0.22
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD22	17	0.22
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD23	17	0.22
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD11	17	0.22
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD12	17	0.22
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD13	17	0.22
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD21	17	0.22
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD22	17	0.22
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD23	17	0.22
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD11	17	0.22
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD12	17	0.22
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD13	17	0.22
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD21	17	0.22
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD22	17	0.22
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD23	17	0.22
(3,118)	1:170:A:GLN:O	1:174:A:LYS:H	6	0.21
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	7	0.21
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	19	0.21
(3,102)	1:151:A:ARG:O	1:155:A:MET:N	10	0.21
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	16	0.21
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	2	0.21
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	7	0.21
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	9	0.21
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	13	0.21
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	17	0.21
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	16	0.21
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	16	0.21
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	16	0.21
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	16	0.21
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	16	0.21
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD11	11	0.21
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD12	11	0.21
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD13	11	0.21
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD21	11	0.21
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD22	11	0.21
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD23	11	0.21
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD11	11	0.21
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD12	11	0.21
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD13	11	0.21
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD21	11	0.21
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD22	11	0.21
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD23	11	0.21
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD11	11	0.21
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD12	11	0.21
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD13	11	0.21
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD21	11	0.21
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD22	11	0.21
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD23	11	0.21
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD11	11	0.21
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD12	11	0.21
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD13	11	0.21
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD21	11	0.21
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD22	11	0.21
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD23	11	0.21
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD11	11	0.21
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD12	11	0.21
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD13	11	0.21
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD21	11	0.21
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD22	11	0.21
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD23	11	0.21
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD11	11	0.21
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD12	11	0.21
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD13	11	0.21
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD21	11	0.21
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD22	11	0.21
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD23	11	0.21
(1,1271)	1:180:A:VAL:H	1:180:A:VAL:HB	19	0.21
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	9	0.21
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	9	0.21
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	4	0.21
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	12	0.21
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	20	0.21
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	9	0.21
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	9	0.21
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	13	0.21
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	13	0.21
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	14	0.21
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	14	0.21
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	14	0.21
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	7	0.21
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	7	0.21
(1,1024)	1:143:A:ASN:H	1:183:A:LEU:HB2	16	0.21
(1,1024)	1:143:A:ASN:H	1:183:A:LEU:HB3	16	0.21
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB2	19	0.21
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB3	19	0.21
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB2	19	0.21
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB3	19	0.21
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB2	19	0.21
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB3	19	0.21
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB2	19	0.21
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB3	19	0.21
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB2	19	0.21
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB3	19	0.21
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB2	19	0.21
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB3	19	0.21
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	7	0.21
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	7	0.21
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	7	0.21
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	10	0.21
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	10	0.21
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	6	0.21
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	6	0.21
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	6	0.21
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	6	0.21
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	15	0.21
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	15	0.21
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	15	0.21
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	15	0.21
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	5	0.21
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	5	0.21
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	5	0.21
(1,800)	1:109:A:ASP:HA	1:116:A:ILE:HA	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	5	0.21
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	5	0.21
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	5	0.21
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	5	0.21
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	5	0.21
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	5	0.21
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	5	0.21
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	5	0.21
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	5	0.21
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	5	0.21
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	5	0.21
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	5	0.21
(1,726)	1:99:A:GLU:H	1:99:A:GLU:HG2	7	0.21
(1,726)	1:99:A:GLU:H	1:99:A:GLU:HG3	7	0.21
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	7	0.21
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	7	0.21
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD11	16	0.21
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD12	16	0.21
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD13	16	0.21
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD11	16	0.21
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD12	16	0.21
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD13	16	0.21
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	4	0.21
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	4	0.21
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	9	0.21
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	9	0.21
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	11	0.21
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	11	0.21
(1,508)	1:65:A:ALA:HB1	1:68:A:VAL:HB	20	0.21
(1,508)	1:65:A:ALA:HB2	1:68:A:VAL:HB	20	0.21
(1,508)	1:65:A:ALA:HB3	1:68:A:VAL:HB	20	0.21
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD11	6	0.21
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD12	6	0.21
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD13	6	0.21
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD11	6	0.21
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD12	6	0.21
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD13	6	0.21
(1,468)	1:58:A:PHE:HA	1:59:A:GLY:H	4	0.21
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	1	0.21
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	1	0.21
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	1	0.21
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:52:A:TYR:HA	1:55:A:PHE:HD1	13	0.21
(1,424)	1:52:A:TYR:HA	1:55:A:PHE:HD2	13	0.21
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	8	0.21
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	9	0.21
(1,277)	1:35:A:ILE:H	1:35:A:ILE:HB	14	0.21
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD11	14	0.21
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD12	14	0.21
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD13	14	0.21
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD2	6	0.21
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD3	6	0.21
(1,195)	1:24:A:GLU:H	1:25:A:LYS:HD2	17	0.21
(1,195)	1:24:A:GLU:H	1:25:A:LYS:HD3	17	0.21
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	13	0.21
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	13	0.21
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	13	0.21
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	15	0.21
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	15	0.21
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	15	0.21
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	7	0.21
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	7	0.21
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	7	0.21
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	7	0.21
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	7	0.21
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	7	0.21
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	7	0.21
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	7	0.21
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	7	0.21
(1,123)	1:17:A:THR:HA	1:24:A:GLU:HA	16	0.21
(1,102)	1:15:A:GLU:HG2	1:18:A:ARG:HD2	16	0.21
(1,102)	1:15:A:GLU:HG2	1:18:A:ARG:HD3	16	0.21
(1,102)	1:15:A:GLU:HG3	1:18:A:ARG:HD2	16	0.21
(1,102)	1:15:A:GLU:HG3	1:18:A:ARG:HD3	16	0.21
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG2	11	0.21
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG3	11	0.21
(1,70)	1:13:A:VAL:H	1:14:A:GLU:HG2	1	0.21
(1,70)	1:13:A:VAL:H	1:14:A:GLU:HG3	1	0.21
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	14	0.2
(3,100)	1:149:A:VAL:O	1:153:A:PHE:N	11	0.2
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	3	0.2
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	17	0.2
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	13	0.2
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:12:A:VAL:O	1:16:A:LEU:N	14	0.2
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	5	0.2
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	10	0.2
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	11	0.2
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	2	0.2
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	2	0.2
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	2	0.2
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	2	0.2
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	2	0.2
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	2	0.2
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE1	5	0.2
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE2	5	0.2
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE1	5	0.2
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE2	5	0.2
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE1	5	0.2
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE2	5	0.2
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE1	5	0.2
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE2	5	0.2
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE1	5	0.2
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE2	5	0.2
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE1	5	0.2
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE2	5	0.2
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	6	0.2
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	6	0.2
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	7	0.2
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	7	0.2
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	11	0.2
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	11	0.2
(1,1073)	1:152:A:ILE:H	1:152:A:ILE:HG12	11	0.2
(1,1073)	1:152:A:ILE:H	1:152:A:ILE:HG13	11	0.2
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG21	18	0.2
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG22	18	0.2
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG23	18	0.2
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG21	18	0.2
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG22	18	0.2
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG23	18	0.2
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG21	18	0.2
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG22	18	0.2
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG23	18	0.2
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG21	18	0.2
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG22	18	0.2
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG23	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG21	18	0.2
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG22	18	0.2
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG23	18	0.2
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG21	18	0.2
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG22	18	0.2
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG23	18	0.2
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD1	3	0.2
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD2	3	0.2
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	4	0.2
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	10	0.2
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	14	0.2
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	12	0.2
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	13	0.2
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB1	5	0.2
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB2	5	0.2
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB3	5	0.2
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB1	5	0.2
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB2	5	0.2
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB3	5	0.2
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB1	5	0.2
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB2	5	0.2
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB3	5	0.2
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	18	0.2
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	18	0.2
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	18	0.2
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG11	18	0.2
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG12	18	0.2
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG13	18	0.2
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG21	18	0.2
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG22	18	0.2
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG23	18	0.2
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG11	18	0.2
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG12	18	0.2
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG13	18	0.2
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG21	18	0.2
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG22	18	0.2
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG23	18	0.2
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG11	2	0.2
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG12	2	0.2
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG13	2	0.2
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG21	2	0.2
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG22	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG23	2	0.2
(1,895)	1:118:A:ARG:H	1:118:A:ARG:HD2	20	0.2
(1,895)	1:118:A:ARG:H	1:118:A:ARG:HD3	20	0.2
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	12	0.2
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	12	0.2
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	12	0.2
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	17	0.2
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	17	0.2
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	17	0.2
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	17	0.2
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	17	0.2
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	17	0.2
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB2	4	0.2
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB3	4	0.2
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB2	4	0.2
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB3	4	0.2
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	3	0.2
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	3	0.2
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	3	0.2
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	3	0.2
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	6	0.2
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	6	0.2
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	6	0.2
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	6	0.2
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	6	0.2
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	6	0.2
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	16	0.2
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	16	0.2
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	16	0.2
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	16	0.2
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	16	0.2
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	16	0.2
(1,823)	1:112:A:ASN:H	1:112:A:ASN:HA	10	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	1	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	1	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	1	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	3	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	3	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	3	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	8	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	8	0.2
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	13	0.2
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	13	0.2
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	13	0.2
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	13	0.2
(1,706)	1:94:A:ARG:H	1:95:A:GLY:H	12	0.2
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	9	0.2
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	9	0.2
(1,593)	1:75:A:ASN:H	1:76:A:LYS:H	12	0.2
(1,563)	1:71:A:VAL:H	1:71:A:VAL:HB	20	0.2
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	7	0.2
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	7	0.2
(1,475)	1:60:A:ASP:HA	1:62:A:THR:H	8	0.2
(1,468)	1:58:A:PHE:HA	1:59:A:GLY:H	19	0.2
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	16	0.2
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	3	0.2
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	3	0.2
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	3	0.2
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	3	0.2
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	16	0.2
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	16	0.2
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	16	0.2
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	16	0.2
(1,444)	1:53:A:LYS:HB2	1:57:A:PRO:HG2	15	0.2
(1,444)	1:53:A:LYS:HB2	1:57:A:PRO:HG3	15	0.2
(1,444)	1:53:A:LYS:HB3	1:57:A:PRO:HG2	15	0.2
(1,444)	1:53:A:LYS:HB3	1:57:A:PRO:HG3	15	0.2
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	5	0.2
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	5	0.2
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	5	0.2
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	5	0.2
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	5	0.2
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	5	0.2
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	5	0.2
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	5	0.2
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	5	0.2
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	5	0.2
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	5	0.2
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	5	0.2
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	16	0.2
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	16	0.2
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	16	0.2
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	16	0.2
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	16	0.2
(1,387)	1:48:A:PHE:HE1	1:80:A:ILE:HG12	9	0.2
(1,387)	1:48:A:PHE:HE1	1:80:A:ILE:HG13	9	0.2
(1,387)	1:48:A:PHE:HE2	1:80:A:ILE:HG12	9	0.2
(1,387)	1:48:A:PHE:HE2	1:80:A:ILE:HG13	9	0.2
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	16	0.2
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	16	0.2
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	16	0.2
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	16	0.2
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	16	0.2
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	16	0.2
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	16	0.2
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	16	0.2
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	16	0.2
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	16	0.2
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	16	0.2
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	16	0.2
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	4	0.2
(1,250)	1:31:A:TYR:HD1	1:86:A:ILE:HG12	2	0.2
(1,250)	1:31:A:TYR:HD1	1:86:A:ILE:HG13	2	0.2
(1,250)	1:31:A:TYR:HD2	1:86:A:ILE:HG12	2	0.2
(1,250)	1:31:A:TYR:HD2	1:86:A:ILE:HG13	2	0.2
(1,200)	1:24:A:GLU:HG2	1:25:A:LYS:HG2	6	0.2
(1,200)	1:24:A:GLU:HG2	1:25:A:LYS:HG3	6	0.2
(1,200)	1:24:A:GLU:HG3	1:25:A:LYS:HG2	6	0.2
(1,200)	1:24:A:GLU:HG3	1:25:A:LYS:HG3	6	0.2
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	2	0.2
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	2	0.2
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	2	0.2
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	4	0.2
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	4	0.2
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	4	0.2
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	12	0.2
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	12	0.2
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	12	0.2
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	16	0.2
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	16	0.2
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	16	0.2
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	4	0.2
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	4	0.2
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	4	0.2
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	4	0.2
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	4	0.2
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	4	0.2
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	4	0.2
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG21	15	0.2
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG22	15	0.2
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG23	15	0.2
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG11	17	0.2
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG12	17	0.2
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG13	17	0.2
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG21	17	0.2
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG22	17	0.2
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG23	17	0.2
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG2	17	0.2
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG3	17	0.2
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG2	17	0.2
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG3	17	0.2
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG2	17	0.2
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG3	17	0.2
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG2	17	0.2
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG3	17	0.2
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG2	17	0.2
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG3	17	0.2
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG2	17	0.2
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG3	17	0.2
(1,109)	1:16:A:LEU:HA	1:19:A:LYS:HB2	20	0.2
(1,109)	1:16:A:LEU:HA	1:19:A:LYS:HB3	20	0.2
(1,64)	1:12:A:VAL:HG21	1:15:A:GLU:HG2	11	0.2
(1,64)	1:12:A:VAL:HG21	1:15:A:GLU:HG3	11	0.2
(1,64)	1:12:A:VAL:HG22	1:15:A:GLU:HG2	11	0.2
(1,64)	1:12:A:VAL:HG22	1:15:A:GLU:HG3	11	0.2
(1,64)	1:12:A:VAL:HG23	1:15:A:GLU:HG2	11	0.2
(1,64)	1:12:A:VAL:HG23	1:15:A:GLU:HG3	11	0.2
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD1	13	0.2
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD2	13	0.2
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD1	13	0.2
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD2	13	0.2
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	11	0.19
(3,94)	1:127:A:ALA:O	1:131:A:MET:H	18	0.19
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	4	0.19
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,27)	1:52:A:TYR:O	1:56:A:PHE:N	11	0.19
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	6	0.19
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	8	0.19
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	15	0.19
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	16	0.19
(1,1241)	1:174:A:LYS:HA	1:175:A:ALA:H	8	0.19
(1,1208)	1:169:A:PHE:HA	1:179:A:ILE:HB	8	0.19
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	5	0.19
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	5	0.19
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD1	8	0.19
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD2	8	0.19
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	10	0.19
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	10	0.19
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	13	0.19
(1,1121)	1:155:A:MET:HG2	1:156:A:MET:HB2	14	0.19
(1,1121)	1:155:A:MET:HG2	1:156:A:MET:HB3	14	0.19
(1,1121)	1:155:A:MET:HG3	1:156:A:MET:HB2	14	0.19
(1,1121)	1:155:A:MET:HG3	1:156:A:MET:HB3	14	0.19
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	3	0.19
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	3	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG21	5	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG22	5	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG23	5	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG21	14	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG22	14	0.19
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG23	14	0.19
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	11	0.19
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	12	0.19
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	12	0.19
(1,924)	1:122:A:LEU:HD11	1:126:A:ASP:HA	12	0.19
(1,924)	1:122:A:LEU:HD12	1:126:A:ASP:HA	12	0.19
(1,924)	1:122:A:LEU:HD13	1:126:A:ASP:HA	12	0.19
(1,924)	1:122:A:LEU:HD21	1:126:A:ASP:HA	12	0.19
(1,924)	1:122:A:LEU:HD22	1:126:A:ASP:HA	12	0.19
(1,924)	1:122:A:LEU:HD23	1:126:A:ASP:HA	12	0.19
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	9	0.19
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	9	0.19
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	11	0.19
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	11	0.19
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	5	0.19
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	5	0.19
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	5	0.19
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	5	0.19
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	5	0.19
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD2	11	0.19
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD3	11	0.19
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD2	11	0.19
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD3	11	0.19
(1,853)	1:115:A:TYR:HD1	1:165:A:THR:HB	11	0.19
(1,853)	1:115:A:TYR:HD2	1:165:A:THR:HB	11	0.19
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	14	0.19
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	14	0.19
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	14	0.19
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	14	0.19
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	4	0.19
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	4	0.19
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	4	0.19
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	4	0.19
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	8	0.19
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	8	0.19
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	8	0.19
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	8	0.19
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	20	0.19
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	20	0.19
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	20	0.19
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	20	0.19
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	20	0.19
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	20	0.19
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	6	0.19
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	6	0.19
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	6	0.19
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	6	0.19
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	6	0.19
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	6	0.19
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	12	0.19
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	12	0.19
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	12	0.19
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	12	0.19
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	12	0.19
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	12	0.19
(1,800)	1:109:A:ASP:HA	1:116:A:ILE:HA	8	0.19
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	4	0.19
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	4	0.19
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	4	0.19
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	6	0.19
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	6	0.19
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	6	0.19
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	6	0.19
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	6	0.19
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	6	0.19
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	6	0.19
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	6	0.19
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	6	0.19
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	6	0.19
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	6	0.19
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	6	0.19
(1,772)	1:107:A:LEU:HG	1:124:A:ILE:HD11	14	0.19
(1,772)	1:107:A:LEU:HG	1:124:A:ILE:HD12	14	0.19
(1,772)	1:107:A:LEU:HG	1:124:A:ILE:HD13	14	0.19
(1,706)	1:94:A:ARG:H	1:95:A:GLY:H	18	0.19
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	17	0.19
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	17	0.19
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	14	0.19
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	14	0.19
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	15	0.19
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	15	0.19
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	11	0.19
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	11	0.19
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	11	0.19
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	18	0.19
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	18	0.19
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	18	0.19
(1,605)	1:77:A:ASP:HA	1:78:A:GLY:H	13	0.19
(1,599)	1:76:A:LYS:HA	1:77:A:ASP:H	12	0.19
(1,595)	1:75:A:ASN:HA	1:76:A:LYS:H	7	0.19
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	3	0.19
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	3	0.19
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	9	0.19
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	9	0.19
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB1	14	0.19
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB2	14	0.19
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB3	14	0.19
(1,555)	1:69:A:PHE:HB2	1:80:A:ILE:HG12	17	0.19
(1,555)	1:69:A:PHE:HB2	1:80:A:ILE:HG13	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:69:A:PHE:HB3	1:80:A:ILE:HG12	17	0.19
(1,555)	1:69:A:PHE:HB3	1:80:A:ILE:HG13	17	0.19
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	5	0.19
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	5	0.19
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	15	0.19
(1,463)	1:57:A:PRO:HD2	1:58:A:PHE:HA	2	0.19
(1,463)	1:57:A:PRO:HD3	1:58:A:PHE:HA	2	0.19
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	4	0.19
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	4	0.19
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	4	0.19
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	4	0.19
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	4	0.19
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	4	0.19
(1,399)	1:49:A:GLN:HB2	1:65:A:ALA:HA	11	0.19
(1,399)	1:49:A:GLN:HB3	1:65:A:ALA:HA	11	0.19
(1,399)	1:49:A:GLN:HB2	1:65:A:ALA:HA	13	0.19
(1,399)	1:49:A:GLN:HB3	1:65:A:ALA:HA	13	0.19
(1,258)	1:32:A:LYS:HA	1:35:A:ILE:HG12	4	0.19
(1,258)	1:32:A:LYS:HA	1:35:A:ILE:HG13	4	0.19
(1,229)	1:30:A:TRP:H	1:30:A:TRP:HD1	16	0.19
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD2	5	0.19
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD3	5	0.19
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	1	0.19
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	1	0.19
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	1	0.19
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	18	0.19
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	18	0.19
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	18	0.19
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	19	0.19
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	19	0.19
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	19	0.19
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	3	0.19
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	3	0.19
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	12	0.19
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	12	0.19
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	12	0.19
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	12	0.19
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	12	0.19
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	12	0.19
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG21	10	0.19
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG22	10	0.19
(1,140)	1:19:A:LYS:HA	1:20:A:THR:HG23	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG2	20	0.19
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG3	20	0.19
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG2	20	0.19
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG3	20	0.19
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG2	20	0.19
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG3	20	0.19
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG2	20	0.19
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG3	20	0.19
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG2	20	0.19
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG3	20	0.19
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG2	20	0.19
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG3	20	0.19
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	18	0.19
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	18	0.19
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	18	0.19
(1,66)	1:12:A:VAL:HG21	1:16:A:LEU:HG	7	0.19
(1,66)	1:12:A:VAL:HG22	1:16:A:LEU:HG	7	0.19
(1,66)	1:12:A:VAL:HG23	1:16:A:LEU:HG	7	0.19
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	10	0.19
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	10	0.19
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	10	0.19
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	10	0.19
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	10	0.19
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	10	0.19
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	14	0.19
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	14	0.19
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	14	0.19
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	14	0.19
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	14	0.19
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	14	0.19
(3,114)	1:166:A:LEU:O	1:170:A:GLN:H	11	0.18
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	10	0.18
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	16	0.18
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	3	0.18
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	11	0.18
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	16	0.18
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	3	0.18
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	20	0.18
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	3	0.18
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD11	13	0.18
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD12	13	0.18
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD13	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD21	13	0.18
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD22	13	0.18
(1,1279)	1:183:A:LEU:H	1:183:A:LEU:HD23	13	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	3	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	3	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	3	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	3	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	3	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	3	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	20	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	20	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	20	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	20	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	20	0.18
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	20	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG11	11	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG12	11	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG13	11	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG21	11	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG22	11	0.18
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG23	11	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG11	11	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG12	11	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG13	11	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG21	11	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG22	11	0.18
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG23	11	0.18
(1,1241)	1:174:A:LYS:HA	1:175:A:ALA:H	7	0.18
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE1	17	0.18
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE2	17	0.18
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE1	17	0.18
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE2	17	0.18
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE1	17	0.18
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE2	17	0.18
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE1	17	0.18
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE2	17	0.18
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE1	17	0.18
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE2	17	0.18
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE1	17	0.18
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE2	17	0.18
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	20	0.18
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG21	19	0.18
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG22	19	0.18
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG23	19	0.18
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG21	19	0.18
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG22	19	0.18
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG23	19	0.18
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	5	0.18
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	11	0.18
(1,1135)	1:157:A:ASP:HA	1:158:A:LYS:H	17	0.18
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	18	0.18
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	18	0.18
(1,1100)	1:153:A:PHE:HD1	1:157:A:ASP:HB2	6	0.18
(1,1100)	1:153:A:PHE:HD1	1:157:A:ASP:HB3	6	0.18
(1,1100)	1:153:A:PHE:HD2	1:157:A:ASP:HB2	6	0.18
(1,1100)	1:153:A:PHE:HD2	1:157:A:ASP:HB3	6	0.18
(1,1065)	1:149:A:VAL:HG11	1:153:A:PHE:HZ	11	0.18
(1,1065)	1:149:A:VAL:HG12	1:153:A:PHE:HZ	11	0.18
(1,1065)	1:149:A:VAL:HG13	1:153:A:PHE:HZ	11	0.18
(1,1065)	1:149:A:VAL:HG21	1:153:A:PHE:HZ	11	0.18
(1,1065)	1:149:A:VAL:HG22	1:153:A:PHE:HZ	11	0.18
(1,1065)	1:149:A:VAL:HG23	1:153:A:PHE:HZ	11	0.18
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	7	0.18
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	7	0.18
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	7	0.18
(1,1034)	1:144:A:THR:HG21	1:146:A:GLU:H	18	0.18
(1,1034)	1:144:A:THR:HG22	1:146:A:GLU:H	18	0.18
(1,1034)	1:144:A:THR:HG23	1:146:A:GLU:H	18	0.18
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	2	0.18
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	10	0.18
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	10	0.18
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	20	0.18
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	20	0.18
(1,1017)	1:142:A:GLU:H	1:143:A:ASN:H	17	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	7	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	7	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	7	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	7	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	7	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	7	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	13	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	13	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	13	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	13	0.18
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	13	0.18
(1,900)	1:118:A:ARG:HB2	1:150:A:ASP:HA	20	0.18
(1,900)	1:118:A:ARG:HB3	1:150:A:ASP:HA	20	0.18
(1,889)	1:117:A:THR:HB	1:163:A:LYS:HG2	11	0.18
(1,889)	1:117:A:THR:HB	1:163:A:LYS:HG3	11	0.18
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	4	0.18
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	4	0.18
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	1	0.18
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	1	0.18
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	1	0.18
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	1	0.18
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	1	0.18
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	1	0.18
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	7	0.18
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	7	0.18
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	7	0.18
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	7	0.18
(1,820)	1:110:A:LEU:HD11	1:112:A:ASN:HB2	16	0.18
(1,820)	1:110:A:LEU:HD11	1:112:A:ASN:HB3	16	0.18
(1,820)	1:110:A:LEU:HD12	1:112:A:ASN:HB2	16	0.18
(1,820)	1:110:A:LEU:HD12	1:112:A:ASN:HB3	16	0.18
(1,820)	1:110:A:LEU:HD13	1:112:A:ASN:HB2	16	0.18
(1,820)	1:110:A:LEU:HD13	1:112:A:ASN:HB3	16	0.18
(1,820)	1:110:A:LEU:HD21	1:112:A:ASN:HB2	16	0.18
(1,820)	1:110:A:LEU:HD21	1:112:A:ASN:HB3	16	0.18
(1,820)	1:110:A:LEU:HD22	1:112:A:ASN:HB2	16	0.18
(1,820)	1:110:A:LEU:HD22	1:112:A:ASN:HB3	16	0.18
(1,820)	1:110:A:LEU:HD23	1:112:A:ASN:HB2	16	0.18
(1,820)	1:110:A:LEU:HD23	1:112:A:ASN:HB3	16	0.18
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	18	0.18
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	18	0.18
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	18	0.18
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	18	0.18
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	18	0.18
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	18	0.18
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD11	2	0.18
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD12	2	0.18
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD13	2	0.18
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD21	2	0.18
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD22	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD23	2	0.18
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD11	2	0.18
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD12	2	0.18
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD13	2	0.18
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD21	2	0.18
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD22	2	0.18
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD23	2	0.18
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	8	0.18
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	8	0.18
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	8	0.18
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	8	0.18
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	17	0.18
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	17	0.18
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	17	0.18
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	17	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	9	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	9	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	9	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	9	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	9	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	9	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	9	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	9	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	9	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	9	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	9	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	9	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	14	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	14	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	14	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	14	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	14	0.18
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	14	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	14	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	14	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	14	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	14	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	14	0.18
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	14	0.18
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD11	16	0.18
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD12	16	0.18
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD13	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD21	16	0.18
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD22	16	0.18
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD23	16	0.18
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD11	16	0.18
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD12	16	0.18
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD13	16	0.18
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD21	16	0.18
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD22	16	0.18
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD23	16	0.18
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD11	16	0.18
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD12	16	0.18
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD13	16	0.18
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD21	16	0.18
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD22	16	0.18
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD23	16	0.18
(1,595)	1:75:A:ASN:HA	1:76:A:LYS:H	19	0.18
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG21	17	0.18
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG22	17	0.18
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG23	17	0.18
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB1	2	0.18
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB2	2	0.18
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB3	2	0.18
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	19	0.18
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	19	0.18
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD11	12	0.18
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD12	12	0.18
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD13	12	0.18
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD11	12	0.18
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD12	12	0.18
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD13	12	0.18
(1,476)	1:60:A:ASP:HB2	1:130:A:GLN:HB2	18	0.18
(1,476)	1:60:A:ASP:HB2	1:130:A:GLN:HB3	18	0.18
(1,476)	1:60:A:ASP:HB3	1:130:A:GLN:HB2	18	0.18
(1,476)	1:60:A:ASP:HB3	1:130:A:GLN:HB3	18	0.18
(1,468)	1:58:A:PHE:HA	1:59:A:GLY:H	9	0.18
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	1	0.18
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	2	0.18
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	8	0.18
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	5	0.18
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	5	0.18
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	5	0.18
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	17	0.18
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	17	0.18
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	17	0.18
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	17	0.18
(1,444)	1:53:A:LYS:HB2	1:57:A:PRO:HG2	2	0.18
(1,444)	1:53:A:LYS:HB2	1:57:A:PRO:HG3	2	0.18
(1,444)	1:53:A:LYS:HB3	1:57:A:PRO:HG2	2	0.18
(1,444)	1:53:A:LYS:HB3	1:57:A:PRO:HG3	2	0.18
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	2	0.18
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	2	0.18
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	2	0.18
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	2	0.18
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	2	0.18
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	2	0.18
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	2	0.18
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	2	0.18
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	2	0.18
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	2	0.18
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	2	0.18
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	2	0.18
(1,403)	1:49:A:GLN:HG2	1:62:A:THR:HG21	5	0.18
(1,403)	1:49:A:GLN:HG2	1:62:A:THR:HG22	5	0.18
(1,403)	1:49:A:GLN:HG2	1:62:A:THR:HG23	5	0.18
(1,403)	1:49:A:GLN:HG3	1:62:A:THR:HG21	5	0.18
(1,403)	1:49:A:GLN:HG3	1:62:A:THR:HG22	5	0.18
(1,403)	1:49:A:GLN:HG3	1:62:A:THR:HG23	5	0.18
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	2	0.18
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	2	0.18
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	2	0.18
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	2	0.18
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	2	0.18
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	2	0.18
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	2	0.18
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	2	0.18
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	2	0.18
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	2	0.18
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	2	0.18
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	2	0.18
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB1	16	0.18
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB2	16	0.18
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB3	16	0.18
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB1	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB2	16	0.18
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB3	16	0.18
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	9	0.18
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	9	0.18
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	9	0.18
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	9	0.18
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	19	0.18
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	19	0.18
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	19	0.18
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	19	0.18
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	7	0.18
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	10	0.18
(1,311)	1:42:A:GLN:HG2	1:79:A:ARG:HA	17	0.18
(1,311)	1:42:A:GLN:HG3	1:79:A:ARG:HA	17	0.18
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	19	0.18
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD2	8	0.18
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD3	8	0.18
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	19	0.18
(1,123)	1:17:A:THR:HA	1:24:A:GLU:HA	15	0.18
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD11	1	0.18
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD12	1	0.18
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD13	1	0.18
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD21	1	0.18
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD22	1	0.18
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD23	1	0.18
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD11	1	0.18
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD12	1	0.18
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD13	1	0.18
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD21	1	0.18
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD22	1	0.18
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD23	1	0.18
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD11	1	0.18
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD12	1	0.18
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD13	1	0.18
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD21	1	0.18
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD22	1	0.18
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD23	1	0.18
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD11	1	0.18
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD12	1	0.18
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD13	1	0.18
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD21	1	0.18
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD22	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD23	1	0.18
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD11	1	0.18
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD12	1	0.18
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD13	1	0.18
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD21	1	0.18
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD22	1	0.18
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD23	1	0.18
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD11	1	0.18
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD12	1	0.18
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD13	1	0.18
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD21	1	0.18
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD22	1	0.18
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD23	1	0.18
(3,114)	1:166:A:LEU:O	1:170:A:GLN:H	16	0.17
(3,103)	1:152:A:ILE:O	1:156:A:MET:N	11	0.17
(3,95)	1:128:A:ILE:O	1:132:A:VAL:H	8	0.17
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	15	0.17
(3,57)	1:85:A:PHE:O	1:89:A:LEU:H	16	0.17
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	3	0.17
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	12	0.17
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	19	0.17
(3,13)	1:29:A:GLN:O	1:33:A:GLY:N	12	0.17
(3,13)	1:29:A:GLN:O	1:33:A:GLY:N	19	0.17
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	1	0.17
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	15	0.17
(2,4)	1:79:A:ARG:O	2:600:A:CA:CA	12	0.17
(1,1289)	1:186:A:TYR:HD1	1:189:A:LEU:HA	6	0.17
(1,1289)	1:186:A:TYR:HD2	1:189:A:LEU:HA	6	0.17
(1,1283)	1:184:A:SER:HB2	1:186:A:TYR:H	1	0.17
(1,1283)	1:184:A:SER:HB3	1:186:A:TYR:H	1	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	14	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	14	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	14	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	14	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	14	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	14	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	16	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	16	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	16	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	16	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	16	0.17
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE1	6	0.17
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE2	6	0.17
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE1	6	0.17
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE2	6	0.17
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE1	6	0.17
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE2	6	0.17
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE1	6	0.17
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE2	6	0.17
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE1	6	0.17
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE2	6	0.17
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE1	6	0.17
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE2	6	0.17
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	15	0.17
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	15	0.17
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	16	0.17
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	16	0.17
(1,1167)	1:164:A:LEU:H	1:165:A:THR:HA	19	0.17
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	14	0.17
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	14	0.17
(1,1136)	1:157:A:ASP:HA	1:158:A:LYS:HG2	8	0.17
(1,1136)	1:157:A:ASP:HA	1:158:A:LYS:HG3	8	0.17
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG21	9	0.17
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG22	9	0.17
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG23	9	0.17
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG21	9	0.17
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG22	9	0.17
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG23	9	0.17
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG21	9	0.17
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG22	9	0.17
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG23	9	0.17
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG21	9	0.17
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG22	9	0.17
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG23	9	0.17
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG21	9	0.17
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG22	9	0.17
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG23	9	0.17
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG21	9	0.17
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG22	9	0.17
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG23	9	0.17
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG21	20	0.17
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG22	20	0.17
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG23	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG21	20	0.17
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG22	20	0.17
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG23	20	0.17
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG21	20	0.17
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG22	20	0.17
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG23	20	0.17
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG21	20	0.17
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG22	20	0.17
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG23	20	0.17
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG21	20	0.17
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG22	20	0.17
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG23	20	0.17
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG21	20	0.17
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG22	20	0.17
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG23	20	0.17
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	5	0.17
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	5	0.17
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	5	0.17
(1,1046)	1:148:A:ARG:HB2	1:152:A:ILE:H	11	0.17
(1,1046)	1:148:A:ARG:HB3	1:152:A:ILE:H	11	0.17
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	13	0.17
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	13	0.17
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	14	0.17
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	14	0.17
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	19	0.17
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	19	0.17
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	11	0.17
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	11	0.17
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	11	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG11	9	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG12	9	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG13	9	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG21	9	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG22	9	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG23	9	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG11	9	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG12	9	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG13	9	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG21	9	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG22	9	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG23	9	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG11	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG12	15	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG13	15	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG21	15	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG22	15	0.17
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG23	15	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG11	15	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG12	15	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG13	15	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG21	15	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG22	15	0.17
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG23	15	0.17
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	20	0.17
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	20	0.17
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	1	0.17
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	1	0.17
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD11	10	0.17
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD12	10	0.17
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD13	10	0.17
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD21	10	0.17
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD22	10	0.17
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD23	10	0.17
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD11	10	0.17
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD12	10	0.17
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD13	10	0.17
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD21	10	0.17
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD22	10	0.17
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD23	10	0.17
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD11	10	0.17
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD12	10	0.17
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD13	10	0.17
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD21	10	0.17
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD22	10	0.17
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD23	10	0.17
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	15	0.17
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	15	0.17
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	15	0.17
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	11	0.17
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	11	0.17
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	11	0.17
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	11	0.17
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	11	0.17
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	4	0.17
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	4	0.17
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	4	0.17
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	4	0.17
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	4	0.17
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	4	0.17
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	5	0.17
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	5	0.17
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	5	0.17
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	5	0.17
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	5	0.17
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	5	0.17
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	7	0.17
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	7	0.17
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	7	0.17
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	15	0.17
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	15	0.17
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	15	0.17
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG21	7	0.17
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG22	7	0.17
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG23	7	0.17
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG21	7	0.17
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG22	7	0.17
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG23	7	0.17
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG21	16	0.17
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG22	16	0.17
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG23	16	0.17
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG21	16	0.17
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG22	16	0.17
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG23	16	0.17
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	10	0.17
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	10	0.17
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	10	0.17
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	10	0.17
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	10	0.17
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	10	0.17
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	10	0.17
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	10	0.17
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	10	0.17
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	10	0.17
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	10	0.17
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	5	0.17
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	5	0.17
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	5	0.17
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	1	0.17
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	1	0.17
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	10	0.17
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	10	0.17
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	10	0.17
(1,595)	1:75:A:ASN:HA	1:76:A:LYS:H	6	0.17
(1,580)	1:72:A:PHE:HZ	1:80:A:ILE:HG12	4	0.17
(1,580)	1:72:A:PHE:HZ	1:80:A:ILE:HG13	4	0.17
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	8	0.17
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	8	0.17
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	12	0.17
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	12	0.17
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	4	0.17
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	4	0.17
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB2	4	0.17
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB3	4	0.17
(1,477)	1:62:A:THR:H	1:62:A:THR:HB	17	0.17
(1,468)	1:58:A:PHE:HA	1:59:A:GLY:H	20	0.17
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	17	0.17
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	13	0.17
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	13	0.17
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	13	0.17
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	13	0.17
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	19	0.17
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	19	0.17
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	19	0.17
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	19	0.17
(1,420)	1:51:A:ILE:HD11	1:85:A:PHE:HB2	13	0.17
(1,420)	1:51:A:ILE:HD11	1:85:A:PHE:HB3	13	0.17
(1,420)	1:51:A:ILE:HD12	1:85:A:PHE:HB2	13	0.17
(1,420)	1:51:A:ILE:HD12	1:85:A:PHE:HB3	13	0.17
(1,420)	1:51:A:ILE:HD13	1:85:A:PHE:HB2	13	0.17
(1,420)	1:51:A:ILE:HD13	1:85:A:PHE:HB3	13	0.17
(1,406)	1:49:A:GLN:HG2	1:66:A:THR:HA	11	0.17
(1,406)	1:49:A:GLN:HG3	1:66:A:THR:HA	11	0.17
(1,399)	1:49:A:GLN:HB2	1:65:A:ALA:HA	18	0.17
(1,399)	1:49:A:GLN:HB3	1:65:A:ALA:HA	18	0.17
(1,387)	1:48:A:PHE:HE1	1:80:A:ILE:HG12	16	0.17
(1,387)	1:48:A:PHE:HE1	1:80:A:ILE:HG13	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:48:A:PHE:HE2	1:80:A:ILE:HG12	16	0.17
(1,387)	1:48:A:PHE:HE2	1:80:A:ILE:HG13	16	0.17
(1,386)	1:48:A:PHE:HE1	1:80:A:ILE:HB	3	0.17
(1,386)	1:48:A:PHE:HE2	1:80:A:ILE:HB	3	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	6	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	6	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	6	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	6	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	6	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	6	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	6	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	6	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	6	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	6	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	6	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	6	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	9	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	9	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	9	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	9	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	9	0.17
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	9	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	9	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	9	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	9	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	9	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	9	0.17
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	9	0.17
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB1	6	0.17
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB2	6	0.17
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB3	6	0.17
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB1	6	0.17
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB2	6	0.17
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB3	6	0.17
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD11	15	0.17
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD12	15	0.17
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD13	15	0.17
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD11	15	0.17
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD12	15	0.17
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD13	15	0.17
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	12	0.17
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	12	0.17
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	12	0.17
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	14	0.17
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	14	0.17
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	14	0.17
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	14	0.17
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	20	0.17
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	20	0.17
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	20	0.17
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	20	0.17
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	2	0.17
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	5	0.17
(1,322)	1:43:A:LEU:HD11	1:44:A:ASP:H	18	0.17
(1,322)	1:43:A:LEU:HD12	1:44:A:ASP:H	18	0.17
(1,322)	1:43:A:LEU:HD13	1:44:A:ASP:H	18	0.17
(1,322)	1:43:A:LEU:HD21	1:44:A:ASP:H	18	0.17
(1,322)	1:43:A:LEU:HD22	1:44:A:ASP:H	18	0.17
(1,322)	1:43:A:LEU:HD23	1:44:A:ASP:H	18	0.17
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	6	0.17
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	6	0.17
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	6	0.17
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	10	0.17
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	10	0.17
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	17	0.17
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	17	0.17
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	10	0.17
(1,145)	1:20:A:THR:H	1:21:A:TYR:H	11	0.17
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	13	0.17
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	13	0.17
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	13	0.17
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	13	0.17
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	13	0.17
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	13	0.17
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG11	2	0.17
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG12	2	0.17
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG13	2	0.17
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG21	2	0.17
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG22	2	0.17
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG23	2	0.17
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	11	0.17
(1,21)	1:8:A:LEU:HD11	1:16:A:LEU:HG	5	0.17
(1,21)	1:8:A:LEU:HD12	1:16:A:LEU:HG	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:8:A:LEU:HD13	1:16:A:LEU:HG	5	0.17
(1,21)	1:8:A:LEU:HD21	1:16:A:LEU:HG	5	0.17
(1,21)	1:8:A:LEU:HD22	1:16:A:LEU:HG	5	0.17
(1,21)	1:8:A:LEU:HD23	1:16:A:LEU:HG	5	0.17
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	18	0.17
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	18	0.17
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	18	0.17
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	18	0.17
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	18	0.17
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	18	0.17
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD1	19	0.17
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD2	19	0.17
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD1	19	0.17
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD2	19	0.17
(3,115)	1:167:A:GLN:O	1:171:A:GLU:H	7	0.16
(3,109)	1:166:A:LEU:O	1:170:A:GLN:N	16	0.16
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	1	0.16
(3,102)	1:151:A:ARG:O	1:155:A:MET:N	4	0.16
(3,97)	1:146:A:GLU:O	1:150:A:ASP:N	11	0.16
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	14	0.16
(3,50)	1:85:A:PHE:O	1:89:A:LEU:N	16	0.16
(3,45)	1:67:A:PHE:O	1:71:A:VAL:H	16	0.16
(3,43)	1:65:A:ALA:O	1:69:A:PHE:H	13	0.16
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	8	0.16
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	17	0.16
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	5	0.16
(3,27)	1:52:A:TYR:O	1:56:A:PHE:N	8	0.16
(3,27)	1:52:A:TYR:O	1:56:A:PHE:N	16	0.16
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	14	0.16
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	4	0.16
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	11	0.16
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	17	0.16
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	19	0.16
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD11	10	0.16
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD12	10	0.16
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD13	10	0.16
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD21	10	0.16
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD22	10	0.16
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD23	10	0.16
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	10	0.16
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	10	0.16
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	10	0.16
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	10	0.16
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	10	0.16
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG11	18	0.16
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG12	18	0.16
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG13	18	0.16
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG21	18	0.16
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG22	18	0.16
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG23	18	0.16
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG11	18	0.16
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG12	18	0.16
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG13	18	0.16
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG21	18	0.16
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG22	18	0.16
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG23	18	0.16
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD2	10	0.16
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD3	10	0.16
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD2	17	0.16
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD3	17	0.16
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	5	0.16
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	5	0.16
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	8	0.16
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	8	0.16
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	8	0.16
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	8	0.16
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	8	0.16
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	8	0.16
(1,1175)	1:164:A:LEU:HD11	1:169:A:PHE:HA	17	0.16
(1,1175)	1:164:A:LEU:HD12	1:169:A:PHE:HA	17	0.16
(1,1175)	1:164:A:LEU:HD13	1:169:A:PHE:HA	17	0.16
(1,1175)	1:164:A:LEU:HD21	1:169:A:PHE:HA	17	0.16
(1,1175)	1:164:A:LEU:HD22	1:169:A:PHE:HA	17	0.16
(1,1175)	1:164:A:LEU:HD23	1:169:A:PHE:HA	17	0.16
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	8	0.16
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	8	0.16
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	1	0.16
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	8	0.16
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	16	0.16
(1,1141)	1:158:A:LYS:H	1:158:A:LYS:HB2	7	0.16
(1,1141)	1:158:A:LYS:H	1:158:A:LYS:HB3	7	0.16
(1,1136)	1:157:A:ASP:HA	1:158:A:LYS:HG2	17	0.16
(1,1136)	1:157:A:ASP:HA	1:158:A:LYS:HG3	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD11	12	0.16
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD12	12	0.16
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD13	12	0.16
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD21	12	0.16
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD22	12	0.16
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD23	12	0.16
(1,1100)	1:153:A:PHE:HD1	1:157:A:ASP:HB2	9	0.16
(1,1100)	1:153:A:PHE:HD1	1:157:A:ASP:HB3	9	0.16
(1,1100)	1:153:A:PHE:HD2	1:157:A:ASP:HB2	9	0.16
(1,1100)	1:153:A:PHE:HD2	1:157:A:ASP:HB3	9	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD11	20	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD12	20	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD13	20	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD21	20	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD22	20	0.16
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD23	20	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD11	20	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD12	20	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD13	20	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD21	20	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD22	20	0.16
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD23	20	0.16
(1,1065)	1:149:A:VAL:HG11	1:153:A:PHE:HZ	4	0.16
(1,1065)	1:149:A:VAL:HG12	1:153:A:PHE:HZ	4	0.16
(1,1065)	1:149:A:VAL:HG13	1:153:A:PHE:HZ	4	0.16
(1,1065)	1:149:A:VAL:HG21	1:153:A:PHE:HZ	4	0.16
(1,1065)	1:149:A:VAL:HG22	1:153:A:PHE:HZ	4	0.16
(1,1065)	1:149:A:VAL:HG23	1:153:A:PHE:HZ	4	0.16
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG21	4	0.16
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG22	4	0.16
(1,1062)	1:149:A:VAL:HG11	1:152:A:ILE:HG23	4	0.16
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG21	4	0.16
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG22	4	0.16
(1,1062)	1:149:A:VAL:HG12	1:152:A:ILE:HG23	4	0.16
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG21	4	0.16
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG22	4	0.16
(1,1062)	1:149:A:VAL:HG13	1:152:A:ILE:HG23	4	0.16
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG21	4	0.16
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG22	4	0.16
(1,1062)	1:149:A:VAL:HG21	1:152:A:ILE:HG23	4	0.16
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG21	4	0.16
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG22	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:149:A:VAL:HG22	1:152:A:ILE:HG23	4	0.16
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG21	4	0.16
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG22	4	0.16
(1,1062)	1:149:A:VAL:HG23	1:152:A:ILE:HG23	4	0.16
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD1	10	0.16
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD2	10	0.16
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	1	0.16
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	5	0.16
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	19	0.16
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	17	0.16
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	17	0.16
(1,1022)	1:143:A:ASN:H	1:144:A:THR:H	16	0.16
(1,1021)	1:142:A:GLU:HG2	1:144:A:THR:H	6	0.16
(1,1021)	1:142:A:GLU:HG3	1:144:A:THR:H	6	0.16
(1,1004)	1:138:A:LEU:H	1:138:A:LEU:HD11	1	0.16
(1,1004)	1:138:A:LEU:H	1:138:A:LEU:HD12	1	0.16
(1,1004)	1:138:A:LEU:H	1:138:A:LEU:HD13	1	0.16
(1,1004)	1:138:A:LEU:H	1:138:A:LEU:HD21	1	0.16
(1,1004)	1:138:A:LEU:H	1:138:A:LEU:HD22	1	0.16
(1,1004)	1:138:A:LEU:H	1:138:A:LEU:HD23	1	0.16
(1,1002)	1:137:A:GLU:HA	1:138:A:LEU:HB2	8	0.16
(1,1002)	1:137:A:GLU:HA	1:138:A:LEU:HB3	8	0.16
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB2	3	0.16
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB3	3	0.16
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB2	3	0.16
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB3	3	0.16
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB2	3	0.16
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB3	3	0.16
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB2	3	0.16
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB3	3	0.16
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB2	3	0.16
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB3	3	0.16
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB2	3	0.16
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB3	3	0.16
(1,995)	1:136:A:VAL:HA	1:137:A:GLU:H	13	0.16
(1,992)	1:136:A:VAL:H	1:136:A:VAL:HB	17	0.16
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	4	0.16
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	11	0.16
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	11	0.16
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	10	0.16
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	10	0.16
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	12	0.16
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	12	0.16
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	12	0.16
(1,927)	1:122:A:LEU:HD11	1:146:A:GLU:HG2	19	0.16
(1,927)	1:122:A:LEU:HD11	1:146:A:GLU:HG3	19	0.16
(1,927)	1:122:A:LEU:HD12	1:146:A:GLU:HG2	19	0.16
(1,927)	1:122:A:LEU:HD12	1:146:A:GLU:HG3	19	0.16
(1,927)	1:122:A:LEU:HD13	1:146:A:GLU:HG2	19	0.16
(1,927)	1:122:A:LEU:HD13	1:146:A:GLU:HG3	19	0.16
(1,927)	1:122:A:LEU:HD21	1:146:A:GLU:HG2	19	0.16
(1,927)	1:122:A:LEU:HD21	1:146:A:GLU:HG3	19	0.16
(1,927)	1:122:A:LEU:HD22	1:146:A:GLU:HG2	19	0.16
(1,927)	1:122:A:LEU:HD22	1:146:A:GLU:HG3	19	0.16
(1,927)	1:122:A:LEU:HD23	1:146:A:GLU:HG2	19	0.16
(1,927)	1:122:A:LEU:HD23	1:146:A:GLU:HG3	19	0.16
(1,900)	1:118:A:ARG:HB2	1:150:A:ASP:HA	16	0.16
(1,900)	1:118:A:ARG:HB3	1:150:A:ASP:HA	16	0.16
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	1	0.16
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	1	0.16
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	1	0.16
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	7	0.16
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	7	0.16
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	7	0.16
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	2	0.16
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	2	0.16
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	2	0.16
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	2	0.16
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	2	0.16
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	2	0.16
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	3	0.16
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	3	0.16
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	3	0.16
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	3	0.16
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	3	0.16
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	3	0.16
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	15	0.16
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	15	0.16
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	15	0.16
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	15	0.16
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	15	0.16
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	15	0.16
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	17	0.16
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	17	0.16
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	17	0.16
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	17	0.16
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	17	0.16
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD2	9	0.16
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD3	9	0.16
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD2	9	0.16
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD3	9	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD11	20	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD12	20	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD13	20	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD21	20	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD22	20	0.16
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD23	20	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD11	20	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD12	20	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD13	20	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD21	20	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD22	20	0.16
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD23	20	0.16
(1,834)	1:114:A:GLY:HA2	1:115:A:TYR:HE1	11	0.16
(1,834)	1:114:A:GLY:HA2	1:115:A:TYR:HE2	11	0.16
(1,834)	1:114:A:GLY:HA3	1:115:A:TYR:HE1	11	0.16
(1,834)	1:114:A:GLY:HA3	1:115:A:TYR:HE2	11	0.16
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	4	0.16
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	4	0.16
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	4	0.16
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	13	0.16
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	13	0.16
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	13	0.16
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	1	0.16
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	1	0.16
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	1	0.16
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	1	0.16
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	1	0.16
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	1	0.16
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	3	0.16
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	3	0.16
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	3	0.16
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	3	0.16
(1,713)	1:96:A:THR:H	1:99:A:GLU:HG2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:96:A:THR:H	1:99:A:GLU:HG3	7	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	1	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	1	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	1	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	6	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	6	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	6	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	13	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	13	0.16
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	13	0.16
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	8	0.16
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	8	0.16
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	19	0.16
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	19	0.16
(1,595)	1:75:A:ASN:HA	1:76:A:LYS:H	15	0.16
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG12	9	0.16
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG13	9	0.16
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	12	0.16
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	12	0.16
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	18	0.16
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	18	0.16
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	20	0.16
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	20	0.16
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	3	0.16
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	3	0.16
(1,549)	1:68:A:VAL:HG11	1:124:A:ILE:HD11	3	0.16
(1,549)	1:68:A:VAL:HG11	1:124:A:ILE:HD12	3	0.16
(1,549)	1:68:A:VAL:HG11	1:124:A:ILE:HD13	3	0.16
(1,549)	1:68:A:VAL:HG12	1:124:A:ILE:HD11	3	0.16
(1,549)	1:68:A:VAL:HG12	1:124:A:ILE:HD12	3	0.16
(1,549)	1:68:A:VAL:HG12	1:124:A:ILE:HD13	3	0.16
(1,549)	1:68:A:VAL:HG13	1:124:A:ILE:HD11	3	0.16
(1,549)	1:68:A:VAL:HG13	1:124:A:ILE:HD12	3	0.16
(1,549)	1:68:A:VAL:HG13	1:124:A:ILE:HD13	3	0.16
(1,549)	1:68:A:VAL:HG21	1:124:A:ILE:HD11	3	0.16
(1,549)	1:68:A:VAL:HG21	1:124:A:ILE:HD12	3	0.16
(1,549)	1:68:A:VAL:HG21	1:124:A:ILE:HD13	3	0.16
(1,549)	1:68:A:VAL:HG22	1:124:A:ILE:HD11	3	0.16
(1,549)	1:68:A:VAL:HG22	1:124:A:ILE:HD12	3	0.16
(1,549)	1:68:A:VAL:HG22	1:124:A:ILE:HD13	3	0.16
(1,549)	1:68:A:VAL:HG23	1:124:A:ILE:HD11	3	0.16
(1,549)	1:68:A:VAL:HG23	1:124:A:ILE:HD12	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:68:A:VAL:HG23	1:124:A:ILE:HD13	3	0.16
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	1	0.16
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	1	0.16
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	20	0.16
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	20	0.16
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	12	0.16
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	13	0.16
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	10	0.16
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	10	0.16
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	10	0.16
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	10	0.16
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	6	0.16
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	6	0.16
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	6	0.16
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	6	0.16
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	6	0.16
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	6	0.16
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	6	0.16
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	6	0.16
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	6	0.16
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	6	0.16
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	6	0.16
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	6	0.16
(1,406)	1:49:A:GLN:HG2	1:66:A:THR:HA	15	0.16
(1,406)	1:49:A:GLN:HG3	1:66:A:THR:HA	15	0.16
(1,399)	1:49:A:GLN:HB2	1:65:A:ALA:HA	5	0.16
(1,399)	1:49:A:GLN:HB3	1:65:A:ALA:HA	5	0.16
(1,386)	1:48:A:PHE:HE1	1:80:A:ILE:HB	1	0.16
(1,386)	1:48:A:PHE:HE2	1:80:A:ILE:HB	1	0.16
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	15	0.16
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	15	0.16
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	15	0.16
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	15	0.16
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	15	0.16
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	15	0.16
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	15	0.16
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	15	0.16
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	15	0.16
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	15	0.16
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	15	0.16
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	15	0.16
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB1	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB2	1	0.16
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB3	1	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB1	1	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB2	1	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB3	1	0.16
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB1	3	0.16
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB2	3	0.16
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB3	3	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB1	3	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB2	3	0.16
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB3	3	0.16
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	11	0.16
(1,312)	1:42:A:GLN:HG2	1:81:A:GLU:HA	6	0.16
(1,312)	1:42:A:GLN:HG3	1:81:A:GLU:HA	6	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD11	1	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD12	1	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD13	1	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD11	18	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD12	18	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD13	18	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD11	20	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD12	20	0.16
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD13	20	0.16
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	3	0.16
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	3	0.16
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	3	0.16
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	20	0.16
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	20	0.16
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	20	0.16
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	5	0.16
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	5	0.16
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	9	0.16
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	14	0.16
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	7	0.16
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	7	0.16
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	7	0.16
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	7	0.16
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	7	0.16
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	7	0.16
(1,117)	1:16:A:LEU:HD11	1:19:A:LYS:HA	6	0.16
(1,117)	1:16:A:LEU:HD12	1:19:A:LYS:HA	6	0.16
(1,117)	1:16:A:LEU:HD13	1:19:A:LYS:HA	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:16:A:LEU:HD21	1:19:A:LYS:HA	6	0.16
(1,117)	1:16:A:LEU:HD22	1:19:A:LYS:HA	6	0.16
(1,117)	1:16:A:LEU:HD23	1:19:A:LYS:HA	6	0.16
(1,117)	1:16:A:LEU:HD11	1:19:A:LYS:HA	19	0.16
(1,117)	1:16:A:LEU:HD12	1:19:A:LYS:HA	19	0.16
(1,117)	1:16:A:LEU:HD13	1:19:A:LYS:HA	19	0.16
(1,117)	1:16:A:LEU:HD21	1:19:A:LYS:HA	19	0.16
(1,117)	1:16:A:LEU:HD22	1:19:A:LYS:HA	19	0.16
(1,117)	1:16:A:LEU:HD23	1:19:A:LYS:HA	19	0.16
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG2	16	0.16
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG3	16	0.16
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	2	0.16
(1,66)	1:12:A:VAL:HG21	1:16:A:LEU:HG	18	0.16
(1,66)	1:12:A:VAL:HG22	1:16:A:LEU:HG	18	0.16
(1,66)	1:12:A:VAL:HG23	1:16:A:LEU:HG	18	0.16
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	12	0.16
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	12	0.16
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	12	0.16
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	12	0.16
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	12	0.16
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	12	0.16
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	19	0.16
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	19	0.16
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	19	0.16
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	19	0.16
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	19	0.16
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	19	0.16
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD1	8	0.16
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD2	8	0.16
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD1	8	0.16
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD2	8	0.16
(3,83)	1:125:A:VAL:O	1:129:A:TYR:N	8	0.15
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	4	0.15
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	10	0.15
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	11	0.15
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	3	0.15
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	11	0.15
(3,45)	1:67:A:PHE:O	1:71:A:VAL:H	10	0.15
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	10	0.15
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	12	0.15
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	8	0.15
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	2	0.15
(3,25)	1:50:A:LYS:O	1:54:A:GLN:N	13	0.15
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	6	0.15
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	7	0.15
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	10	0.15
(3,9)	1:25:A:LYS:O	1:29:A:GLN:N	2	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD11	5	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD12	5	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD13	5	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD21	5	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD22	5	0.15
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD23	5	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD11	5	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD12	5	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD13	5	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD21	5	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD22	5	0.15
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD23	5	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD11	5	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD12	5	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD13	5	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD21	5	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD22	5	0.15
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD23	5	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD11	5	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD12	5	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD13	5	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD21	5	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD22	5	0.15
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD23	5	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD11	5	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD12	5	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD13	5	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD21	5	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD22	5	0.15
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD23	5	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD11	5	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD12	5	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD13	5	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD21	5	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD22	5	0.15
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD23	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:174:A:LYS:H	1:174:A:LYS:HE2	14	0.15
(1,1236)	1:174:A:LYS:H	1:174:A:LYS:HE3	14	0.15
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	6	0.15
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	16	0.15
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE1	20	0.15
(1,1197)	1:166:A:LEU:HD11	1:169:A:PHE:HE2	20	0.15
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE1	20	0.15
(1,1197)	1:166:A:LEU:HD12	1:169:A:PHE:HE2	20	0.15
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE1	20	0.15
(1,1197)	1:166:A:LEU:HD13	1:169:A:PHE:HE2	20	0.15
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE1	20	0.15
(1,1197)	1:166:A:LEU:HD21	1:169:A:PHE:HE2	20	0.15
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE1	20	0.15
(1,1197)	1:166:A:LEU:HD22	1:169:A:PHE:HE2	20	0.15
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE1	20	0.15
(1,1197)	1:166:A:LEU:HD23	1:169:A:PHE:HE2	20	0.15
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	14	0.15
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	14	0.15
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	17	0.15
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	17	0.15
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	18	0.15
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	18	0.15
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	6	0.15
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	6	0.15
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG21	8	0.15
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG22	8	0.15
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG23	8	0.15
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG21	8	0.15
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG22	8	0.15
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG23	8	0.15
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	2	0.15
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	2	0.15
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	18	0.15
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	18	0.15
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	2	0.15
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	9	0.15
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	18	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD11	17	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD12	17	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD13	17	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD21	17	0.15
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD22	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD23	17	0.15
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	1	0.15
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	1	0.15
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	10	0.15
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	10	0.15
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	13	0.15
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	13	0.15
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	17	0.15
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	17	0.15
(1,1073)	1:152:A:ILE:H	1:152:A:ILE:HG12	16	0.15
(1,1073)	1:152:A:ILE:H	1:152:A:ILE:HG13	16	0.15
(1,1034)	1:144:A:THR:HG21	1:146:A:GLU:H	15	0.15
(1,1034)	1:144:A:THR:HG22	1:146:A:GLU:H	15	0.15
(1,1034)	1:144:A:THR:HG23	1:146:A:GLU:H	15	0.15
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	3	0.15
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	8	0.15
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG21	14	0.15
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG22	14	0.15
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG23	14	0.15
(1,1024)	1:143:A:ASN:H	1:183:A:LEU:HB2	2	0.15
(1,1024)	1:143:A:ASN:H	1:183:A:LEU:HB3	2	0.15
(1,1008)	1:138:A:LEU:HD11	1:139:A:PRO:HA	12	0.15
(1,1008)	1:138:A:LEU:HD12	1:139:A:PRO:HA	12	0.15
(1,1008)	1:138:A:LEU:HD13	1:139:A:PRO:HA	12	0.15
(1,1008)	1:138:A:LEU:HD21	1:139:A:PRO:HA	12	0.15
(1,1008)	1:138:A:LEU:HD22	1:139:A:PRO:HA	12	0.15
(1,1008)	1:138:A:LEU:HD23	1:139:A:PRO:HA	12	0.15
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD11	8	0.15
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD12	8	0.15
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD13	8	0.15
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD21	8	0.15
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD22	8	0.15
(1,996)	1:136:A:VAL:HB	1:138:A:LEU:HD23	8	0.15
(1,990)	1:135:A:THR:HG21	1:138:A:LEU:HD11	5	0.15
(1,990)	1:135:A:THR:HG21	1:138:A:LEU:HD12	5	0.15
(1,990)	1:135:A:THR:HG21	1:138:A:LEU:HD13	5	0.15
(1,990)	1:135:A:THR:HG21	1:138:A:LEU:HD21	5	0.15
(1,990)	1:135:A:THR:HG21	1:138:A:LEU:HD22	5	0.15
(1,990)	1:135:A:THR:HG21	1:138:A:LEU:HD23	5	0.15
(1,990)	1:135:A:THR:HG22	1:138:A:LEU:HD11	5	0.15
(1,990)	1:135:A:THR:HG22	1:138:A:LEU:HD12	5	0.15
(1,990)	1:135:A:THR:HG22	1:138:A:LEU:HD13	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:135:A:THR:HG22	1:138:A:LEU:HD21	5	0.15
(1,990)	1:135:A:THR:HG22	1:138:A:LEU:HD22	5	0.15
(1,990)	1:135:A:THR:HG22	1:138:A:LEU:HD23	5	0.15
(1,990)	1:135:A:THR:HG23	1:138:A:LEU:HD11	5	0.15
(1,990)	1:135:A:THR:HG23	1:138:A:LEU:HD12	5	0.15
(1,990)	1:135:A:THR:HG23	1:138:A:LEU:HD13	5	0.15
(1,990)	1:135:A:THR:HG23	1:138:A:LEU:HD21	5	0.15
(1,990)	1:135:A:THR:HG23	1:138:A:LEU:HD22	5	0.15
(1,990)	1:135:A:THR:HG23	1:138:A:LEU:HD23	5	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	14	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	14	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	14	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	14	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	14	0.15
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	14	0.15
(1,988)	1:135:A:THR:HB	1:138:A:LEU:H	14	0.15
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD11	6	0.15
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD12	6	0.15
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD13	6	0.15
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD21	6	0.15
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD22	6	0.15
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD23	6	0.15
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD11	6	0.15
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD12	6	0.15
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD13	6	0.15
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD21	6	0.15
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD22	6	0.15
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD23	6	0.15
(1,953)	1:125:A:VAL:HG11	1:129:A:TYR:H	8	0.15
(1,953)	1:125:A:VAL:HG12	1:129:A:TYR:H	8	0.15
(1,953)	1:125:A:VAL:HG13	1:129:A:TYR:H	8	0.15
(1,953)	1:125:A:VAL:HG21	1:129:A:TYR:H	8	0.15
(1,953)	1:125:A:VAL:HG22	1:129:A:TYR:H	8	0.15
(1,953)	1:125:A:VAL:HG23	1:129:A:TYR:H	8	0.15
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	5	0.15
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	5	0.15
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	5	0.15
(1,924)	1:122:A:LEU:HD11	1:126:A:ASP:HA	7	0.15
(1,924)	1:122:A:LEU:HD12	1:126:A:ASP:HA	7	0.15
(1,924)	1:122:A:LEU:HD13	1:126:A:ASP:HA	7	0.15
(1,924)	1:122:A:LEU:HD21	1:126:A:ASP:HA	7	0.15
(1,924)	1:122:A:LEU:HD22	1:126:A:ASP:HA	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,924)	1:122:A:LEU:HD23	1:126:A:ASP:HA	7	0.15
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	1	0.15
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	1	0.15
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	2	0.15
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	2	0.15
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	12	0.15
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	12	0.15
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	2	0.15
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	2	0.15
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	2	0.15
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	2	0.15
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	2	0.15
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	2	0.15
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB2	14	0.15
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB3	14	0.15
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB2	14	0.15
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB3	14	0.15
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	2	0.15
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	2	0.15
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	2	0.15
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	2	0.15
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	9	0.15
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	9	0.15
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	9	0.15
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	9	0.15
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	13	0.15
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	13	0.15
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	13	0.15
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	13	0.15
(1,816)	1:110:A:LEU:HB2	1:111:A:ASP:H	5	0.15
(1,816)	1:110:A:LEU:HB3	1:111:A:ASP:H	5	0.15
(1,816)	1:110:A:LEU:HB2	1:111:A:ASP:H	6	0.15
(1,816)	1:110:A:LEU:HB3	1:111:A:ASP:H	6	0.15
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	17	0.15
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	17	0.15
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	17	0.15
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	13	0.15
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	13	0.15
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	13	0.15
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	13	0.15
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	13	0.15
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:109:A:ASP:HA	1:116:A:ILE:HA	17	0.15
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG21	13	0.15
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG22	13	0.15
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG23	13	0.15
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG21	13	0.15
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG22	13	0.15
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG23	13	0.15
(1,792)	1:108:A:TYR:HD1	1:124:A:ILE:HD11	15	0.15
(1,792)	1:108:A:TYR:HD1	1:124:A:ILE:HD12	15	0.15
(1,792)	1:108:A:TYR:HD1	1:124:A:ILE:HD13	15	0.15
(1,792)	1:108:A:TYR:HD2	1:124:A:ILE:HD11	15	0.15
(1,792)	1:108:A:TYR:HD2	1:124:A:ILE:HD12	15	0.15
(1,792)	1:108:A:TYR:HD2	1:124:A:ILE:HD13	15	0.15
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	7	0.15
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	7	0.15
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	7	0.15
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	7	0.15
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	16	0.15
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	16	0.15
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	16	0.15
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	16	0.15
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	16	0.15
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	16	0.15
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	16	0.15
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	16	0.15
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	16	0.15
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	16	0.15
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	16	0.15
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	16	0.15
(1,773)	1:107:A:LEU:HD11	1:108:A:TYR:H	10	0.15
(1,773)	1:107:A:LEU:HD12	1:108:A:TYR:H	10	0.15
(1,773)	1:107:A:LEU:HD13	1:108:A:TYR:H	10	0.15
(1,773)	1:107:A:LEU:HD21	1:108:A:TYR:H	10	0.15
(1,773)	1:107:A:LEU:HD22	1:108:A:TYR:H	10	0.15
(1,773)	1:107:A:LEU:HD23	1:108:A:TYR:H	10	0.15
(1,744)	1:101:A:LEU:HD11	1:169:A:PHE:HE1	5	0.15
(1,744)	1:101:A:LEU:HD11	1:169:A:PHE:HE2	5	0.15
(1,744)	1:101:A:LEU:HD12	1:169:A:PHE:HE1	5	0.15
(1,744)	1:101:A:LEU:HD12	1:169:A:PHE:HE2	5	0.15
(1,744)	1:101:A:LEU:HD13	1:169:A:PHE:HE1	5	0.15
(1,744)	1:101:A:LEU:HD13	1:169:A:PHE:HE2	5	0.15
(1,744)	1:101:A:LEU:HD21	1:169:A:PHE:HE1	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:101:A:LEU:HD21	1:169:A:PHE:HE2	5	0.15
(1,744)	1:101:A:LEU:HD22	1:169:A:PHE:HE1	5	0.15
(1,744)	1:101:A:LEU:HD22	1:169:A:PHE:HE2	5	0.15
(1,744)	1:101:A:LEU:HD23	1:169:A:PHE:HE1	5	0.15
(1,744)	1:101:A:LEU:HD23	1:169:A:PHE:HE2	5	0.15
(1,715)	1:96:A:THR:HB	1:98:A:ASP:H	12	0.15
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	17	0.15
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	17	0.15
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	17	0.15
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	7	0.15
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	7	0.15
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	7	0.15
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	19	0.15
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	19	0.15
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	19	0.15
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	6	0.15
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	6	0.15
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	16	0.15
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	16	0.15
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	13	0.15
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	13	0.15
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	19	0.15
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	19	0.15
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB2	20	0.15
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB3	20	0.15
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD11	7	0.15
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD12	7	0.15
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD13	7	0.15
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD11	7	0.15
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD12	7	0.15
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD13	7	0.15
(1,490)	1:63:A:LYS:HB2	1:65:A:ALA:HB1	7	0.15
(1,490)	1:63:A:LYS:HB2	1:65:A:ALA:HB2	7	0.15
(1,490)	1:63:A:LYS:HB2	1:65:A:ALA:HB3	7	0.15
(1,490)	1:63:A:LYS:HB3	1:65:A:ALA:HB1	7	0.15
(1,490)	1:63:A:LYS:HB3	1:65:A:ALA:HB2	7	0.15
(1,490)	1:63:A:LYS:HB3	1:65:A:ALA:HB3	7	0.15
(1,476)	1:60:A:ASP:HB2	1:130:A:GLN:HB2	7	0.15
(1,476)	1:60:A:ASP:HB2	1:130:A:GLN:HB3	7	0.15
(1,476)	1:60:A:ASP:HB3	1:130:A:GLN:HB2	7	0.15
(1,476)	1:60:A:ASP:HB3	1:130:A:GLN:HB3	7	0.15
(1,468)	1:58:A:PHE:HA	1:59:A:GLY:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	7	0.15
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	9	0.15
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	9	0.15
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	9	0.15
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	9	0.15
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	11	0.15
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	11	0.15
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	11	0.15
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	11	0.15
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	11	0.15
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	11	0.15
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	11	0.15
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	11	0.15
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	11	0.15
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	11	0.15
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	11	0.15
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	11	0.15
(1,386)	1:48:A:PHE:HE1	1:80:A:ILE:HB	17	0.15
(1,386)	1:48:A:PHE:HE2	1:80:A:ILE:HB	17	0.15
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	15	0.15
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	15	0.15
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	15	0.15
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	15	0.15
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	17	0.15
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	17	0.15
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	17	0.15
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	17	0.15
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	17	0.15
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	20	0.15
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	18	0.15
(1,293)	1:35:A:ILE:HD11	1:39:A:PRO:HA	6	0.15
(1,293)	1:35:A:ILE:HD12	1:39:A:PRO:HA	6	0.15
(1,293)	1:35:A:ILE:HD13	1:39:A:PRO:HA	6	0.15
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	3	0.15
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	12	0.15
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	13	0.15
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD11	17	0.15
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD12	17	0.15
(1,215)	1:27:A:VAL:HB	1:86:A:ILE:HD13	17	0.15
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	5	0.15
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	5	0.15
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	7	0.15
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	7	0.15
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	7	0.15
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	14	0.15
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	14	0.15
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	14	0.15
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	9	0.15
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	9	0.15
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	16	0.15
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	16	0.15
(1,160)	1:21:A:TYR:HA	1:22:A:PHE:H	16	0.15
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	5	0.15
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	5	0.15
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	5	0.15
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	5	0.15
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	5	0.15
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	5	0.15
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	5	0.15
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	14	0.15
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	14	0.15
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	14	0.15
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	14	0.15
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	14	0.15
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	14	0.15
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	17	0.15
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	17	0.15
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	17	0.15
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	17	0.15
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	17	0.15
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	17	0.15
(1,126)	1:17:A:THR:HB	1:24:A:GLU:HG2	20	0.15
(1,126)	1:17:A:THR:HB	1:24:A:GLU:HG3	20	0.15
(1,117)	1:16:A:LEU:HD11	1:19:A:LYS:HA	2	0.15
(1,117)	1:16:A:LEU:HD12	1:19:A:LYS:HA	2	0.15
(1,117)	1:16:A:LEU:HD13	1:19:A:LYS:HA	2	0.15
(1,117)	1:16:A:LEU:HD21	1:19:A:LYS:HA	2	0.15
(1,117)	1:16:A:LEU:HD22	1:19:A:LYS:HA	2	0.15
(1,117)	1:16:A:LEU:HD23	1:19:A:LYS:HA	2	0.15
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	13	0.15
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	13	0.15
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	13	0.15
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	15	0.15
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	15	0.15
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG2	13	0.15
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG3	13	0.15
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	4	0.15
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	9	0.15
(1,70)	1:13:A:VAL:H	1:14:A:GLU:HG2	20	0.15
(1,70)	1:13:A:VAL:H	1:14:A:GLU:HG3	20	0.15
(1,54)	1:12:A:VAL:HA	1:14:A:GLU:HB2	1	0.15
(1,54)	1:12:A:VAL:HA	1:14:A:GLU:HB3	1	0.15
(3,109)	1:166:A:LEU:O	1:170:A:GLN:N	11	0.14
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	20	0.14
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	4	0.14
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	8	0.14
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	19	0.14
(3,96)	1:129:A:TYR:O	1:133:A:GLY:H	15	0.14
(3,94)	1:127:A:ALA:O	1:131:A:MET:H	14	0.14
(3,92)	1:125:A:VAL:O	1:129:A:TYR:H	8	0.14
(3,92)	1:125:A:VAL:O	1:129:A:TYR:H	15	0.14
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	5	0.14
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	11	0.14
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	10	0.14
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	17	0.14
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	20	0.14
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	15	0.14
(3,17)	1:28:A:GLN:O	1:32:A:LYS:H	6	0.14
(3,14)	1:30:A:TRP:O	1:34:A:PHE:N	13	0.14
(3,9)	1:25:A:LYS:O	1:29:A:GLN:N	10	0.14
(3,9)	1:25:A:LYS:O	1:29:A:GLN:N	11	0.14
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	5	0.14
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	10	0.14
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	18	0.14
(3,4)	1:11:A:GLU:O	1:15:A:GLU:H	5	0.14
(2,4)	1:79:A:ARG:O	2:600:A:CA:CA	13	0.14
(1,1296)	1:189:A:LEU:HA	1:190:A:VAL:H	14	0.14
(1,1290)	1:186:A:TYR:HD1	1:189:A:LEU:HB2	15	0.14
(1,1290)	1:186:A:TYR:HD1	1:189:A:LEU:HB3	15	0.14
(1,1290)	1:186:A:TYR:HD2	1:189:A:LEU:HB2	15	0.14
(1,1290)	1:186:A:TYR:HD2	1:189:A:LEU:HB3	15	0.14
(1,1283)	1:184:A:SER:HB2	1:186:A:TYR:H	4	0.14
(1,1283)	1:184:A:SER:HB3	1:186:A:TYR:H	4	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD11	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD12	7	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD13	7	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD21	7	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD22	7	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD23	7	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD11	7	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD12	7	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD13	7	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD21	7	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD22	7	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD23	7	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD11	7	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD12	7	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD13	7	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD21	7	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD22	7	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD23	7	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD11	7	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD12	7	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD13	7	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD21	7	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD22	7	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD23	7	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD11	7	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD12	7	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD13	7	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD21	7	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD22	7	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD23	7	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD11	7	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD12	7	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD13	7	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD21	7	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD22	7	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD23	7	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD11	19	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD12	19	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD13	19	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD21	19	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD22	19	0.14
(1,1276)	1:180:A:VAL:HG11	1:183:A:LEU:HD23	19	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD11	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD12	19	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD13	19	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD21	19	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD22	19	0.14
(1,1276)	1:180:A:VAL:HG12	1:183:A:LEU:HD23	19	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD11	19	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD12	19	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD13	19	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD21	19	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD22	19	0.14
(1,1276)	1:180:A:VAL:HG13	1:183:A:LEU:HD23	19	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD11	19	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD12	19	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD13	19	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD21	19	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD22	19	0.14
(1,1276)	1:180:A:VAL:HG21	1:183:A:LEU:HD23	19	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD11	19	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD12	19	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD13	19	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD21	19	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD22	19	0.14
(1,1276)	1:180:A:VAL:HG22	1:183:A:LEU:HD23	19	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD11	19	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD12	19	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD13	19	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD21	19	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD22	19	0.14
(1,1276)	1:180:A:VAL:HG23	1:183:A:LEU:HD23	19	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	12	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	12	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	12	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	12	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	12	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	12	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	19	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	19	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	19	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	19	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	19	0.14
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	19	0.14
(1,1247)	1:175:A:ALA:H	1:180:A:VAL:HG11	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:175:A:ALA:H	1:180:A:VAL:HG12	13	0.14
(1,1247)	1:175:A:ALA:H	1:180:A:VAL:HG13	13	0.14
(1,1247)	1:175:A:ALA:H	1:180:A:VAL:HG21	13	0.14
(1,1247)	1:175:A:ALA:H	1:180:A:VAL:HG22	13	0.14
(1,1247)	1:175:A:ALA:H	1:180:A:VAL:HG23	13	0.14
(1,1241)	1:174:A:LYS:HA	1:175:A:ALA:H	13	0.14
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG21	1	0.14
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG22	1	0.14
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG23	1	0.14
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	3	0.14
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	15	0.14
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	18	0.14
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	7	0.14
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	7	0.14
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB2	20	0.14
(1,1192)	1:166:A:LEU:HG	1:170:A:GLN:HB3	20	0.14
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	8	0.14
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	8	0.14
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD1	14	0.14
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD2	14	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	6	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	6	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	6	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	6	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	6	0.14
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	6	0.14
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	9	0.14
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	9	0.14
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	14	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	1	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	1	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	1	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	12	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	12	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	12	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	15	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	15	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	15	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	19	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	19	0.14
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	19	0.14
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:143:A:ASN:H	1:183:A:LEU:HB2	5	0.14
(1,1024)	1:143:A:ASN:H	1:183:A:LEU:HB3	5	0.14
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	8	0.14
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	8	0.14
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	14	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	9	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	9	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	9	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	9	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	9	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	9	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	11	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	11	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	11	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	11	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	11	0.14
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	11	0.14
(1,988)	1:135:A:THR:HB	1:138:A:LEU:H	4	0.14
(1,988)	1:135:A:THR:HB	1:138:A:LEU:H	10	0.14
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD11	19	0.14
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD12	19	0.14
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD13	19	0.14
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD21	19	0.14
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD22	19	0.14
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD23	19	0.14
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD11	19	0.14
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD12	19	0.14
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD13	19	0.14
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD21	19	0.14
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD22	19	0.14
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD23	19	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB1	11	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB2	11	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB3	11	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB1	11	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB2	11	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB3	11	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB1	11	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB2	11	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB3	11	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB1	16	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB2	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB3	16	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB1	16	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB2	16	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB3	16	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB1	16	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB2	16	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB3	16	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB1	18	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB2	18	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB3	18	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB1	18	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB2	18	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB3	18	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB1	18	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB2	18	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB3	18	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB1	19	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB2	19	0.14
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB3	19	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB1	19	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB2	19	0.14
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB3	19	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB1	19	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB2	19	0.14
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB3	19	0.14
(1,953)	1:125:A:VAL:HG11	1:129:A:TYR:H	15	0.14
(1,953)	1:125:A:VAL:HG12	1:129:A:TYR:H	15	0.14
(1,953)	1:125:A:VAL:HG13	1:129:A:TYR:H	15	0.14
(1,953)	1:125:A:VAL:HG21	1:129:A:TYR:H	15	0.14
(1,953)	1:125:A:VAL:HG22	1:129:A:TYR:H	15	0.14
(1,953)	1:125:A:VAL:HG23	1:129:A:TYR:H	15	0.14
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD11	19	0.14
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD12	19	0.14
(1,951)	1:125:A:VAL:HB	1:128:A:ILE:HD13	19	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	1	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	1	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	4	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	4	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	7	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	7	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	10	0.14
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	20	0.14
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	20	0.14
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	20	0.14
(1,928)	1:122:A:LEU:HD11	1:149:A:VAL:HB	20	0.14
(1,928)	1:122:A:LEU:HD12	1:149:A:VAL:HB	20	0.14
(1,928)	1:122:A:LEU:HD13	1:149:A:VAL:HB	20	0.14
(1,928)	1:122:A:LEU:HD21	1:149:A:VAL:HB	20	0.14
(1,928)	1:122:A:LEU:HD22	1:149:A:VAL:HB	20	0.14
(1,928)	1:122:A:LEU:HD23	1:149:A:VAL:HB	20	0.14
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG11	7	0.14
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG12	7	0.14
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG13	7	0.14
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG21	7	0.14
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG22	7	0.14
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG23	7	0.14
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG11	7	0.14
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG12	7	0.14
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG13	7	0.14
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG21	7	0.14
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG22	7	0.14
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG23	7	0.14
(1,900)	1:118:A:ARG:HB2	1:150:A:ASP:HA	11	0.14
(1,900)	1:118:A:ARG:HB3	1:150:A:ASP:HA	11	0.14
(1,895)	1:118:A:ARG:H	1:118:A:ARG:HD2	3	0.14
(1,895)	1:118:A:ARG:H	1:118:A:ARG:HD3	3	0.14
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	2	0.14
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	2	0.14
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	3	0.14
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	3	0.14
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	10	0.14
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	10	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD11	9	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD12	9	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD13	9	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD21	9	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD22	9	0.14
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD23	9	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD11	9	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD12	9	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD13	9	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD21	9	0.14
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD22	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD23	9	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD11	9	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD12	9	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD13	9	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD21	9	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD22	9	0.14
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD23	9	0.14
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	19	0.14
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	19	0.14
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	19	0.14
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	18	0.14
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	18	0.14
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	18	0.14
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	18	0.14
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	6	0.14
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	6	0.14
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	6	0.14
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	10	0.14
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	10	0.14
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	10	0.14
(1,812)	1:110:A:LEU:H	1:110:A:LEU:HD11	5	0.14
(1,812)	1:110:A:LEU:H	1:110:A:LEU:HD12	5	0.14
(1,812)	1:110:A:LEU:H	1:110:A:LEU:HD13	5	0.14
(1,812)	1:110:A:LEU:H	1:110:A:LEU:HD21	5	0.14
(1,812)	1:110:A:LEU:H	1:110:A:LEU:HD22	5	0.14
(1,812)	1:110:A:LEU:H	1:110:A:LEU:HD23	5	0.14
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG21	9	0.14
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG22	9	0.14
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG23	9	0.14
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG21	9	0.14
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG22	9	0.14
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG23	9	0.14
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG21	17	0.14
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG22	17	0.14
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG23	17	0.14
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG21	17	0.14
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG22	17	0.14
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG23	17	0.14
(1,775)	1:107:A:LEU:HD11	1:110:A:LEU:HB2	15	0.14
(1,775)	1:107:A:LEU:HD11	1:110:A:LEU:HB3	15	0.14
(1,775)	1:107:A:LEU:HD12	1:110:A:LEU:HB2	15	0.14
(1,775)	1:107:A:LEU:HD12	1:110:A:LEU:HB3	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:107:A:LEU:HD13	1:110:A:LEU:HB2	15	0.14
(1,775)	1:107:A:LEU:HD13	1:110:A:LEU:HB3	15	0.14
(1,775)	1:107:A:LEU:HD21	1:110:A:LEU:HB2	15	0.14
(1,775)	1:107:A:LEU:HD21	1:110:A:LEU:HB3	15	0.14
(1,775)	1:107:A:LEU:HD22	1:110:A:LEU:HB2	15	0.14
(1,775)	1:107:A:LEU:HD22	1:110:A:LEU:HB3	15	0.14
(1,775)	1:107:A:LEU:HD23	1:110:A:LEU:HB2	15	0.14
(1,775)	1:107:A:LEU:HD23	1:110:A:LEU:HB3	15	0.14
(1,759)	1:104:A:ALA:HB1	1:169:A:PHE:HE1	19	0.14
(1,759)	1:104:A:ALA:HB1	1:169:A:PHE:HE2	19	0.14
(1,759)	1:104:A:ALA:HB2	1:169:A:PHE:HE1	19	0.14
(1,759)	1:104:A:ALA:HB2	1:169:A:PHE:HE2	19	0.14
(1,759)	1:104:A:ALA:HB3	1:169:A:PHE:HE1	19	0.14
(1,759)	1:104:A:ALA:HB3	1:169:A:PHE:HE2	19	0.14
(1,699)	1:91:A:VAL:HG11	1:103:A:TRP:HD1	9	0.14
(1,699)	1:91:A:VAL:HG12	1:103:A:TRP:HD1	9	0.14
(1,699)	1:91:A:VAL:HG13	1:103:A:TRP:HD1	9	0.14
(1,699)	1:91:A:VAL:HG21	1:103:A:TRP:HD1	9	0.14
(1,699)	1:91:A:VAL:HG22	1:103:A:TRP:HD1	9	0.14
(1,699)	1:91:A:VAL:HG23	1:103:A:TRP:HD1	9	0.14
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	8	0.14
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	8	0.14
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	8	0.14
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	18	0.14
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	18	0.14
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	18	0.14
(1,679)	1:89:A:LEU:HD11	1:91:A:VAL:HG11	2	0.14
(1,679)	1:89:A:LEU:HD11	1:91:A:VAL:HG12	2	0.14
(1,679)	1:89:A:LEU:HD11	1:91:A:VAL:HG13	2	0.14
(1,679)	1:89:A:LEU:HD11	1:91:A:VAL:HG21	2	0.14
(1,679)	1:89:A:LEU:HD11	1:91:A:VAL:HG22	2	0.14
(1,679)	1:89:A:LEU:HD11	1:91:A:VAL:HG23	2	0.14
(1,679)	1:89:A:LEU:HD12	1:91:A:VAL:HG11	2	0.14
(1,679)	1:89:A:LEU:HD12	1:91:A:VAL:HG12	2	0.14
(1,679)	1:89:A:LEU:HD12	1:91:A:VAL:HG13	2	0.14
(1,679)	1:89:A:LEU:HD12	1:91:A:VAL:HG21	2	0.14
(1,679)	1:89:A:LEU:HD12	1:91:A:VAL:HG22	2	0.14
(1,679)	1:89:A:LEU:HD12	1:91:A:VAL:HG23	2	0.14
(1,679)	1:89:A:LEU:HD13	1:91:A:VAL:HG11	2	0.14
(1,679)	1:89:A:LEU:HD13	1:91:A:VAL:HG12	2	0.14
(1,679)	1:89:A:LEU:HD13	1:91:A:VAL:HG13	2	0.14
(1,679)	1:89:A:LEU:HD13	1:91:A:VAL:HG21	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:89:A:LEU:HD13	1:91:A:VAL:HG22	2	0.14
(1,679)	1:89:A:LEU:HD13	1:91:A:VAL:HG23	2	0.14
(1,679)	1:89:A:LEU:HD21	1:91:A:VAL:HG11	2	0.14
(1,679)	1:89:A:LEU:HD21	1:91:A:VAL:HG12	2	0.14
(1,679)	1:89:A:LEU:HD21	1:91:A:VAL:HG13	2	0.14
(1,679)	1:89:A:LEU:HD21	1:91:A:VAL:HG21	2	0.14
(1,679)	1:89:A:LEU:HD21	1:91:A:VAL:HG22	2	0.14
(1,679)	1:89:A:LEU:HD21	1:91:A:VAL:HG23	2	0.14
(1,679)	1:89:A:LEU:HD22	1:91:A:VAL:HG11	2	0.14
(1,679)	1:89:A:LEU:HD22	1:91:A:VAL:HG12	2	0.14
(1,679)	1:89:A:LEU:HD22	1:91:A:VAL:HG13	2	0.14
(1,679)	1:89:A:LEU:HD22	1:91:A:VAL:HG21	2	0.14
(1,679)	1:89:A:LEU:HD22	1:91:A:VAL:HG22	2	0.14
(1,679)	1:89:A:LEU:HD22	1:91:A:VAL:HG23	2	0.14
(1,679)	1:89:A:LEU:HD23	1:91:A:VAL:HG11	2	0.14
(1,679)	1:89:A:LEU:HD23	1:91:A:VAL:HG12	2	0.14
(1,679)	1:89:A:LEU:HD23	1:91:A:VAL:HG13	2	0.14
(1,679)	1:89:A:LEU:HD23	1:91:A:VAL:HG21	2	0.14
(1,679)	1:89:A:LEU:HD23	1:91:A:VAL:HG22	2	0.14
(1,679)	1:89:A:LEU:HD23	1:91:A:VAL:HG23	2	0.14
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	6	0.14
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	6	0.14
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	13	0.14
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	13	0.14
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD11	19	0.14
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD12	19	0.14
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD13	19	0.14
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD11	19	0.14
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD12	19	0.14
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD13	19	0.14
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG12	6	0.14
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG13	6	0.14
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG21	10	0.14
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG22	10	0.14
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG23	10	0.14
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB1	17	0.14
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB2	17	0.14
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB3	17	0.14
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	10	0.14
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	10	0.14
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	2	0.14
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,476)	1:60:A:ASP:HB2	1:130:A:GLN:HB2	3	0.14
(1,476)	1:60:A:ASP:HB2	1:130:A:GLN:HB3	3	0.14
(1,476)	1:60:A:ASP:HB3	1:130:A:GLN:HB2	3	0.14
(1,476)	1:60:A:ASP:HB3	1:130:A:GLN:HB3	3	0.14
(1,463)	1:57:A:PRO:HD2	1:58:A:PHE:HA	18	0.14
(1,463)	1:57:A:PRO:HD3	1:58:A:PHE:HA	18	0.14
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	11	0.14
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	11	0.14
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	11	0.14
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	11	0.14
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	20	0.14
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	20	0.14
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	20	0.14
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	20	0.14
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD11	12	0.14
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD12	12	0.14
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD13	12	0.14
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD21	12	0.14
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD22	12	0.14
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD23	12	0.14
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD11	12	0.14
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD12	12	0.14
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD13	12	0.14
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD21	12	0.14
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD22	12	0.14
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD23	12	0.14
(1,420)	1:51:A:ILE:HD11	1:85:A:PHE:HB2	11	0.14
(1,420)	1:51:A:ILE:HD11	1:85:A:PHE:HB3	11	0.14
(1,420)	1:51:A:ILE:HD12	1:85:A:PHE:HB2	11	0.14
(1,420)	1:51:A:ILE:HD12	1:85:A:PHE:HB3	11	0.14
(1,420)	1:51:A:ILE:HD13	1:85:A:PHE:HB2	11	0.14
(1,420)	1:51:A:ILE:HD13	1:85:A:PHE:HB3	11	0.14
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG11	17	0.14
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG12	17	0.14
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG13	17	0.14
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG21	17	0.14
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG22	17	0.14
(1,407)	1:49:A:GLN:HG2	1:68:A:VAL:HG23	17	0.14
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG11	17	0.14
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG12	17	0.14
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG13	17	0.14
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG21	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG22	17	0.14
(1,407)	1:49:A:GLN:HG3	1:68:A:VAL:HG23	17	0.14
(1,387)	1:48:A:PHE:HE1	1:80:A:ILE:HG12	12	0.14
(1,387)	1:48:A:PHE:HE1	1:80:A:ILE:HG13	12	0.14
(1,387)	1:48:A:PHE:HE2	1:80:A:ILE:HG12	12	0.14
(1,387)	1:48:A:PHE:HE2	1:80:A:ILE:HG13	12	0.14
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	20	0.14
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	20	0.14
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	20	0.14
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	20	0.14
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	20	0.14
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	20	0.14
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	20	0.14
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	20	0.14
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	20	0.14
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	20	0.14
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	20	0.14
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	20	0.14
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD11	2	0.14
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD12	2	0.14
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD13	2	0.14
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD11	2	0.14
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD12	2	0.14
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD13	2	0.14
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	9	0.14
(1,367)	1:47:A:GLY:HA2	1:51:A:ILE:HG12	16	0.14
(1,367)	1:47:A:GLY:HA2	1:51:A:ILE:HG13	16	0.14
(1,367)	1:47:A:GLY:HA3	1:51:A:ILE:HG12	16	0.14
(1,367)	1:47:A:GLY:HA3	1:51:A:ILE:HG13	16	0.14
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	9	0.14
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	1	0.14
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	16	0.14
(1,311)	1:42:A:GLN:HG2	1:79:A:ARG:HA	14	0.14
(1,311)	1:42:A:GLN:HG3	1:79:A:ARG:HA	14	0.14
(1,306)	1:42:A:GLN:HA	1:81:A:GLU:H	13	0.14
(1,272)	1:34:A:PHE:HD1	1:35:A:ILE:HD11	14	0.14
(1,272)	1:34:A:PHE:HD1	1:35:A:ILE:HD12	14	0.14
(1,272)	1:34:A:PHE:HD1	1:35:A:ILE:HD13	14	0.14
(1,272)	1:34:A:PHE:HD2	1:35:A:ILE:HD11	14	0.14
(1,272)	1:34:A:PHE:HD2	1:35:A:ILE:HD12	14	0.14
(1,272)	1:34:A:PHE:HD2	1:35:A:ILE:HD13	14	0.14
(1,267)	1:34:A:PHE:HB2	1:41:A:GLY:HA2	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:34:A:PHE:HB2	1:41:A:GLY:HA3	16	0.14
(1,267)	1:34:A:PHE:HB3	1:41:A:GLY:HA2	16	0.14
(1,267)	1:34:A:PHE:HB3	1:41:A:GLY:HA3	16	0.14
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	10	0.14
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD11	4	0.14
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD12	4	0.14
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD13	4	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD11	4	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD12	4	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD13	4	0.14
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD11	15	0.14
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD12	15	0.14
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD13	15	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD11	15	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD12	15	0.14
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD13	15	0.14
(1,229)	1:30:A:TRP:H	1:30:A:TRP:HD1	5	0.14
(1,199)	1:24:A:GLU:HB2	1:27:A:VAL:H	4	0.14
(1,199)	1:24:A:GLU:HB3	1:27:A:VAL:H	4	0.14
(1,199)	1:24:A:GLU:HB2	1:27:A:VAL:H	12	0.14
(1,199)	1:24:A:GLU:HB3	1:27:A:VAL:H	12	0.14
(1,193)	1:24:A:GLU:H	1:24:A:GLU:HG2	11	0.14
(1,193)	1:24:A:GLU:H	1:24:A:GLU:HG3	11	0.14
(1,192)	1:23:A:THR:HG21	1:24:A:GLU:HB2	10	0.14
(1,192)	1:23:A:THR:HG21	1:24:A:GLU:HB3	10	0.14
(1,192)	1:23:A:THR:HG22	1:24:A:GLU:HB2	10	0.14
(1,192)	1:23:A:THR:HG22	1:24:A:GLU:HB3	10	0.14
(1,192)	1:23:A:THR:HG23	1:24:A:GLU:HB2	10	0.14
(1,192)	1:23:A:THR:HG23	1:24:A:GLU:HB3	10	0.14
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	9	0.14
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	9	0.14
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	9	0.14
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	11	0.14
(1,150)	1:20:A:THR:HG21	1:22:A:PHE:H	13	0.14
(1,150)	1:20:A:THR:HG22	1:22:A:PHE:H	13	0.14
(1,150)	1:20:A:THR:HG23	1:22:A:PHE:H	13	0.14
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	16	0.14
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	16	0.14
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	16	0.14
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	16	0.14
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	16	0.14
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:19:A:LYS:HB2	1:20:A:THR:HG21	15	0.14
(1,142)	1:19:A:LYS:HB2	1:20:A:THR:HG22	15	0.14
(1,142)	1:19:A:LYS:HB2	1:20:A:THR:HG23	15	0.14
(1,142)	1:19:A:LYS:HB3	1:20:A:THR:HG21	15	0.14
(1,142)	1:19:A:LYS:HB3	1:20:A:THR:HG22	15	0.14
(1,142)	1:19:A:LYS:HB3	1:20:A:THR:HG23	15	0.14
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG11	11	0.14
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG12	11	0.14
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG13	11	0.14
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG21	11	0.14
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG22	11	0.14
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG23	11	0.14
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD11	6	0.14
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD12	6	0.14
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD13	6	0.14
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD21	6	0.14
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD22	6	0.14
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD23	6	0.14
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD11	6	0.14
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD12	6	0.14
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD13	6	0.14
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD21	6	0.14
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD22	6	0.14
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD23	6	0.14
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD11	6	0.14
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD12	6	0.14
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD13	6	0.14
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD21	6	0.14
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD22	6	0.14
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD23	6	0.14
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD11	6	0.14
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD12	6	0.14
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD13	6	0.14
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD21	6	0.14
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD22	6	0.14
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD23	6	0.14
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD11	6	0.14
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD12	6	0.14
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD13	6	0.14
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD21	6	0.14
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD22	6	0.14
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD23	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD11	6	0.14
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD12	6	0.14
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD13	6	0.14
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD21	6	0.14
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD22	6	0.14
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD23	6	0.14
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG2	7	0.14
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG3	7	0.14
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG2	7	0.14
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG3	7	0.14
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG2	7	0.14
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG3	7	0.14
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG2	7	0.14
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG3	7	0.14
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG2	7	0.14
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG3	7	0.14
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG2	7	0.14
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG3	7	0.14
(1,102)	1:15:A:GLU:HG2	1:18:A:ARG:HD2	19	0.14
(1,102)	1:15:A:GLU:HG2	1:18:A:ARG:HD3	19	0.14
(1,102)	1:15:A:GLU:HG3	1:18:A:ARG:HD2	19	0.14
(1,102)	1:15:A:GLU:HG3	1:18:A:ARG:HD3	19	0.14
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	1	0.14
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	13	0.14
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	15	0.14
(1,66)	1:12:A:VAL:HG21	1:16:A:LEU:HG	3	0.14
(1,66)	1:12:A:VAL:HG22	1:16:A:LEU:HG	3	0.14
(1,66)	1:12:A:VAL:HG23	1:16:A:LEU:HG	3	0.14
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD1	12	0.14
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD2	12	0.14
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD1	12	0.14
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD2	12	0.14
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD1	16	0.14
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD2	16	0.14
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD1	16	0.14
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD2	16	0.14
(3,115)	1:167:A:GLN:O	1:171:A:GLU:H	11	0.13
(3,114)	1:166:A:LEU:O	1:170:A:GLN:H	2	0.13
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	11	0.13
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	17	0.13
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	1	0.13
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	15	0.13
(3,61)	1:89:A:LEU:O	1:93:A:SER:H	7	0.13
(3,59)	1:87:A:GLN:O	1:91:A:VAL:H	10	0.13
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	18	0.13
(3,45)	1:67:A:PHE:O	1:71:A:VAL:H	4	0.13
(3,45)	1:67:A:PHE:O	1:71:A:VAL:H	8	0.13
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	4	0.13
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	9	0.13
(3,27)	1:52:A:TYR:O	1:56:A:PHE:N	12	0.13
(3,27)	1:52:A:TYR:O	1:56:A:PHE:N	14	0.13
(3,27)	1:52:A:TYR:O	1:56:A:PHE:N	20	0.13
(3,23)	1:48:A:PHE:O	1:52:A:TYR:N	13	0.13
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	8	0.13
(3,14)	1:30:A:TRP:O	1:34:A:PHE:N	14	0.13
(3,4)	1:11:A:GLU:O	1:15:A:GLU:H	11	0.13
(3,4)	1:11:A:GLU:O	1:15:A:GLU:H	20	0.13
(3,2)	1:12:A:VAL:O	1:16:A:LEU:N	7	0.13
(2,14)	1:159:A:ASN:OD1	2:602:A:CA:CA	10	0.13
(2,2)	1:75:A:ASN:OD1	2:600:A:CA:CA	13	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	6	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	6	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	6	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	6	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	6	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	6	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	9	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	9	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	9	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	9	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	9	0.13
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	9	0.13
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD11	4	0.13
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD12	4	0.13
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD13	4	0.13
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD11	13	0.13
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD12	13	0.13
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD13	13	0.13
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD2	13	0.13
(1,1239)	1:174:A:LYS:HA	1:174:A:LYS:HD3	13	0.13
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG21	14	0.13
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG22	14	0.13
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG23	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	1	0.13
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	7	0.13
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	12	0.13
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	14	0.13
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	19	0.13
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	20	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG11	6	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG12	6	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG13	6	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG21	6	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG22	6	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG23	6	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG11	20	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG12	20	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG13	20	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG21	20	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG22	20	0.13
(1,1215)	1:170:A:GLN:HA	1:180:A:VAL:HG23	20	0.13
(1,1208)	1:169:A:PHE:HA	1:179:A:ILE:HB	11	0.13
(1,1208)	1:169:A:PHE:HA	1:179:A:ILE:HB	13	0.13
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	2	0.13
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	2	0.13
(1,1189)	1:166:A:LEU:HB2	1:170:A:GLN:HA	17	0.13
(1,1189)	1:166:A:LEU:HB3	1:170:A:GLN:HA	17	0.13
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	5	0.13
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	5	0.13
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	5	0.13
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	5	0.13
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	5	0.13
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	5	0.13
(1,1172)	1:164:A:LEU:HG	1:165:A:THR:H	11	0.13
(1,1167)	1:164:A:LEU:H	1:165:A:THR:HA	5	0.13
(1,1167)	1:164:A:LEU:H	1:165:A:THR:HA	16	0.13
(1,1148)	1:159:A:ASN:H	1:160:A:ALA:H	19	0.13
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	1	0.13
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	1	0.13
(1,1146)	1:158:A:LYS:HB2	1:159:A:ASN:H	15	0.13
(1,1146)	1:158:A:LYS:HB3	1:159:A:ASN:H	15	0.13
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	7	0.13
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	6	0.13
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	6	0.13
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	8	0.13
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	8	0.13
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	8	0.13
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	13	0.13
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG21	5	0.13
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG22	5	0.13
(1,1025)	1:144:A:THR:H	1:144:A:THR:HG23	5	0.13
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG21	12	0.13
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG22	12	0.13
(1,1023)	1:143:A:ASN:H	1:144:A:THR:HG23	12	0.13
(1,1017)	1:142:A:GLU:H	1:143:A:ASN:H	5	0.13
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	16	0.13
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	16	0.13
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD11	8	0.13
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD12	8	0.13
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD13	8	0.13
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD21	8	0.13
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD22	8	0.13
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD23	8	0.13
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD11	8	0.13
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD12	8	0.13
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD13	8	0.13
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD21	8	0.13
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD22	8	0.13
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD23	8	0.13
(1,973)	1:129:A:TYR:HB2	1:144:A:THR:HG21	4	0.13
(1,973)	1:129:A:TYR:HB2	1:144:A:THR:HG22	4	0.13
(1,973)	1:129:A:TYR:HB2	1:144:A:THR:HG23	4	0.13
(1,973)	1:129:A:TYR:HB3	1:144:A:THR:HG21	4	0.13
(1,973)	1:129:A:TYR:HB3	1:144:A:THR:HG22	4	0.13
(1,973)	1:129:A:TYR:HB3	1:144:A:THR:HG23	4	0.13
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB1	9	0.13
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB2	9	0.13
(1,967)	1:128:A:ILE:HD11	1:182:A:ALA:HB3	9	0.13
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB1	9	0.13
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB2	9	0.13
(1,967)	1:128:A:ILE:HD12	1:182:A:ALA:HB3	9	0.13
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB1	9	0.13
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB2	9	0.13
(1,967)	1:128:A:ILE:HD13	1:182:A:ALA:HB3	9	0.13
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	13	0.13
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	13	0.13
(1,927)	1:122:A:LEU:HD11	1:146:A:GLU:HG2	8	0.13
(1,927)	1:122:A:LEU:HD11	1:146:A:GLU:HG3	8	0.13
(1,927)	1:122:A:LEU:HD12	1:146:A:GLU:HG2	8	0.13
(1,927)	1:122:A:LEU:HD12	1:146:A:GLU:HG3	8	0.13
(1,927)	1:122:A:LEU:HD13	1:146:A:GLU:HG2	8	0.13
(1,927)	1:122:A:LEU:HD13	1:146:A:GLU:HG3	8	0.13
(1,927)	1:122:A:LEU:HD21	1:146:A:GLU:HG2	8	0.13
(1,927)	1:122:A:LEU:HD21	1:146:A:GLU:HG3	8	0.13
(1,927)	1:122:A:LEU:HD22	1:146:A:GLU:HG2	8	0.13
(1,927)	1:122:A:LEU:HD22	1:146:A:GLU:HG3	8	0.13
(1,927)	1:122:A:LEU:HD23	1:146:A:GLU:HG2	8	0.13
(1,927)	1:122:A:LEU:HD23	1:146:A:GLU:HG3	8	0.13
(1,905)	1:119:A:ASN:HA	1:122:A:LEU:HG	17	0.13
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	12	0.13
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	12	0.13
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	14	0.13
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	14	0.13
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	6	0.13
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	6	0.13
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	17	0.13
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	17	0.13
(1,865)	1:116:A:ILE:HB	1:164:A:LEU:HA	7	0.13
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD2	17	0.13
(1,857)	1:115:A:TYR:HE1	1:163:A:LYS:HD3	17	0.13
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD2	17	0.13
(1,857)	1:115:A:TYR:HE2	1:163:A:LYS:HD3	17	0.13
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	10	0.13
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	10	0.13
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	10	0.13
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	10	0.13
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	18	0.13
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	18	0.13
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	18	0.13
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD11	3	0.13
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD12	3	0.13
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD13	3	0.13
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD11	3	0.13
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD12	3	0.13
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD13	3	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	2	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	2	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	2	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	2	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	2	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	2	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	2	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	2	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	2	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	2	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	2	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD11	18	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD12	18	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD13	18	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD21	18	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD22	18	0.13
(1,787)	1:108:A:TYR:HB2	1:164:A:LEU:HD23	18	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD11	18	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD12	18	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD13	18	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD21	18	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD22	18	0.13
(1,787)	1:108:A:TYR:HB3	1:164:A:LEU:HD23	18	0.13
(1,773)	1:107:A:LEU:HD11	1:108:A:TYR:H	5	0.13
(1,773)	1:107:A:LEU:HD12	1:108:A:TYR:H	5	0.13
(1,773)	1:107:A:LEU:HD13	1:108:A:TYR:H	5	0.13
(1,773)	1:107:A:LEU:HD21	1:108:A:TYR:H	5	0.13
(1,773)	1:107:A:LEU:HD22	1:108:A:TYR:H	5	0.13
(1,773)	1:107:A:LEU:HD23	1:108:A:TYR:H	5	0.13
(1,773)	1:107:A:LEU:HD11	1:108:A:TYR:H	9	0.13
(1,773)	1:107:A:LEU:HD12	1:108:A:TYR:H	9	0.13
(1,773)	1:107:A:LEU:HD13	1:108:A:TYR:H	9	0.13
(1,773)	1:107:A:LEU:HD21	1:108:A:TYR:H	9	0.13
(1,773)	1:107:A:LEU:HD22	1:108:A:TYR:H	9	0.13
(1,773)	1:107:A:LEU:HD23	1:108:A:TYR:H	9	0.13
(1,715)	1:96:A:THR:HB	1:98:A:ASP:H	1	0.13
(1,715)	1:96:A:THR:HB	1:98:A:ASP:H	11	0.13
(1,715)	1:96:A:THR:HB	1:98:A:ASP:H	18	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD11	2	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD12	2	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD13	2	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD21	2	0.13
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD22	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD23	2	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD11	2	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD12	2	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD13	2	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD21	2	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD22	2	0.13
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD23	2	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD11	2	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD12	2	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD13	2	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD21	2	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD22	2	0.13
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD23	2	0.13
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	18	0.13
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	18	0.13
(1,641)	1:85:A:PHE:HD1	1:89:A:LEU:HA	11	0.13
(1,641)	1:85:A:PHE:HD2	1:89:A:LEU:HA	11	0.13
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD11	4	0.13
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD12	4	0.13
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD13	4	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD11	4	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD12	4	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD13	4	0.13
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD11	12	0.13
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD12	12	0.13
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD13	12	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD11	12	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD12	12	0.13
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD13	12	0.13
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	4	0.13
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	4	0.13
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	6	0.13
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	6	0.13
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	10	0.13
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	10	0.13
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	12	0.13
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	12	0.13
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB1	9	0.13
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB2	9	0.13
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB3	9	0.13
(1,567)	1:71:A:VAL:HG11	1:72:A:PHE:H	9	0.13
(1,567)	1:71:A:VAL:HG12	1:72:A:PHE:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:71:A:VAL:HG13	1:72:A:PHE:H	9	0.13
(1,567)	1:71:A:VAL:HG21	1:72:A:PHE:H	9	0.13
(1,567)	1:71:A:VAL:HG22	1:72:A:PHE:H	9	0.13
(1,567)	1:71:A:VAL:HG23	1:72:A:PHE:H	9	0.13
(1,557)	1:69:A:PHE:HD1	1:80:A:ILE:HA	13	0.13
(1,557)	1:69:A:PHE:HD2	1:80:A:ILE:HA	13	0.13
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	9	0.13
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	9	0.13
(1,540)	1:68:A:VAL:HB	1:71:A:VAL:HG11	7	0.13
(1,540)	1:68:A:VAL:HB	1:71:A:VAL:HG12	7	0.13
(1,540)	1:68:A:VAL:HB	1:71:A:VAL:HG13	7	0.13
(1,540)	1:68:A:VAL:HB	1:71:A:VAL:HG21	7	0.13
(1,540)	1:68:A:VAL:HB	1:71:A:VAL:HG22	7	0.13
(1,540)	1:68:A:VAL:HB	1:71:A:VAL:HG23	7	0.13
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	3	0.13
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	3	0.13
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	15	0.13
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	15	0.13
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD11	4	0.13
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD12	4	0.13
(1,524)	1:67:A:PHE:HA	1:124:A:ILE:HD13	4	0.13
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB2	16	0.13
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB3	16	0.13
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD11	9	0.13
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD12	9	0.13
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD13	9	0.13
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD11	9	0.13
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD12	9	0.13
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD13	9	0.13
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD11	14	0.13
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD12	14	0.13
(1,503)	1:64:A:PHE:HB2	1:124:A:ILE:HD13	14	0.13
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD11	14	0.13
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD12	14	0.13
(1,503)	1:64:A:PHE:HB3	1:124:A:ILE:HD13	14	0.13
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	6	0.13
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	6	0.13
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	6	0.13
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	6	0.13
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	6	0.13
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	18	0.13
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	18	0.13
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	18	0.13
(1,444)	1:53:A:LYS:HB2	1:57:A:PRO:HG2	1	0.13
(1,444)	1:53:A:LYS:HB2	1:57:A:PRO:HG3	1	0.13
(1,444)	1:53:A:LYS:HB3	1:57:A:PRO:HG2	1	0.13
(1,444)	1:53:A:LYS:HB3	1:57:A:PRO:HG3	1	0.13
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	14	0.13
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	14	0.13
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	14	0.13
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	14	0.13
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	14	0.13
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	14	0.13
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	14	0.13
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	14	0.13
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	14	0.13
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	14	0.13
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	14	0.13
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	14	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD11	4	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD12	4	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD13	4	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD21	4	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD22	4	0.13
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD23	4	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD11	4	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD12	4	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD13	4	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD21	4	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD22	4	0.13
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD23	4	0.13
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	17	0.13
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	17	0.13
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	17	0.13
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	17	0.13
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	17	0.13
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	17	0.13
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB1	17	0.13
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB2	17	0.13
(1,383)	1:48:A:PHE:HD1	1:88:A:ALA:HB3	17	0.13
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB1	17	0.13
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB2	17	0.13
(1,383)	1:48:A:PHE:HD2	1:88:A:ALA:HB3	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:48:A:PHE:HD1	1:65:A:ALA:HA	3	0.13
(1,379)	1:48:A:PHE:HD2	1:65:A:ALA:HA	3	0.13
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	4	0.13
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	4	0.13
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	4	0.13
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	4	0.13
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	4	0.13
(1,367)	1:47:A:GLY:HA2	1:51:A:ILE:HG12	11	0.13
(1,367)	1:47:A:GLY:HA2	1:51:A:ILE:HG13	11	0.13
(1,367)	1:47:A:GLY:HA3	1:51:A:ILE:HG12	11	0.13
(1,367)	1:47:A:GLY:HA3	1:51:A:ILE:HG13	11	0.13
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	19	0.13
(1,276)	1:34:A:PHE:HZ	1:86:A:ILE:HA	14	0.13
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	11	0.13
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	17	0.13
(1,229)	1:30:A:TRP:H	1:30:A:TRP:HD1	1	0.13
(1,177)	1:22:A:PHE:HB2	1:86:A:ILE:HD11	2	0.13
(1,177)	1:22:A:PHE:HB2	1:86:A:ILE:HD12	2	0.13
(1,177)	1:22:A:PHE:HB2	1:86:A:ILE:HD13	2	0.13
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	7	0.13
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	7	0.13
(1,160)	1:21:A:TYR:HA	1:22:A:PHE:H	12	0.13
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG21	7	0.13
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG22	7	0.13
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG23	7	0.13
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG21	7	0.13
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG22	7	0.13
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG23	7	0.13
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG21	7	0.13
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG22	7	0.13
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG23	7	0.13
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	8	0.13
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	8	0.13
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	8	0.13
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	8	0.13
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	8	0.13
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	8	0.13
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	10	0.13
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	10	0.13
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	10	0.13
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	10	0.13
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	10	0.13
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	13	0.13
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	13	0.13
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	13	0.13
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	13	0.13
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	13	0.13
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	13	0.13
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	9	0.13
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	9	0.13
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	9	0.13
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	14	0.13
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	14	0.13
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	14	0.13
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	18	0.13
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	18	0.13
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	18	0.13
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	20	0.13
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	20	0.13
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	20	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG11	4	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG12	4	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG13	4	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG21	4	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG22	4	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG23	4	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG11	16	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG12	16	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG13	16	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG21	16	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG22	16	0.13
(1,127)	1:17:A:THR:HB	1:27:A:VAL:HG23	16	0.13
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD11	4	0.13
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD12	4	0.13
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD13	4	0.13
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD21	4	0.13
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD22	4	0.13
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD23	4	0.13
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD11	4	0.13
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD12	4	0.13
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD13	4	0.13
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD21	4	0.13
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD22	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD23	4	0.13
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD11	4	0.13
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD12	4	0.13
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD13	4	0.13
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD21	4	0.13
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD22	4	0.13
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD23	4	0.13
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD11	4	0.13
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD12	4	0.13
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD13	4	0.13
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD21	4	0.13
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD22	4	0.13
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD23	4	0.13
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD11	4	0.13
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD12	4	0.13
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD13	4	0.13
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD21	4	0.13
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD22	4	0.13
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD23	4	0.13
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD11	4	0.13
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD12	4	0.13
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD13	4	0.13
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD21	4	0.13
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD22	4	0.13
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD23	4	0.13
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	5	0.13
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	5	0.13
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	5	0.13
(1,98)	1:15:A:GLU:HA	1:18:A:ARG:HD2	7	0.13
(1,98)	1:15:A:GLU:HA	1:18:A:ARG:HD3	7	0.13
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	7	0.13
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	8	0.13
(1,83)	1:13:A:VAL:HG11	1:24:A:GLU:HA	18	0.13
(1,83)	1:13:A:VAL:HG12	1:24:A:GLU:HA	18	0.13
(1,83)	1:13:A:VAL:HG13	1:24:A:GLU:HA	18	0.13
(1,83)	1:13:A:VAL:HG21	1:24:A:GLU:HA	18	0.13
(1,83)	1:13:A:VAL:HG22	1:24:A:GLU:HA	18	0.13
(1,83)	1:13:A:VAL:HG23	1:24:A:GLU:HA	18	0.13
(1,66)	1:12:A:VAL:HG21	1:16:A:LEU:HG	20	0.13
(1,66)	1:12:A:VAL:HG22	1:16:A:LEU:HG	20	0.13
(1,66)	1:12:A:VAL:HG23	1:16:A:LEU:HG	20	0.13
(1,65)	1:12:A:VAL:HG21	1:16:A:LEU:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:12:A:VAL:HG22	1:16:A:LEU:H	19	0.13
(1,65)	1:12:A:VAL:HG23	1:16:A:LEU:H	19	0.13
(1,64)	1:12:A:VAL:HG21	1:15:A:GLU:HG2	4	0.13
(1,64)	1:12:A:VAL:HG21	1:15:A:GLU:HG3	4	0.13
(1,64)	1:12:A:VAL:HG22	1:15:A:GLU:HG2	4	0.13
(1,64)	1:12:A:VAL:HG22	1:15:A:GLU:HG3	4	0.13
(1,64)	1:12:A:VAL:HG23	1:15:A:GLU:HG2	4	0.13
(1,64)	1:12:A:VAL:HG23	1:15:A:GLU:HG3	4	0.13
(1,54)	1:12:A:VAL:HA	1:14:A:GLU:HB2	13	0.13
(1,54)	1:12:A:VAL:HA	1:14:A:GLU:HB3	13	0.13
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	13	0.13
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	13	0.13
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	13	0.13
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	13	0.13
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	13	0.13
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	13	0.13
(3,124)	1:164:A:LEU:O	1:116:A:ILE:H	7	0.12
(3,124)	1:164:A:LEU:O	1:116:A:ILE:H	10	0.12
(3,118)	1:170:A:GLN:O	1:174:A:LYS:H	5	0.12
(3,118)	1:170:A:GLN:O	1:174:A:LYS:H	12	0.12
(3,115)	1:167:A:GLN:O	1:171:A:GLU:H	1	0.12
(3,114)	1:166:A:LEU:O	1:170:A:GLN:H	6	0.12
(3,113)	1:170:A:GLN:O	1:174:A:LYS:N	6	0.12
(3,112)	1:169:A:PHE:O	1:173:A:SER:N	10	0.12
(3,109)	1:166:A:LEU:O	1:170:A:GLN:N	13	0.12
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	4	0.12
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	8	0.12
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	16	0.12
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	12	0.12
(3,102)	1:151:A:ARG:O	1:155:A:MET:N	18	0.12
(3,100)	1:149:A:VAL:O	1:153:A:PHE:N	17	0.12
(3,91)	1:124:A:ILE:O	1:128:A:ILE:H	12	0.12
(3,87)	1:120:A:GLU:O	1:124:A:ILE:H	13	0.12
(3,83)	1:125:A:VAL:O	1:129:A:TYR:N	14	0.12
(3,74)	1:103:A:TRP:O	1:107:A:LEU:H	14	0.12
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	14	0.12
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	15	0.12
(3,46)	1:68:A:VAL:O	1:72:A:PHE:H	19	0.12
(3,45)	1:67:A:PHE:O	1:71:A:VAL:H	1	0.12
(3,37)	1:65:A:ALA:O	1:69:A:PHE:N	13	0.12
(3,33)	1:50:A:LYS:O	1:54:A:GLN:H	2	0.12
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	15	0.12
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	16	0.12
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	19	0.12
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	20	0.12
(3,30)	1:47:A:GLY:O	1:51:A:ILE:H	3	0.12
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	8	0.12
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	1	0.12
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	20	0.12
(3,7)	1:14:A:GLU:O	1:18:A:ARG:H	9	0.12
(3,5)	1:12:A:VAL:O	1:16:A:LEU:H	14	0.12
(3,4)	1:11:A:GLU:O	1:15:A:GLU:H	9	0.12
(2,17)	1:168:A:GLU:OE1	2:602:A:CA:CA	16	0.12
(2,16)	1:163:A:LYS:O	2:602:A:CA:CA	10	0.12
(2,15)	1:161:A:ASP:OD2	2:602:A:CA:CA	5	0.12
(2,3)	1:77:A:ASP:OD1	2:600:A:CA:CA	7	0.12
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	15	0.12
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	15	0.12
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	15	0.12
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	15	0.12
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	15	0.12
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	15	0.12
(1,1233)	1:173:A:SER:HB2	1:179:A:ILE:HD11	6	0.12
(1,1233)	1:173:A:SER:HB2	1:179:A:ILE:HD12	6	0.12
(1,1233)	1:173:A:SER:HB2	1:179:A:ILE:HD13	6	0.12
(1,1233)	1:173:A:SER:HB3	1:179:A:ILE:HD11	6	0.12
(1,1233)	1:173:A:SER:HB3	1:179:A:ILE:HD12	6	0.12
(1,1233)	1:173:A:SER:HB3	1:179:A:ILE:HD13	6	0.12
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	2	0.12
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	4	0.12
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	5	0.12
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	9	0.12
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	10	0.12
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	11	0.12
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	13	0.12
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	17	0.12
(1,1211)	1:169:A:PHE:HE1	1:179:A:ILE:HG12	6	0.12
(1,1211)	1:169:A:PHE:HE1	1:179:A:ILE:HG13	6	0.12
(1,1211)	1:169:A:PHE:HE2	1:179:A:ILE:HG12	6	0.12
(1,1211)	1:169:A:PHE:HE2	1:179:A:ILE:HG13	6	0.12
(1,1208)	1:169:A:PHE:HA	1:179:A:ILE:HB	1	0.12
(1,1208)	1:169:A:PHE:HA	1:179:A:ILE:HB	4	0.12
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	20	0.12
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	20	0.12
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	20	0.12
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	20	0.12
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	20	0.12
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG21	16	0.12
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG22	16	0.12
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG23	16	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG21	16	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG22	16	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG23	16	0.12
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG21	18	0.12
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG22	18	0.12
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG23	18	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG21	18	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG22	18	0.12
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG23	18	0.12
(1,1153)	1:160:A:ALA:HA	1:161:A:ASP:H	15	0.12
(1,1142)	1:158:A:LYS:H	1:158:A:LYS:HG2	7	0.12
(1,1142)	1:158:A:LYS:H	1:158:A:LYS:HG3	7	0.12
(1,1139)	1:157:A:ASP:HB2	1:164:A:LEU:HB2	16	0.12
(1,1139)	1:157:A:ASP:HB2	1:164:A:LEU:HB3	16	0.12
(1,1139)	1:157:A:ASP:HB3	1:164:A:LEU:HB2	16	0.12
(1,1139)	1:157:A:ASP:HB3	1:164:A:LEU:HB3	16	0.12
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	3	0.12
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	5	0.12
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	8	0.12
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	14	0.12
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	7	0.12
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	7	0.12
(1,1101)	1:153:A:PHE:HD1	1:164:A:LEU:HG	20	0.12
(1,1101)	1:153:A:PHE:HD2	1:164:A:LEU:HG	20	0.12
(1,1073)	1:152:A:ILE:H	1:152:A:ILE:HG12	10	0.12
(1,1073)	1:152:A:ILE:H	1:152:A:ILE:HG13	10	0.12
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	17	0.12
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	17	0.12
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	17	0.12
(1,1021)	1:142:A:GLU:HG2	1:144:A:THR:H	7	0.12
(1,1021)	1:142:A:GLU:HG3	1:144:A:THR:H	7	0.12
(1,1021)	1:142:A:GLU:HG2	1:144:A:THR:H	15	0.12
(1,1021)	1:142:A:GLU:HG3	1:144:A:THR:H	15	0.12
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB3	10	0.12
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB2	10	0.12
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB3	10	0.12
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB2	10	0.12
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB3	10	0.12
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB2	10	0.12
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB3	10	0.12
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB2	10	0.12
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB3	10	0.12
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB2	10	0.12
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB3	10	0.12
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB2	14	0.12
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB3	14	0.12
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB2	14	0.12
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB3	14	0.12
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB2	14	0.12
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB3	14	0.12
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB2	14	0.12
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB3	14	0.12
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB2	14	0.12
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB3	14	0.12
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB2	14	0.12
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB3	14	0.12
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB2	18	0.12
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB3	18	0.12
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB2	18	0.12
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB3	18	0.12
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB2	18	0.12
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB3	18	0.12
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB2	18	0.12
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB3	18	0.12
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB2	18	0.12
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB3	18	0.12
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB2	18	0.12
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB3	18	0.12
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	7	0.12
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	10	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	6	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	6	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	6	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	6	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	6	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD11	16	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD12	16	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD13	16	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD21	16	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD22	16	0.12
(1,989)	1:135:A:THR:HB	1:138:A:LEU:HD23	16	0.12
(1,988)	1:135:A:THR:HB	1:138:A:LEU:H	11	0.12
(1,988)	1:135:A:THR:HB	1:138:A:LEU:H	16	0.12
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	13	0.12
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	13	0.12
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	18	0.12
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	18	0.12
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	2	0.12
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	2	0.12
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	2	0.12
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	8	0.12
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	8	0.12
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	8	0.12
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	17	0.12
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	17	0.12
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	17	0.12
(1,910)	1:120:A:GLU:HA	1:124:A:ILE:HD11	8	0.12
(1,910)	1:120:A:GLU:HA	1:124:A:ILE:HD12	8	0.12
(1,910)	1:120:A:GLU:HA	1:124:A:ILE:HD13	8	0.12
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG11	6	0.12
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG12	6	0.12
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG13	6	0.12
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG21	6	0.12
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG22	6	0.12
(1,898)	1:118:A:ARG:HA	1:149:A:VAL:HG23	6	0.12
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	7	0.12
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	7	0.12
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	5	0.12
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	5	0.12
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	7	0.12
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	7	0.12
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	6	0.12
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	6	0.12
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	6	0.12
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	12	0.12
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	12	0.12
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	12	0.12
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	12	0.12
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	12	0.12
(1,872)	1:116:A:ILE:HG21	1:118:A:ARG:HG2	16	0.12
(1,872)	1:116:A:ILE:HG21	1:118:A:ARG:HG3	16	0.12
(1,872)	1:116:A:ILE:HG22	1:118:A:ARG:HG2	16	0.12
(1,872)	1:116:A:ILE:HG22	1:118:A:ARG:HG3	16	0.12
(1,872)	1:116:A:ILE:HG23	1:118:A:ARG:HG2	16	0.12
(1,872)	1:116:A:ILE:HG23	1:118:A:ARG:HG3	16	0.12
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	9	0.12
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	9	0.12
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	9	0.12
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	9	0.12
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	9	0.12
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	9	0.12
(1,853)	1:115:A:TYR:HD1	1:165:A:THR:HB	1	0.12
(1,853)	1:115:A:TYR:HD2	1:165:A:THR:HB	1	0.12
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG2	20	0.12
(1,847)	1:115:A:TYR:HD1	1:163:A:LYS:HG3	20	0.12
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG2	20	0.12
(1,847)	1:115:A:TYR:HD2	1:163:A:LYS:HG3	20	0.12
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG21	8	0.12
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG22	8	0.12
(1,827)	1:112:A:ASN:HB2	1:116:A:ILE:HG23	8	0.12
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG21	8	0.12
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG22	8	0.12
(1,827)	1:112:A:ASN:HB3	1:116:A:ILE:HG23	8	0.12
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD11	11	0.12
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD12	11	0.12
(1,810)	1:109:A:ASP:HB2	1:124:A:ILE:HD13	11	0.12
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD11	11	0.12
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD12	11	0.12
(1,810)	1:109:A:ASP:HB3	1:124:A:ILE:HD13	11	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD11	7	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD12	7	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD13	7	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD21	7	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD22	7	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD23	7	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD11	7	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD12	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD13	7	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD21	7	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD22	7	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD23	7	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD11	13	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD12	13	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD13	13	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD21	13	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD22	13	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD23	13	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD11	13	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD12	13	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD13	13	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD21	13	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD22	13	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD23	13	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD11	18	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD12	18	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD13	18	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD21	18	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD22	18	0.12
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD23	18	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD11	18	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD12	18	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD13	18	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD21	18	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD22	18	0.12
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD23	18	0.12
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG12	9	0.12
(1,789)	1:108:A:TYR:HD1	1:116:A:ILE:HG13	9	0.12
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG12	9	0.12
(1,789)	1:108:A:TYR:HD2	1:116:A:ILE:HG13	9	0.12
(1,775)	1:107:A:LEU:HD11	1:110:A:LEU:HB2	9	0.12
(1,775)	1:107:A:LEU:HD11	1:110:A:LEU:HB3	9	0.12
(1,775)	1:107:A:LEU:HD12	1:110:A:LEU:HB2	9	0.12
(1,775)	1:107:A:LEU:HD12	1:110:A:LEU:HB3	9	0.12
(1,775)	1:107:A:LEU:HD13	1:110:A:LEU:HB2	9	0.12
(1,775)	1:107:A:LEU:HD13	1:110:A:LEU:HB3	9	0.12
(1,775)	1:107:A:LEU:HD21	1:110:A:LEU:HB2	9	0.12
(1,775)	1:107:A:LEU:HD21	1:110:A:LEU:HB3	9	0.12
(1,775)	1:107:A:LEU:HD22	1:110:A:LEU:HB2	9	0.12
(1,775)	1:107:A:LEU:HD22	1:110:A:LEU:HB3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:107:A:LEU:HD23	1:110:A:LEU:HB2	9	0.12
(1,775)	1:107:A:LEU:HD23	1:110:A:LEU:HB3	9	0.12
(1,749)	1:102:A:ARG:HB2	1:103:A:TRP:H	18	0.12
(1,749)	1:102:A:ARG:HB3	1:103:A:TRP:H	18	0.12
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB2	17	0.12
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB3	17	0.12
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB2	17	0.12
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB3	17	0.12
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB2	17	0.12
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB3	17	0.12
(1,698)	1:91:A:VAL:HG11	1:103:A:TRP:HB2	16	0.12
(1,698)	1:91:A:VAL:HG11	1:103:A:TRP:HB3	16	0.12
(1,698)	1:91:A:VAL:HG12	1:103:A:TRP:HB2	16	0.12
(1,698)	1:91:A:VAL:HG12	1:103:A:TRP:HB3	16	0.12
(1,698)	1:91:A:VAL:HG13	1:103:A:TRP:HB2	16	0.12
(1,698)	1:91:A:VAL:HG13	1:103:A:TRP:HB3	16	0.12
(1,698)	1:91:A:VAL:HG21	1:103:A:TRP:HB2	16	0.12
(1,698)	1:91:A:VAL:HG21	1:103:A:TRP:HB3	16	0.12
(1,698)	1:91:A:VAL:HG22	1:103:A:TRP:HB2	16	0.12
(1,698)	1:91:A:VAL:HG22	1:103:A:TRP:HB3	16	0.12
(1,698)	1:91:A:VAL:HG23	1:103:A:TRP:HB2	16	0.12
(1,698)	1:91:A:VAL:HG23	1:103:A:TRP:HB3	16	0.12
(1,683)	1:90:A:SER:H	1:92:A:THR:HG21	14	0.12
(1,683)	1:90:A:SER:H	1:92:A:THR:HG22	14	0.12
(1,683)	1:90:A:SER:H	1:92:A:THR:HG23	14	0.12
(1,643)	1:85:A:PHE:HD1	1:89:A:LEU:HG	5	0.12
(1,643)	1:85:A:PHE:HD2	1:89:A:LEU:HG	5	0.12
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG12	7	0.12
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG13	7	0.12
(1,587)	1:74:A:GLU:H	1:74:A:GLU:HB2	12	0.12
(1,587)	1:74:A:GLU:H	1:74:A:GLU:HB3	12	0.12
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG21	15	0.12
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG22	15	0.12
(1,585)	1:73:A:ASP:HA	1:80:A:ILE:HG23	15	0.12
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB1	12	0.12
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB2	12	0.12
(1,576)	1:72:A:PHE:HA	1:88:A:ALA:HB3	12	0.12
(1,556)	1:69:A:PHE:HB2	1:80:A:ILE:HD11	16	0.12
(1,556)	1:69:A:PHE:HB2	1:80:A:ILE:HD12	16	0.12
(1,556)	1:69:A:PHE:HB2	1:80:A:ILE:HD13	16	0.12
(1,556)	1:69:A:PHE:HB3	1:80:A:ILE:HD11	16	0.12
(1,556)	1:69:A:PHE:HB3	1:80:A:ILE:HD12	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:69:A:PHE:HB3	1:80:A:ILE:HD13	16	0.12
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	1	0.12
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	1	0.12
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	10	0.12
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	10	0.12
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	13	0.12
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	13	0.12
(1,554)	1:69:A:PHE:HB2	1:80:A:ILE:HB	14	0.12
(1,554)	1:69:A:PHE:HB3	1:80:A:ILE:HB	14	0.12
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	6	0.12
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	6	0.12
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	18	0.12
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	18	0.12
(1,518)	1:66:A:THR:HG21	1:67:A:PHE:HB2	18	0.12
(1,518)	1:66:A:THR:HG21	1:67:A:PHE:HB3	18	0.12
(1,518)	1:66:A:THR:HG22	1:67:A:PHE:HB2	18	0.12
(1,518)	1:66:A:THR:HG22	1:67:A:PHE:HB3	18	0.12
(1,518)	1:66:A:THR:HG23	1:67:A:PHE:HB2	18	0.12
(1,518)	1:66:A:THR:HG23	1:67:A:PHE:HB3	18	0.12
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB2	8	0.12
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB3	8	0.12
(1,463)	1:57:A:PRO:HD2	1:58:A:PHE:HA	6	0.12
(1,463)	1:57:A:PRO:HD3	1:58:A:PHE:HA	6	0.12
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	2	0.12
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	2	0.12
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	2	0.12
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	2	0.12
(1,406)	1:49:A:GLN:HG2	1:66:A:THR:HA	18	0.12
(1,406)	1:49:A:GLN:HG3	1:66:A:THR:HA	18	0.12
(1,399)	1:49:A:GLN:HB2	1:65:A:ALA:HA	12	0.12
(1,399)	1:49:A:GLN:HB3	1:65:A:ALA:HA	12	0.12
(1,386)	1:48:A:PHE:HE1	1:80:A:ILE:HB	6	0.12
(1,386)	1:48:A:PHE:HE2	1:80:A:ILE:HB	6	0.12
(1,386)	1:48:A:PHE:HE1	1:80:A:ILE:HB	15	0.12
(1,386)	1:48:A:PHE:HE2	1:80:A:ILE:HB	15	0.12
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	11	0.12
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	11	0.12
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	11	0.12
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	11	0.12
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	11	0.12
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	11	0.12
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	11	0.12
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	11	0.12
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	11	0.12
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	11	0.12
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	11	0.12
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	3	0.12
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	3	0.12
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	3	0.12
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	3	0.12
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	10	0.12
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	10	0.12
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	10	0.12
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	10	0.12
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	5	0.12
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	14	0.12
(1,333)	1:44:A:ASP:H	1:79:A:ARG:HA	20	0.12
(1,306)	1:42:A:GLN:HA	1:81:A:GLU:H	4	0.12
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	7	0.12
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD2	19	0.12
(1,204)	1:25:A:LYS:HA	1:25:A:LYS:HD3	19	0.12
(1,192)	1:23:A:THR:HG21	1:24:A:GLU:HB2	8	0.12
(1,192)	1:23:A:THR:HG21	1:24:A:GLU:HB3	8	0.12
(1,192)	1:23:A:THR:HG22	1:24:A:GLU:HB2	8	0.12
(1,192)	1:23:A:THR:HG22	1:24:A:GLU:HB3	8	0.12
(1,192)	1:23:A:THR:HG23	1:24:A:GLU:HB2	8	0.12
(1,192)	1:23:A:THR:HG23	1:24:A:GLU:HB3	8	0.12
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	8	0.12
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	8	0.12
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	8	0.12
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	19	0.12
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	19	0.12
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG21	13	0.12
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG22	13	0.12
(1,154)	1:20:A:THR:HG21	1:86:A:ILE:HG23	13	0.12
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG21	13	0.12
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG22	13	0.12
(1,154)	1:20:A:THR:HG22	1:86:A:ILE:HG23	13	0.12
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG21	13	0.12
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG22	13	0.12
(1,154)	1:20:A:THR:HG23	1:86:A:ILE:HG23	13	0.12
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	1	0.12
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	1	0.12
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	1	0.12
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	1	0.12
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	1	0.12
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	19	0.12
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	19	0.12
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	19	0.12
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	19	0.12
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	19	0.12
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	19	0.12
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	2	0.12
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	2	0.12
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	2	0.12
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	2	0.12
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	2	0.12
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	2	0.12
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	1	0.12
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	1	0.12
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	1	0.12
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	5	0.12
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	5	0.12
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	5	0.12
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	2	0.12
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	2	0.12
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	2	0.12
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	12	0.12
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	12	0.12
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	12	0.12
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	3	0.12
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	6	0.12
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	20	0.12
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	6	0.12
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	6	0.12
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	6	0.12
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	6	0.12
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	6	0.12
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	6	0.12
(1,4)	1:7:A:LYS:HA	1:32:A:LYS:HG2	9	0.12
(1,4)	1:7:A:LYS:HA	1:32:A:LYS:HG3	9	0.12
(3,115)	1:167:A:GLN:O	1:171:A:GLU:H	19	0.11
(3,114)	1:166:A:LEU:O	1:170:A:GLN:H	5	0.11
(3,114)	1:166:A:LEU:O	1:170:A:GLN:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,114)	1:166:A:LEU:O	1:170:A:GLN:H	18	0.11
(3,112)	1:169:A:PHE:O	1:173:A:SER:N	11	0.11
(3,112)	1:169:A:PHE:O	1:173:A:SER:N	20	0.11
(3,109)	1:166:A:LEU:O	1:170:A:GLN:N	1	0.11
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	14	0.11
(3,104)	1:146:A:GLU:O	1:150:A:ASP:H	16	0.11
(3,103)	1:152:A:ILE:O	1:156:A:MET:N	4	0.11
(3,102)	1:151:A:ARG:O	1:155:A:MET:N	9	0.11
(3,100)	1:149:A:VAL:O	1:153:A:PHE:N	7	0.11
(3,95)	1:128:A:ILE:O	1:132:A:VAL:H	12	0.11
(3,94)	1:127:A:ALA:O	1:131:A:MET:H	6	0.11
(3,94)	1:127:A:ALA:O	1:131:A:MET:H	8	0.11
(3,85)	1:118:A:ARG:O	1:122:A:LEU:H	18	0.11
(3,74)	1:103:A:TRP:O	1:107:A:LEU:H	8	0.11
(3,59)	1:87:A:GLN:O	1:91:A:VAL:H	9	0.11
(3,58)	1:86:A:ILE:O	1:90:A:SER:H	5	0.11
(3,57)	1:85:A:PHE:O	1:89:A:LEU:H	18	0.11
(3,55)	1:83:A:SER:O	1:87:A:GLN:H	13	0.11
(3,50)	1:85:A:PHE:O	1:89:A:LEU:N	14	0.11
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	3	0.11
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	5	0.11
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	9	0.11
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	10	0.11
(3,23)	1:48:A:PHE:O	1:52:A:TYR:N	12	0.11
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	2	0.11
(3,18)	1:29:A:GLN:O	1:33:A:GLY:H	14	0.11
(3,11)	1:27:A:VAL:O	1:31:A:TYR:N	18	0.11
(3,6)	1:13:A:VAL:O	1:17:A:THR:H	5	0.11
(3,6)	1:13:A:VAL:O	1:17:A:THR:H	12	0.11
(3,6)	1:13:A:VAL:O	1:17:A:THR:H	20	0.11
(3,4)	1:11:A:GLU:O	1:15:A:GLU:H	2	0.11
(3,4)	1:11:A:GLU:O	1:15:A:GLU:H	4	0.11
(3,3)	1:10:A:PRO:O	1:14:A:GLU:H	14	0.11
(3,2)	1:12:A:VAL:O	1:16:A:LEU:N	3	0.11
(3,1)	1:11:A:GLU:O	1:15:A:GLU:N	5	0.11
(2,17)	1:168:A:GLU:OE1	2:602:A:CA:CA	5	0.11
(2,12)	1:120:A:GLU:OE2	2:601:A:CA:CA	8	0.11
(2,2)	1:75:A:ASN:OD1	2:600:A:CA:CA	16	0.11
(1,1283)	1:184:A:SER:HB2	1:186:A:TYR:H	19	0.11
(1,1283)	1:184:A:SER:HB3	1:186:A:TYR:H	19	0.11
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD11	9	0.11
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD13	9	0.11
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD21	9	0.11
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD22	9	0.11
(1,1281)	1:183:A:LEU:HA	1:185:A:LEU:HD23	9	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	5	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	5	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	5	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	5	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	5	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	5	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	7	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	7	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	7	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	7	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	7	0.11
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	7	0.11
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD11	8	0.11
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD12	8	0.11
(1,1263)	1:179:A:ILE:HA	1:179:A:ILE:HD13	8	0.11
(1,1241)	1:174:A:LYS:HA	1:175:A:ALA:H	17	0.11
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG21	11	0.11
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG22	11	0.11
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG23	11	0.11
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG21	16	0.11
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG22	16	0.11
(1,1228)	1:173:A:SER:HA	1:179:A:ILE:HG23	16	0.11
(1,1223)	1:173:A:SER:H	1:173:A:SER:HA	8	0.11
(1,1208)	1:169:A:PHE:HA	1:179:A:ILE:HB	14	0.11
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD1	1	0.11
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD2	1	0.11
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD1	19	0.11
(1,1186)	1:166:A:LEU:H	1:169:A:PHE:HD2	19	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	3	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	3	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	3	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	3	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	3	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	3	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD11	14	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD12	14	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD13	14	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD21	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD22	14	0.11
(1,1184)	1:166:A:LEU:H	1:166:A:LEU:HD23	14	0.11
(1,1167)	1:164:A:LEU:H	1:165:A:THR:HA	11	0.11
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG21	6	0.11
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG22	6	0.11
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG23	6	0.11
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG21	6	0.11
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG22	6	0.11
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG23	6	0.11
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG21	12	0.11
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG22	12	0.11
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG23	12	0.11
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG21	12	0.11
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG22	12	0.11
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG23	12	0.11
(1,1144)	1:158:A:LYS:H	1:164:A:LEU:HD11	5	0.11
(1,1144)	1:158:A:LYS:H	1:164:A:LEU:HD12	5	0.11
(1,1144)	1:158:A:LYS:H	1:164:A:LEU:HD13	5	0.11
(1,1144)	1:158:A:LYS:H	1:164:A:LEU:HD21	5	0.11
(1,1144)	1:158:A:LYS:H	1:164:A:LEU:HD22	5	0.11
(1,1144)	1:158:A:LYS:H	1:164:A:LEU:HD23	5	0.11
(1,1131)	1:156:A:MET:HB2	1:179:A:ILE:HG12	16	0.11
(1,1131)	1:156:A:MET:HB2	1:179:A:ILE:HG13	16	0.11
(1,1131)	1:156:A:MET:HB3	1:179:A:ILE:HG12	16	0.11
(1,1131)	1:156:A:MET:HB3	1:179:A:ILE:HG13	16	0.11
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD11	6	0.11
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD12	6	0.11
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD13	6	0.11
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD21	6	0.11
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD22	6	0.11
(1,1129)	1:156:A:MET:HA	1:164:A:LEU:HD23	6	0.11
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	1	0.11
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	2	0.11
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	4	0.11
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	9	0.11
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	12	0.11
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	13	0.11
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	15	0.11
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	19	0.11
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	15	0.11
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	15	0.11
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	19	0.11
(1,1098)	1:153:A:PHE:HD1	1:154:A:ALA:HA	15	0.11
(1,1098)	1:153:A:PHE:HD2	1:154:A:ALA:HA	15	0.11
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD11	16	0.11
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD12	16	0.11
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD13	16	0.11
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD21	16	0.11
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD22	16	0.11
(1,1097)	1:153:A:PHE:HB2	1:164:A:LEU:HD23	16	0.11
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD11	16	0.11
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD12	16	0.11
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD13	16	0.11
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD21	16	0.11
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD22	16	0.11
(1,1097)	1:153:A:PHE:HB3	1:164:A:LEU:HD23	16	0.11
(1,1065)	1:149:A:VAL:HG11	1:153:A:PHE:HZ	12	0.11
(1,1065)	1:149:A:VAL:HG12	1:153:A:PHE:HZ	12	0.11
(1,1065)	1:149:A:VAL:HG13	1:153:A:PHE:HZ	12	0.11
(1,1065)	1:149:A:VAL:HG21	1:153:A:PHE:HZ	12	0.11
(1,1065)	1:149:A:VAL:HG22	1:153:A:PHE:HZ	12	0.11
(1,1065)	1:149:A:VAL:HG23	1:153:A:PHE:HZ	12	0.11
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD1	20	0.11
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD2	20	0.11
(1,1056)	1:149:A:VAL:HB	1:153:A:PHE:H	10	0.11
(1,1056)	1:149:A:VAL:HB	1:153:A:PHE:H	17	0.11
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB2	11	0.11
(1,1027)	1:144:A:THR:H	1:183:A:LEU:HB3	11	0.11
(1,1017)	1:142:A:GLU:H	1:143:A:ASN:H	3	0.11
(1,1017)	1:142:A:GLU:H	1:143:A:ASN:H	6	0.11
(1,1017)	1:142:A:GLU:H	1:143:A:ASN:H	13	0.11
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	13	0.11
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	13	0.11
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB2	4	0.11
(1,998)	1:136:A:VAL:HG11	1:138:A:LEU:HB3	4	0.11
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB2	4	0.11
(1,998)	1:136:A:VAL:HG12	1:138:A:LEU:HB3	4	0.11
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB2	4	0.11
(1,998)	1:136:A:VAL:HG13	1:138:A:LEU:HB3	4	0.11
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB2	4	0.11
(1,998)	1:136:A:VAL:HG21	1:138:A:LEU:HB3	4	0.11
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB2	4	0.11
(1,998)	1:136:A:VAL:HG22	1:138:A:LEU:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB2	4	0.11
(1,998)	1:136:A:VAL:HG23	1:138:A:LEU:HB3	4	0.11
(1,991)	1:136:A:VAL:H	1:136:A:VAL:HA	17	0.11
(1,988)	1:135:A:THR:HB	1:138:A:LEU:H	7	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD11	3	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD12	3	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD13	3	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD21	3	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD22	3	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD23	3	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD11	3	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD12	3	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD13	3	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD21	3	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD22	3	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD23	3	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD11	12	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD12	12	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD13	12	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD21	12	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD22	12	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD23	12	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD11	12	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD12	12	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD13	12	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD21	12	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD22	12	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD23	12	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD11	16	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD12	16	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD13	16	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD21	16	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD22	16	0.11
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD23	16	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD11	16	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD12	16	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD13	16	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD21	16	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD22	16	0.11
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD23	16	0.11
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	9	0.11
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	19	0.11
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	19	0.11
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	19	0.11
(1,923)	1:122:A:LEU:HG	1:123:A:ASP:H	4	0.11
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG11	13	0.11
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG12	13	0.11
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG13	13	0.11
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG21	13	0.11
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG22	13	0.11
(1,901)	1:118:A:ARG:HD2	1:149:A:VAL:HG23	13	0.11
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG11	13	0.11
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG12	13	0.11
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG13	13	0.11
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG21	13	0.11
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG22	13	0.11
(1,901)	1:118:A:ARG:HD3	1:149:A:VAL:HG23	13	0.11
(1,894)	1:118:A:ARG:H	1:118:A:ARG:HG2	16	0.11
(1,894)	1:118:A:ARG:H	1:118:A:ARG:HG3	16	0.11
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	6	0.11
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	6	0.11
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	16	0.11
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	16	0.11
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD2	15	0.11
(1,882)	1:117:A:THR:H	1:118:A:ARG:HD3	15	0.11
(1,875)	1:116:A:ILE:HG21	1:164:A:LEU:HA	13	0.11
(1,875)	1:116:A:ILE:HG22	1:164:A:LEU:HA	13	0.11
(1,875)	1:116:A:ILE:HG23	1:164:A:LEU:HA	13	0.11
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	6	0.11
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	6	0.11
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	6	0.11
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	6	0.11
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	6	0.11
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	6	0.11
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD1	9	0.11
(1,874)	1:116:A:ILE:HG21	1:153:A:PHE:HD2	9	0.11
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD1	9	0.11
(1,874)	1:116:A:ILE:HG22	1:153:A:PHE:HD2	9	0.11
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD1	9	0.11
(1,874)	1:116:A:ILE:HG23	1:153:A:PHE:HD2	9	0.11
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	1	0.11
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	1	0.11
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	1	0.11
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	1	0.11
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	1	0.11
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	5	0.11
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	5	0.11
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	5	0.11
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	5	0.11
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	5	0.11
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	5	0.11
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB2	6	0.11
(1,871)	1:116:A:ILE:HG21	1:118:A:ARG:HB3	6	0.11
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB2	6	0.11
(1,871)	1:116:A:ILE:HG22	1:118:A:ARG:HB3	6	0.11
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB2	6	0.11
(1,871)	1:116:A:ILE:HG23	1:118:A:ARG:HB3	6	0.11
(1,865)	1:116:A:ILE:HB	1:164:A:LEU:HA	14	0.11
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD11	12	0.11
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD12	12	0.11
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD13	12	0.11
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD21	12	0.11
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD22	12	0.11
(1,851)	1:115:A:TYR:HD1	1:164:A:LEU:HD23	12	0.11
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD11	12	0.11
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD12	12	0.11
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD13	12	0.11
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD21	12	0.11
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD22	12	0.11
(1,851)	1:115:A:TYR:HD2	1:164:A:LEU:HD23	12	0.11
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	8	0.11
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	8	0.11
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	8	0.11
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	8	0.11
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	14	0.11
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	14	0.11
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	14	0.11
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD11	16	0.11
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD12	16	0.11
(1,814)	1:110:A:LEU:H	1:116:A:ILE:HD13	16	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	2	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	2	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	2	0.11
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	2	0.11
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	2	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	5	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	5	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	5	0.11
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	5	0.11
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	5	0.11
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	5	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG21	10	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG22	10	0.11
(1,809)	1:109:A:ASP:HB2	1:124:A:ILE:HG23	10	0.11
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG21	10	0.11
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG22	10	0.11
(1,809)	1:109:A:ASP:HB3	1:124:A:ILE:HG23	10	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD11	3	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD12	3	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD13	3	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD21	3	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD22	3	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD23	3	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD11	3	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD12	3	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD13	3	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD21	3	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD22	3	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD23	3	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD11	15	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD12	15	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD13	15	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD21	15	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD22	15	0.11
(1,804)	1:109:A:ASP:HB2	1:110:A:LEU:HD23	15	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD11	15	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD12	15	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD13	15	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD21	15	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD22	15	0.11
(1,804)	1:109:A:ASP:HB3	1:110:A:LEU:HD23	15	0.11
(1,800)	1:109:A:ASP:HA	1:116:A:ILE:HA	4	0.11
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG21	18	0.11
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG22	18	0.11
(1,796)	1:108:A:TYR:HE1	1:124:A:ILE:HG23	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG21	18	0.11
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG22	18	0.11
(1,796)	1:108:A:TYR:HE2	1:124:A:ILE:HG23	18	0.11
(1,795)	1:108:A:TYR:HE1	1:124:A:ILE:HB	14	0.11
(1,795)	1:108:A:TYR:HE2	1:124:A:ILE:HB	14	0.11
(1,775)	1:107:A:LEU:HD11	1:110:A:LEU:HB2	8	0.11
(1,775)	1:107:A:LEU:HD11	1:110:A:LEU:HB3	8	0.11
(1,775)	1:107:A:LEU:HD12	1:110:A:LEU:HB2	8	0.11
(1,775)	1:107:A:LEU:HD12	1:110:A:LEU:HB3	8	0.11
(1,775)	1:107:A:LEU:HD13	1:110:A:LEU:HB2	8	0.11
(1,775)	1:107:A:LEU:HD13	1:110:A:LEU:HB3	8	0.11
(1,775)	1:107:A:LEU:HD21	1:110:A:LEU:HB2	8	0.11
(1,775)	1:107:A:LEU:HD21	1:110:A:LEU:HB3	8	0.11
(1,775)	1:107:A:LEU:HD22	1:110:A:LEU:HB2	8	0.11
(1,775)	1:107:A:LEU:HD22	1:110:A:LEU:HB3	8	0.11
(1,775)	1:107:A:LEU:HD23	1:110:A:LEU:HB2	8	0.11
(1,775)	1:107:A:LEU:HD23	1:110:A:LEU:HB3	8	0.11
(1,773)	1:107:A:LEU:HD11	1:108:A:TYR:H	1	0.11
(1,773)	1:107:A:LEU:HD12	1:108:A:TYR:H	1	0.11
(1,773)	1:107:A:LEU:HD13	1:108:A:TYR:H	1	0.11
(1,773)	1:107:A:LEU:HD21	1:108:A:TYR:H	1	0.11
(1,773)	1:107:A:LEU:HD22	1:108:A:TYR:H	1	0.11
(1,773)	1:107:A:LEU:HD23	1:108:A:TYR:H	1	0.11
(1,773)	1:107:A:LEU:HD11	1:108:A:TYR:H	17	0.11
(1,773)	1:107:A:LEU:HD12	1:108:A:TYR:H	17	0.11
(1,773)	1:107:A:LEU:HD13	1:108:A:TYR:H	17	0.11
(1,773)	1:107:A:LEU:HD21	1:108:A:TYR:H	17	0.11
(1,773)	1:107:A:LEU:HD22	1:108:A:TYR:H	17	0.11
(1,773)	1:107:A:LEU:HD23	1:108:A:TYR:H	17	0.11
(1,773)	1:107:A:LEU:HD11	1:108:A:TYR:H	18	0.11
(1,773)	1:107:A:LEU:HD12	1:108:A:TYR:H	18	0.11
(1,773)	1:107:A:LEU:HD13	1:108:A:TYR:H	18	0.11
(1,773)	1:107:A:LEU:HD21	1:108:A:TYR:H	18	0.11
(1,773)	1:107:A:LEU:HD22	1:108:A:TYR:H	18	0.11
(1,773)	1:107:A:LEU:HD23	1:108:A:TYR:H	18	0.11
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB2	14	0.11
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB3	14	0.11
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB2	14	0.11
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB3	14	0.11
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB2	14	0.11
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB3	14	0.11
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB2	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB3	16	0.11
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB2	16	0.11
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB3	16	0.11
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB2	16	0.11
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB3	16	0.11
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB2	19	0.11
(1,718)	1:96:A:THR:HG21	1:98:A:ASP:HB3	19	0.11
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB2	19	0.11
(1,718)	1:96:A:THR:HG22	1:98:A:ASP:HB3	19	0.11
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB2	19	0.11
(1,718)	1:96:A:THR:HG23	1:98:A:ASP:HB3	19	0.11
(1,715)	1:96:A:THR:HB	1:98:A:ASP:H	2	0.11
(1,696)	1:91:A:VAL:HG11	1:100:A:LYS:HA	19	0.11
(1,696)	1:91:A:VAL:HG12	1:100:A:LYS:HA	19	0.11
(1,696)	1:91:A:VAL:HG13	1:100:A:LYS:HA	19	0.11
(1,696)	1:91:A:VAL:HG21	1:100:A:LYS:HA	19	0.11
(1,696)	1:91:A:VAL:HG22	1:100:A:LYS:HA	19	0.11
(1,696)	1:91:A:VAL:HG23	1:100:A:LYS:HA	19	0.11
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD11	7	0.11
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD12	7	0.11
(1,628)	1:82:A:PHE:HE1	1:86:A:ILE:HD13	7	0.11
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD11	7	0.11
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD12	7	0.11
(1,628)	1:82:A:PHE:HE2	1:86:A:ILE:HD13	7	0.11
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG12	19	0.11
(1,589)	1:74:A:GLU:H	1:80:A:ILE:HG13	19	0.11
(1,580)	1:72:A:PHE:HZ	1:80:A:ILE:HG12	1	0.11
(1,580)	1:72:A:PHE:HZ	1:80:A:ILE:HG13	1	0.11
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	3	0.11
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	3	0.11
(1,579)	1:72:A:PHE:HD1	1:103:A:TRP:HA	17	0.11
(1,579)	1:72:A:PHE:HD2	1:103:A:TRP:HA	17	0.11
(1,546)	1:68:A:VAL:HG11	1:80:A:ILE:HD11	12	0.11
(1,546)	1:68:A:VAL:HG11	1:80:A:ILE:HD12	12	0.11
(1,546)	1:68:A:VAL:HG11	1:80:A:ILE:HD13	12	0.11
(1,546)	1:68:A:VAL:HG12	1:80:A:ILE:HD11	12	0.11
(1,546)	1:68:A:VAL:HG12	1:80:A:ILE:HD12	12	0.11
(1,546)	1:68:A:VAL:HG12	1:80:A:ILE:HD13	12	0.11
(1,546)	1:68:A:VAL:HG13	1:80:A:ILE:HD11	12	0.11
(1,546)	1:68:A:VAL:HG13	1:80:A:ILE:HD12	12	0.11
(1,546)	1:68:A:VAL:HG13	1:80:A:ILE:HD13	12	0.11
(1,546)	1:68:A:VAL:HG21	1:80:A:ILE:HD11	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:68:A:VAL:HG21	1:80:A:ILE:HD12	12	0.11
(1,546)	1:68:A:VAL:HG21	1:80:A:ILE:HD13	12	0.11
(1,546)	1:68:A:VAL:HG22	1:80:A:ILE:HD11	12	0.11
(1,546)	1:68:A:VAL:HG22	1:80:A:ILE:HD12	12	0.11
(1,546)	1:68:A:VAL:HG22	1:80:A:ILE:HD13	12	0.11
(1,546)	1:68:A:VAL:HG23	1:80:A:ILE:HD11	12	0.11
(1,546)	1:68:A:VAL:HG23	1:80:A:ILE:HD12	12	0.11
(1,546)	1:68:A:VAL:HG23	1:80:A:ILE:HD13	12	0.11
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	8	0.11
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	8	0.11
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	15	0.11
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	15	0.11
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	16	0.11
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	16	0.11
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD1	14	0.11
(1,537)	1:68:A:VAL:HA	1:72:A:PHE:HD2	14	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD11	4	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD12	4	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD13	4	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD21	4	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD22	4	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD23	4	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD11	15	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD12	15	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD13	15	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD21	15	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD22	15	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD23	15	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD11	17	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD12	17	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD13	17	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD21	17	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD22	17	0.11
(1,523)	1:67:A:PHE:HA	1:107:A:LEU:HD23	17	0.11
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB2	10	0.11
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB3	10	0.11
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB2	17	0.11
(1,514)	1:66:A:THR:HB	1:69:A:PHE:HB3	17	0.11
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD1	8	0.11
(1,454)	1:55:A:PHE:HD1	1:56:A:PHE:HD2	8	0.11
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD1	8	0.11
(1,454)	1:55:A:PHE:HD2	1:56:A:PHE:HD2	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	18	0.11
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	18	0.11
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	18	0.11
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	18	0.11
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	18	0.11
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	18	0.11
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	18	0.11
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	18	0.11
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	18	0.11
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	18	0.11
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	18	0.11
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	18	0.11
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD11	11	0.11
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD12	11	0.11
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD13	11	0.11
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD21	11	0.11
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD22	11	0.11
(1,434)	1:52:A:TYR:HD1	1:89:A:LEU:HD23	11	0.11
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD11	11	0.11
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD12	11	0.11
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD13	11	0.11
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD21	11	0.11
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD22	11	0.11
(1,434)	1:52:A:TYR:HD2	1:89:A:LEU:HD23	11	0.11
(1,425)	1:52:A:TYR:HA	1:56:A:PHE:H	14	0.11
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	9	0.11
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	9	0.11
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	9	0.11
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	9	0.11
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	9	0.11
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	9	0.11
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	18	0.11
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	18	0.11
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	18	0.11
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	18	0.11
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	18	0.11
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	18	0.11
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE1	19	0.11
(1,419)	1:51:A:ILE:HD11	1:56:A:PHE:HE2	19	0.11
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE1	19	0.11
(1,419)	1:51:A:ILE:HD12	1:56:A:PHE:HE2	19	0.11
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE1	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:51:A:ILE:HD13	1:56:A:PHE:HE2	19	0.11
(1,386)	1:48:A:PHE:HE1	1:80:A:ILE:HB	20	0.11
(1,386)	1:48:A:PHE:HE2	1:80:A:ILE:HB	20	0.11
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD11	7	0.11
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD12	7	0.11
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD13	7	0.11
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD21	7	0.11
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD22	7	0.11
(1,384)	1:48:A:PHE:HD1	1:89:A:LEU:HD23	7	0.11
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD11	7	0.11
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD12	7	0.11
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD13	7	0.11
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD21	7	0.11
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD22	7	0.11
(1,384)	1:48:A:PHE:HD2	1:89:A:LEU:HD23	7	0.11
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	5	0.11
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	5	0.11
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	5	0.11
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	5	0.11
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	8	0.11
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	10	0.11
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	18	0.11
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	6	0.11
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	12	0.11
(1,321)	1:43:A:LEU:HG	1:44:A:ASP:H	17	0.11
(1,311)	1:42:A:GLN:HG2	1:79:A:ARG:HA	15	0.11
(1,311)	1:42:A:GLN:HG3	1:79:A:ARG:HA	15	0.11
(1,311)	1:42:A:GLN:HG2	1:79:A:ARG:HA	20	0.11
(1,311)	1:42:A:GLN:HG3	1:79:A:ARG:HA	20	0.11
(1,274)	1:34:A:PHE:HE1	1:86:A:ILE:HA	6	0.11
(1,274)	1:34:A:PHE:HE2	1:86:A:ILE:HA	6	0.11
(1,273)	1:34:A:PHE:HE1	1:35:A:ILE:HB	14	0.11
(1,273)	1:34:A:PHE:HE2	1:35:A:ILE:HB	14	0.11
(1,258)	1:32:A:LYS:HA	1:35:A:ILE:HG12	2	0.11
(1,258)	1:32:A:LYS:HA	1:35:A:ILE:HG13	2	0.11
(1,258)	1:32:A:LYS:HA	1:35:A:ILE:HG12	9	0.11
(1,258)	1:32:A:LYS:HA	1:35:A:ILE:HG13	9	0.11
(1,251)	1:31:A:TYR:HE1	1:35:A:ILE:HG21	14	0.11
(1,251)	1:31:A:TYR:HE1	1:35:A:ILE:HG22	14	0.11
(1,251)	1:31:A:TYR:HE1	1:35:A:ILE:HG23	14	0.11
(1,251)	1:31:A:TYR:HE2	1:35:A:ILE:HG21	14	0.11
(1,251)	1:31:A:TYR:HE2	1:35:A:ILE:HG22	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:31:A:TYR:HE2	1:35:A:ILE:HG23	14	0.11
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	8	0.11
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	15	0.11
(1,242)	1:31:A:TYR:HA	1:86:A:ILE:HB	16	0.11
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD11	19	0.11
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD12	19	0.11
(1,236)	1:30:A:TRP:HB2	1:86:A:ILE:HD13	19	0.11
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD11	19	0.11
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD12	19	0.11
(1,236)	1:30:A:TRP:HB3	1:86:A:ILE:HD13	19	0.11
(1,193)	1:24:A:GLU:H	1:24:A:GLU:HG2	10	0.11
(1,193)	1:24:A:GLU:H	1:24:A:GLU:HG3	10	0.11
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	12	0.11
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	12	0.11
(1,159)	1:21:A:TYR:H	1:22:A:PHE:HB2	15	0.11
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	18	0.11
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	18	0.11
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	18	0.11
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	18	0.11
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	18	0.11
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	18	0.11
(1,145)	1:20:A:THR:H	1:21:A:TYR:H	15	0.11
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	4	0.11
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	4	0.11
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	4	0.11
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	4	0.11
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	4	0.11
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	4	0.11
(1,130)	1:17:A:THR:HG21	1:23:A:THR:HB	17	0.11
(1,130)	1:17:A:THR:HG22	1:23:A:THR:HB	17	0.11
(1,130)	1:17:A:THR:HG23	1:23:A:THR:HB	17	0.11
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG2	2	0.11
(1,120)	1:16:A:LEU:HD11	1:24:A:GLU:HG3	2	0.11
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG2	2	0.11
(1,120)	1:16:A:LEU:HD12	1:24:A:GLU:HG3	2	0.11
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG2	2	0.11
(1,120)	1:16:A:LEU:HD13	1:24:A:GLU:HG3	2	0.11
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG2	2	0.11
(1,120)	1:16:A:LEU:HD21	1:24:A:GLU:HG3	2	0.11
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG2	2	0.11
(1,120)	1:16:A:LEU:HD22	1:24:A:GLU:HG3	2	0.11
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:16:A:LEU:HD23	1:24:A:GLU:HG3	2	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	6	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	6	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	6	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	8	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	8	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	8	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG21	9	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG22	9	0.11
(1,107)	1:16:A:LEU:H	1:17:A:THR:HG23	9	0.11
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG2	6	0.11
(1,97)	1:15:A:GLU:HA	1:18:A:ARG:HG3	6	0.11
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	12	0.11
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	19	0.11
(1,70)	1:13:A:VAL:H	1:14:A:GLU:HG2	19	0.11
(1,70)	1:13:A:VAL:H	1:14:A:GLU:HG3	19	0.11
(1,54)	1:12:A:VAL:HA	1:14:A:GLU:HB2	19	0.11
(1,54)	1:12:A:VAL:HA	1:14:A:GLU:HB3	19	0.11
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	4	0.11
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	4	0.11
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	4	0.11
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	4	0.11
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	4	0.11
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	4	0.11
(1,19)	1:8:A:LEU:HD11	1:13:A:VAL:HB	20	0.11
(1,19)	1:8:A:LEU:HD12	1:13:A:VAL:HB	20	0.11
(1,19)	1:8:A:LEU:HD13	1:13:A:VAL:HB	20	0.11
(1,19)	1:8:A:LEU:HD21	1:13:A:VAL:HB	20	0.11
(1,19)	1:8:A:LEU:HD22	1:13:A:VAL:HB	20	0.11
(1,19)	1:8:A:LEU:HD23	1:13:A:VAL:HB	20	0.11
(1,9)	1:8:A:LEU:HB2	1:28:A:GLN:HG2	18	0.11
(1,9)	1:8:A:LEU:HB2	1:28:A:GLN:HG3	18	0.11
(1,9)	1:8:A:LEU:HB3	1:28:A:GLN:HG2	18	0.11
(1,9)	1:8:A:LEU:HB3	1:28:A:GLN:HG3	18	0.11
(1,4)	1:7:A:LYS:HA	1:32:A:LYS:HG2	6	0.11
(1,4)	1:7:A:LYS:HA	1:32:A:LYS:HG3	6	0.11
(1,4)	1:7:A:LYS:HA	1:32:A:LYS:HG2	20	0.11
(1,4)	1:7:A:LYS:HA	1:32:A:LYS:HG3	20	0.11
(3,124)	1:164:A:LEU:O	1:116:A:ILE:H	1	0.1
(3,118)	1:170:A:GLN:O	1:174:A:LYS:H	3	0.1
(3,118)	1:170:A:GLN:O	1:174:A:LYS:H	11	0.1
(3,118)	1:170:A:GLN:O	1:174:A:LYS:H	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,112)	1:169:A:PHE:O	1:173:A:SER:N	5	0.1
(3,112)	1:169:A:PHE:O	1:173:A:SER:N	14	0.1
(3,112)	1:169:A:PHE:O	1:173:A:SER:N	16	0.1
(3,109)	1:166:A:LEU:O	1:170:A:GLN:N	10	0.1
(3,109)	1:166:A:LEU:O	1:170:A:GLN:N	14	0.1
(3,109)	1:166:A:LEU:O	1:170:A:GLN:N	19	0.1
(3,108)	1:150:A:ASP:O	1:154:A:ALA:H	6	0.1
(3,105)	1:147:A:LYS:O	1:151:A:ARG:H	20	0.1
(3,92)	1:125:A:VAL:O	1:129:A:TYR:H	12	0.1
(3,69)	1:98:A:ASP:O	1:102:A:ARG:H	19	0.1
(3,59)	1:87:A:GLN:O	1:91:A:VAL:H	8	0.1
(3,58)	1:86:A:ILE:O	1:90:A:SER:H	14	0.1
(3,43)	1:65:A:ALA:O	1:69:A:PHE:H	6	0.1
(3,31)	1:48:A:PHE:O	1:52:A:TYR:H	4	0.1
(3,27)	1:52:A:TYR:O	1:56:A:PHE:N	18	0.1
(3,26)	1:51:A:ILE:O	1:55:A:PHE:N	18	0.1
(3,25)	1:50:A:LYS:O	1:54:A:GLN:N	15	0.1
(3,19)	1:30:A:TRP:O	1:34:A:PHE:H	17	0.1
(3,14)	1:30:A:TRP:O	1:34:A:PHE:N	19	0.1
(3,13)	1:29:A:GLN:O	1:33:A:GLY:N	13	0.1
(3,5)	1:12:A:VAL:O	1:16:A:LEU:H	7	0.1
(2,17)	1:168:A:GLU:OE1	2:602:A:CA:CA	12	0.1
(2,14)	1:159:A:ASN:OD1	2:602:A:CA:CA	5	0.1
(2,10)	1:115:A:TYR:O	2:601:A:CA:CA	8	0.1
(1,1283)	1:184:A:SER:HB2	1:186:A:TYR:H	7	0.1
(1,1283)	1:184:A:SER:HB3	1:186:A:TYR:H	7	0.1
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD11	8	0.1
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD12	8	0.1
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD13	8	0.1
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD21	8	0.1
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD22	8	0.1
(1,1274)	1:180:A:VAL:HA	1:183:A:LEU:HD23	8	0.1
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG11	5	0.1
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG12	5	0.1
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG13	5	0.1
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG21	5	0.1
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG22	5	0.1
(1,1245)	1:174:A:LYS:HB2	1:180:A:VAL:HG23	5	0.1
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG11	5	0.1
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG12	5	0.1
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG13	5	0.1
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG21	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG22	5	0.1
(1,1245)	1:174:A:LYS:HB3	1:180:A:VAL:HG23	5	0.1
(1,1220)	1:172:A:GLY:HA2	1:175:A:ALA:HA	14	0.1
(1,1220)	1:172:A:GLY:HA3	1:175:A:ALA:HA	14	0.1
(1,1172)	1:164:A:LEU:HG	1:165:A:THR:H	16	0.1
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG21	4	0.1
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG22	4	0.1
(1,1164)	1:163:A:LYS:HE2	1:165:A:THR:HG23	4	0.1
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG21	4	0.1
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG22	4	0.1
(1,1164)	1:163:A:LYS:HE3	1:165:A:THR:HG23	4	0.1
(1,1145)	1:158:A:LYS:HA	1:159:A:ASN:H	10	0.1
(1,1136)	1:157:A:ASP:HA	1:158:A:LYS:HG2	11	0.1
(1,1136)	1:157:A:ASP:HA	1:158:A:LYS:HG3	11	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE1	2	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE2	2	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE3	2	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE1	2	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE2	2	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE3	2	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE1	2	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE2	2	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE3	2	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE1	3	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE2	3	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE3	3	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE1	3	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE2	3	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE3	3	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE1	3	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE2	3	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE3	3	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE1	8	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE2	8	0.1
(1,1114)	1:154:A:ALA:HB1	1:155:A:MET:HE3	8	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE1	8	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE2	8	0.1
(1,1114)	1:154:A:ALA:HB2	1:155:A:MET:HE3	8	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE1	8	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE2	8	0.1
(1,1114)	1:154:A:ALA:HB3	1:155:A:MET:HE3	8	0.1
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	18	0.1
(1,1108)	1:154:A:ALA:H	1:154:A:ALA:HA	20	0.1
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB2	6	0.1
(1,1105)	1:153:A:PHE:HZ	1:156:A:MET:HB3	6	0.1
(1,1080)	1:152:A:ILE:HA	1:155:A:MET:HG2	3	0.1
(1,1080)	1:152:A:ILE:HA	1:155:A:MET:HG3	3	0.1
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD1	11	0.1
(1,1057)	1:149:A:VAL:HB	1:153:A:PHE:HD2	11	0.1
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG21	13	0.1
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG22	13	0.1
(1,1052)	1:149:A:VAL:HA	1:152:A:ILE:HG23	13	0.1
(1,1029)	1:144:A:THR:HA	1:146:A:GLU:H	4	0.1
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	1	0.1
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	1	0.1
(1,1011)	1:139:A:PRO:HD2	1:144:A:THR:HA	10	0.1
(1,1011)	1:139:A:PRO:HD3	1:144:A:THR:HA	10	0.1
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD11	2	0.1
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD12	2	0.1
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD13	2	0.1
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD21	2	0.1
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD22	2	0.1
(1,975)	1:129:A:TYR:HD1	1:138:A:LEU:HD23	2	0.1
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD11	2	0.1
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD12	2	0.1
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD13	2	0.1
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD21	2	0.1
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD22	2	0.1
(1,975)	1:129:A:TYR:HD2	1:138:A:LEU:HD23	2	0.1
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD1	6	0.1
(1,949)	1:125:A:VAL:HA	1:129:A:TYR:HD2	6	0.1
(1,943)	1:124:A:ILE:HD11	1:127:A:ALA:HA	11	0.1
(1,943)	1:124:A:ILE:HD12	1:127:A:ALA:HA	11	0.1
(1,943)	1:124:A:ILE:HD13	1:127:A:ALA:HA	11	0.1
(1,924)	1:122:A:LEU:HD11	1:126:A:ASP:HA	5	0.1
(1,924)	1:122:A:LEU:HD12	1:126:A:ASP:HA	5	0.1
(1,924)	1:122:A:LEU:HD13	1:126:A:ASP:HA	5	0.1
(1,924)	1:122:A:LEU:HD21	1:126:A:ASP:HA	5	0.1
(1,924)	1:122:A:LEU:HD22	1:126:A:ASP:HA	5	0.1
(1,924)	1:122:A:LEU:HD23	1:126:A:ASP:HA	5	0.1
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	17	0.1
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	17	0.1
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD2	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,887)	1:117:A:THR:HA	1:163:A:LYS:HD3	18	0.1
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD11	18	0.1
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD12	18	0.1
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD13	18	0.1
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD21	18	0.1
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD22	18	0.1
(1,877)	1:116:A:ILE:HG21	1:164:A:LEU:HD23	18	0.1
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD11	18	0.1
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD12	18	0.1
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD13	18	0.1
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD21	18	0.1
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD22	18	0.1
(1,877)	1:116:A:ILE:HG22	1:164:A:LEU:HD23	18	0.1
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD11	18	0.1
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD12	18	0.1
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD13	18	0.1
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD21	18	0.1
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD22	18	0.1
(1,877)	1:116:A:ILE:HG23	1:164:A:LEU:HD23	18	0.1
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD11	12	0.1
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD12	12	0.1
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD13	12	0.1
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD21	12	0.1
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD22	12	0.1
(1,858)	1:115:A:TYR:HE1	1:166:A:LEU:HD23	12	0.1
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD11	12	0.1
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD12	12	0.1
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD13	12	0.1
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD21	12	0.1
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD22	12	0.1
(1,858)	1:115:A:TYR:HE2	1:166:A:LEU:HD23	12	0.1
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB2	8	0.1
(1,856)	1:115:A:TYR:HE1	1:163:A:LYS:HB3	8	0.1
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB2	8	0.1
(1,856)	1:115:A:TYR:HE2	1:163:A:LYS:HB3	8	0.1
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB2	16	0.1
(1,850)	1:115:A:TYR:HD1	1:164:A:LEU:HB3	16	0.1
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB2	16	0.1
(1,850)	1:115:A:TYR:HD2	1:164:A:LEU:HB3	16	0.1
(1,751)	1:103:A:TRP:H	1:103:A:TRP:HD1	12	0.1
(1,750)	1:102:A:ARG:HD2	1:166:A:LEU:HD11	18	0.1
(1,750)	1:102:A:ARG:HD2	1:166:A:LEU:HD12	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:102:A:ARG:HD2	1:166:A:LEU:HD13	18	0.1
(1,750)	1:102:A:ARG:HD2	1:166:A:LEU:HD21	18	0.1
(1,750)	1:102:A:ARG:HD2	1:166:A:LEU:HD22	18	0.1
(1,750)	1:102:A:ARG:HD2	1:166:A:LEU:HD23	18	0.1
(1,750)	1:102:A:ARG:HD3	1:166:A:LEU:HD11	18	0.1
(1,750)	1:102:A:ARG:HD3	1:166:A:LEU:HD12	18	0.1
(1,750)	1:102:A:ARG:HD3	1:166:A:LEU:HD13	18	0.1
(1,750)	1:102:A:ARG:HD3	1:166:A:LEU:HD21	18	0.1
(1,750)	1:102:A:ARG:HD3	1:166:A:LEU:HD22	18	0.1
(1,750)	1:102:A:ARG:HD3	1:166:A:LEU:HD23	18	0.1
(1,715)	1:96:A:THR:HB	1:98:A:ASP:H	15	0.1
(1,710)	1:96:A:THR:H	1:96:A:THR:HG21	11	0.1
(1,710)	1:96:A:THR:H	1:96:A:THR:HG22	11	0.1
(1,710)	1:96:A:THR:H	1:96:A:THR:HG23	11	0.1
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD11	18	0.1
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD12	18	0.1
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD13	18	0.1
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD21	18	0.1
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD22	18	0.1
(1,658)	1:86:A:ILE:HD11	1:89:A:LEU:HD23	18	0.1
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD11	18	0.1
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD12	18	0.1
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD13	18	0.1
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD21	18	0.1
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD22	18	0.1
(1,658)	1:86:A:ILE:HD12	1:89:A:LEU:HD23	18	0.1
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD11	18	0.1
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD12	18	0.1
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD13	18	0.1
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD21	18	0.1
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD22	18	0.1
(1,658)	1:86:A:ILE:HD13	1:89:A:LEU:HD23	18	0.1
(1,622)	1:80:A:ILE:HD11	1:84:A:GLU:H	3	0.1
(1,622)	1:80:A:ILE:HD12	1:84:A:GLU:H	3	0.1
(1,622)	1:80:A:ILE:HD13	1:84:A:GLU:H	3	0.1
(1,605)	1:77:A:ASP:HA	1:78:A:GLY:H	5	0.1
(1,603)	1:77:A:ASP:H	1:78:A:GLY:H	12	0.1
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB2	14	0.1
(1,581)	1:72:A:PHE:HZ	1:89:A:LEU:HB3	14	0.1
(1,580)	1:72:A:PHE:HZ	1:80:A:ILE:HG12	8	0.1
(1,580)	1:72:A:PHE:HZ	1:80:A:ILE:HG13	8	0.1
(1,557)	1:69:A:PHE:HD1	1:80:A:ILE:HA	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:69:A:PHE:HD2	1:80:A:ILE:HA	16	0.1
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD1	3	0.1
(1,541)	1:68:A:VAL:HB	1:72:A:PHE:HD2	3	0.1
(1,502)	1:64:A:PHE:HB2	1:124:A:ILE:HG21	6	0.1
(1,502)	1:64:A:PHE:HB2	1:124:A:ILE:HG22	6	0.1
(1,502)	1:64:A:PHE:HB2	1:124:A:ILE:HG23	6	0.1
(1,502)	1:64:A:PHE:HB3	1:124:A:ILE:HG21	6	0.1
(1,502)	1:64:A:PHE:HB3	1:124:A:ILE:HG22	6	0.1
(1,502)	1:64:A:PHE:HB3	1:124:A:ILE:HG23	6	0.1
(1,491)	1:63:A:LYS:HB2	1:67:A:PHE:H	14	0.1
(1,491)	1:63:A:LYS:HB3	1:67:A:PHE:H	14	0.1
(1,467)	1:58:A:PHE:H	1:136:A:VAL:H	11	0.1
(1,462)	1:57:A:PRO:HG2	1:58:A:PHE:HZ	13	0.1
(1,462)	1:57:A:PRO:HG3	1:58:A:PHE:HZ	13	0.1
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD11	10	0.1
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD12	10	0.1
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD13	10	0.1
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD21	10	0.1
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD22	10	0.1
(1,435)	1:52:A:TYR:HD1	1:107:A:LEU:HD23	10	0.1
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD11	10	0.1
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD12	10	0.1
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD13	10	0.1
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD21	10	0.1
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD22	10	0.1
(1,435)	1:52:A:TYR:HD2	1:107:A:LEU:HD23	10	0.1
(1,431)	1:52:A:TYR:HD1	1:64:A:PHE:HB2	6	0.1
(1,431)	1:52:A:TYR:HD1	1:64:A:PHE:HB3	6	0.1
(1,431)	1:52:A:TYR:HD2	1:64:A:PHE:HB2	6	0.1
(1,431)	1:52:A:TYR:HD2	1:64:A:PHE:HB3	6	0.1
(1,412)	1:51:A:ILE:H	1:51:A:ILE:HG12	11	0.1
(1,412)	1:51:A:ILE:H	1:51:A:ILE:HG13	11	0.1
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD11	6	0.1
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD12	6	0.1
(1,382)	1:48:A:PHE:HD1	1:80:A:ILE:HD13	6	0.1
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD11	6	0.1
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD12	6	0.1
(1,382)	1:48:A:PHE:HD2	1:80:A:ILE:HD13	6	0.1
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG12	11	0.1
(1,378)	1:48:A:PHE:HD1	1:51:A:ILE:HG13	11	0.1
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG12	11	0.1
(1,378)	1:48:A:PHE:HD2	1:51:A:ILE:HG13	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:48:A:PHE:HA	1:51:A:ILE:HB	19	0.1
(1,337)	1:44:A:ASP:HB2	1:45:A:ALA:H	20	0.1
(1,311)	1:42:A:GLN:HG2	1:79:A:ARG:HA	6	0.1
(1,311)	1:42:A:GLN:HG3	1:79:A:ARG:HA	6	0.1
(1,292)	1:35:A:ILE:HG12	1:39:A:PRO:HA	12	0.1
(1,292)	1:35:A:ILE:HG13	1:39:A:PRO:HA	12	0.1
(1,285)	1:35:A:ILE:HB	1:39:A:PRO:HA	3	0.1
(1,273)	1:34:A:PHE:HE1	1:35:A:ILE:HB	1	0.1
(1,273)	1:34:A:PHE:HE2	1:35:A:ILE:HB	1	0.1
(1,273)	1:34:A:PHE:HE1	1:35:A:ILE:HB	18	0.1
(1,273)	1:34:A:PHE:HE2	1:35:A:ILE:HB	18	0.1
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	10	0.1
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	10	0.1
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	10	0.1
(1,191)	1:23:A:THR:HG21	1:24:A:GLU:HA	17	0.1
(1,191)	1:23:A:THR:HG22	1:24:A:GLU:HA	17	0.1
(1,191)	1:23:A:THR:HG23	1:24:A:GLU:HA	17	0.1
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	6	0.1
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	6	0.1
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB2	20	0.1
(1,161)	1:21:A:TYR:HA	1:93:A:SER:HB3	20	0.1
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB2	9	0.1
(1,152)	1:20:A:THR:HG21	1:24:A:GLU:HB3	9	0.1
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB2	9	0.1
(1,152)	1:20:A:THR:HG22	1:24:A:GLU:HB3	9	0.1
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB2	9	0.1
(1,152)	1:20:A:THR:HG23	1:24:A:GLU:HB3	9	0.1
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG21	19	0.1
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG22	19	0.1
(1,144)	1:19:A:LYS:HE2	1:20:A:THR:HG23	19	0.1
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG21	19	0.1
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG22	19	0.1
(1,144)	1:19:A:LYS:HE3	1:20:A:THR:HG23	19	0.1
(1,134)	1:17:A:THR:HG21	1:27:A:VAL:HG11	17	0.1
(1,134)	1:17:A:THR:HG21	1:27:A:VAL:HG12	17	0.1
(1,134)	1:17:A:THR:HG21	1:27:A:VAL:HG13	17	0.1
(1,134)	1:17:A:THR:HG21	1:27:A:VAL:HG21	17	0.1
(1,134)	1:17:A:THR:HG21	1:27:A:VAL:HG22	17	0.1
(1,134)	1:17:A:THR:HG21	1:27:A:VAL:HG23	17	0.1
(1,134)	1:17:A:THR:HG22	1:27:A:VAL:HG11	17	0.1
(1,134)	1:17:A:THR:HG22	1:27:A:VAL:HG12	17	0.1
(1,134)	1:17:A:THR:HG22	1:27:A:VAL:HG13	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:17:A:THR:HG22	1:27:A:VAL:HG21	17	0.1
(1,134)	1:17:A:THR:HG22	1:27:A:VAL:HG22	17	0.1
(1,134)	1:17:A:THR:HG22	1:27:A:VAL:HG23	17	0.1
(1,134)	1:17:A:THR:HG23	1:27:A:VAL:HG11	17	0.1
(1,134)	1:17:A:THR:HG23	1:27:A:VAL:HG12	17	0.1
(1,134)	1:17:A:THR:HG23	1:27:A:VAL:HG13	17	0.1
(1,134)	1:17:A:THR:HG23	1:27:A:VAL:HG21	17	0.1
(1,134)	1:17:A:THR:HG23	1:27:A:VAL:HG22	17	0.1
(1,134)	1:17:A:THR:HG23	1:27:A:VAL:HG23	17	0.1
(1,125)	1:17:A:THR:HB	1:23:A:THR:HA	9	0.1
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD11	5	0.1
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD12	5	0.1
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD13	5	0.1
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD21	5	0.1
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD22	5	0.1
(1,121)	1:16:A:LEU:HD11	1:89:A:LEU:HD23	5	0.1
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD11	5	0.1
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD12	5	0.1
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD13	5	0.1
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD21	5	0.1
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD22	5	0.1
(1,121)	1:16:A:LEU:HD12	1:89:A:LEU:HD23	5	0.1
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD11	5	0.1
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD12	5	0.1
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD13	5	0.1
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD21	5	0.1
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD22	5	0.1
(1,121)	1:16:A:LEU:HD13	1:89:A:LEU:HD23	5	0.1
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD11	5	0.1
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD12	5	0.1
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD13	5	0.1
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD21	5	0.1
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD22	5	0.1
(1,121)	1:16:A:LEU:HD21	1:89:A:LEU:HD23	5	0.1
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD11	5	0.1
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD12	5	0.1
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD13	5	0.1
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD21	5	0.1
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD22	5	0.1
(1,121)	1:16:A:LEU:HD22	1:89:A:LEU:HD23	5	0.1
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD11	5	0.1
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD12	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD13	5	0.1
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD21	5	0.1
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD22	5	0.1
(1,121)	1:16:A:LEU:HD23	1:89:A:LEU:HD23	5	0.1
(1,117)	1:16:A:LEU:HD11	1:19:A:LYS:HA	4	0.1
(1,117)	1:16:A:LEU:HD12	1:19:A:LYS:HA	4	0.1
(1,117)	1:16:A:LEU:HD13	1:19:A:LYS:HA	4	0.1
(1,117)	1:16:A:LEU:HD21	1:19:A:LYS:HA	4	0.1
(1,117)	1:16:A:LEU:HD22	1:19:A:LYS:HA	4	0.1
(1,117)	1:16:A:LEU:HD23	1:19:A:LYS:HA	4	0.1
(1,95)	1:15:A:GLU:HA	1:18:A:ARG:HA	5	0.1
(1,83)	1:13:A:VAL:HG11	1:24:A:GLU:HA	10	0.1
(1,83)	1:13:A:VAL:HG12	1:24:A:GLU:HA	10	0.1
(1,83)	1:13:A:VAL:HG13	1:24:A:GLU:HA	10	0.1
(1,83)	1:13:A:VAL:HG21	1:24:A:GLU:HA	10	0.1
(1,83)	1:13:A:VAL:HG22	1:24:A:GLU:HA	10	0.1
(1,83)	1:13:A:VAL:HG23	1:24:A:GLU:HA	10	0.1
(1,65)	1:12:A:VAL:HG21	1:16:A:LEU:H	13	0.1
(1,65)	1:12:A:VAL:HG22	1:16:A:LEU:H	13	0.1
(1,65)	1:12:A:VAL:HG23	1:16:A:LEU:H	13	0.1
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD1	4	0.1
(1,11)	1:8:A:LEU:HB2	1:82:A:PHE:HD2	4	0.1
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD1	4	0.1
(1,11)	1:8:A:LEU:HB3	1:82:A:PHE:HD2	4	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found