Full wwPDB NMR Structure Validation Report (i)

Mar 2, 2026 – 02:01 AM UTC

PDB ID	:	2N1D / pdb_00002n1d
BMRB ID	:	25556
Title	:	Solution structure of the MRG15-MRGBP complex
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Deposited on	:	2015-03-27

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

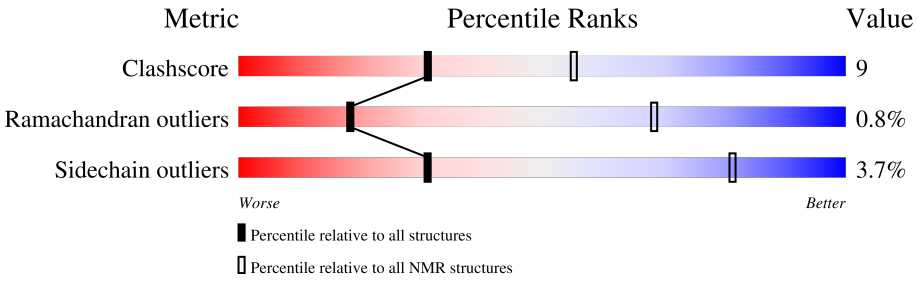
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	54	56% 22% • 20%
2	B	172	77% 17% 6%

2 Ensemble composition and analysis

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

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:75-A:117, B:156-B:203, B:211-B:323 (204)	0.98	8

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3684 atoms, of which 1839 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MRG/MORF4L-binding protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	54	874	279	432	76	85	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	SER	-	expression tag	UNP Q9NV56
A	67	ASN	-	expression tag	UNP Q9NV56
A	68	ALA	-	expression tag	UNP Q9NV56

- Molecule 2 is a protein called Mortality factor 4-like protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	172	2810	912	1407	229	259	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	152	SER	-	expression tag	UNP Q9UBU8
B	153	ASN	-	expression tag	UNP Q9UBU8
B	154	ALA	-	expression tag	UNP Q9UBU8

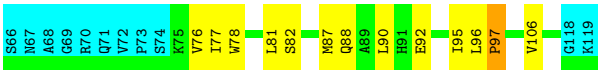
4 Residue-property plots

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.

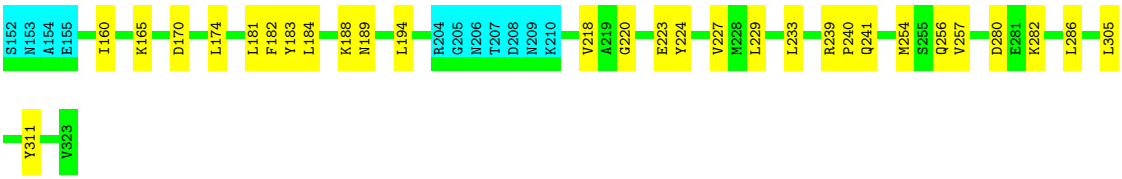
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

Chain B:



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

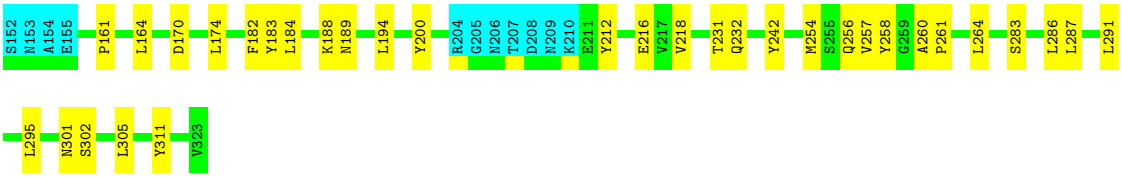
4.2.1 Score per residue for model 1

• Molecule 1: MRG/MORF4L-binding protein

Chain A:

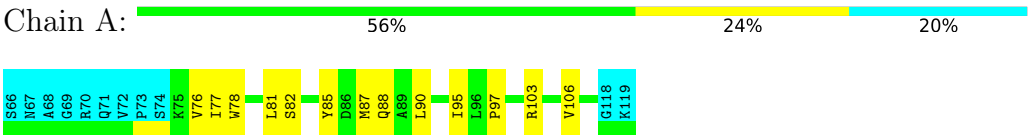
• Molecule 2: Mortality factor 4-like protein 1

Chain B:

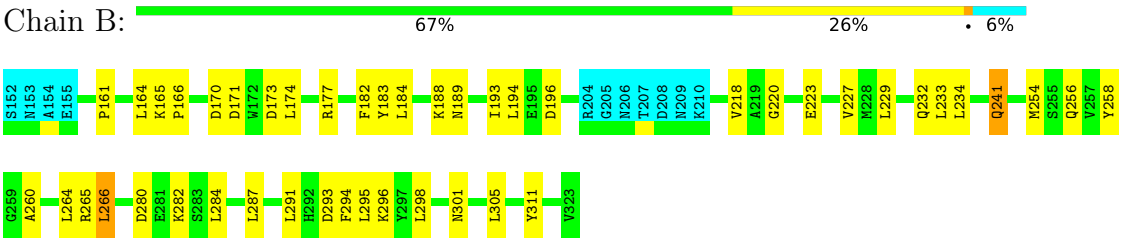


4.2.2 Score per residue for model 2

• Molecule 1: MRG/MORF4L-binding protein

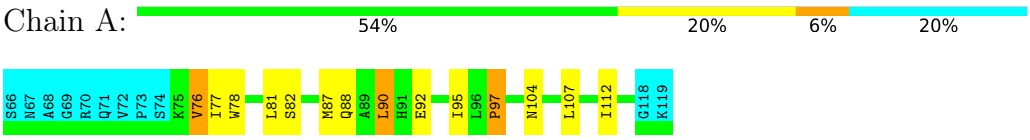


• Molecule 2: Mortality factor 4-like protein 1

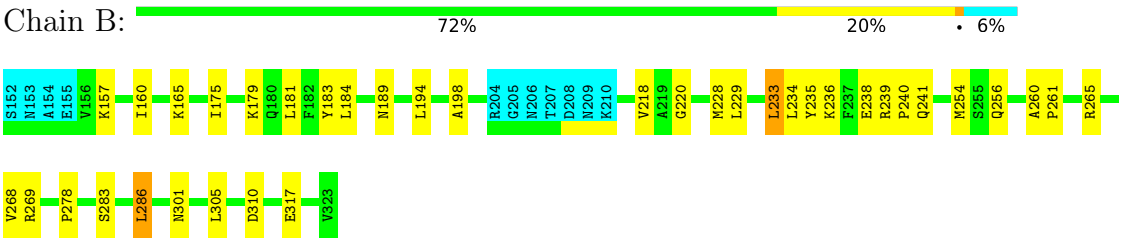


4.2.3 Score per residue for model 3

• Molecule 1: MRG/MORF4L-binding protein



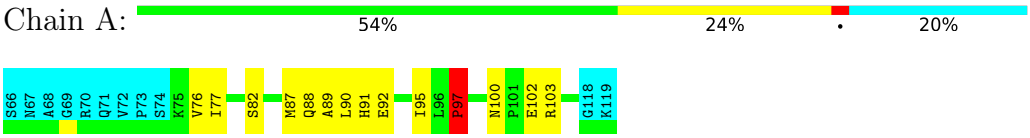
• Molecule 2: Mortality factor 4-like protein 1



4.2.4 Score per residue for model 4

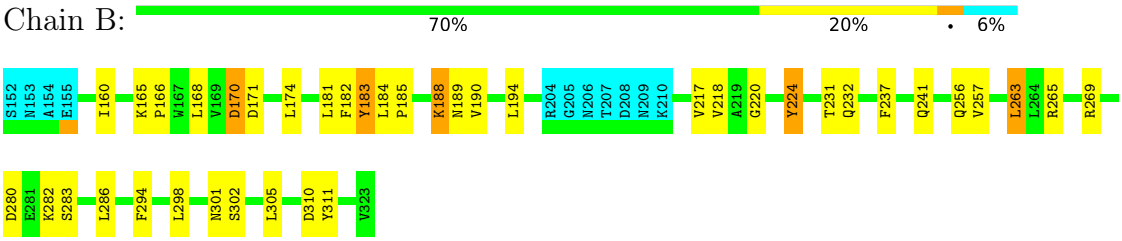
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

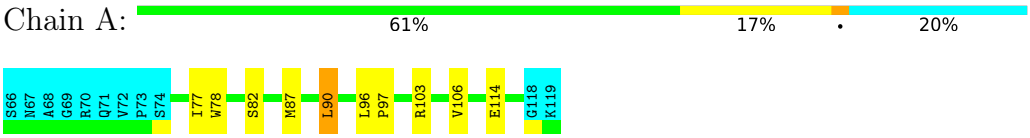
Chain B:



4.2.5 Score per residue for model 5

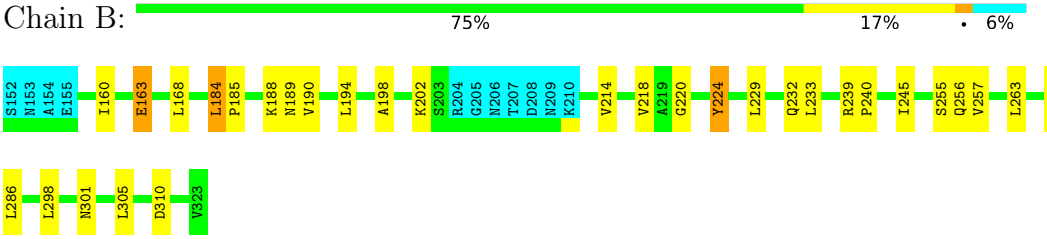
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

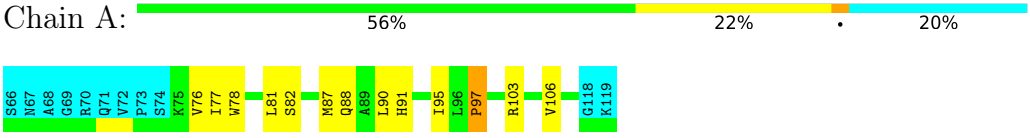
Chain B:



4.2.6 Score per residue for model 6

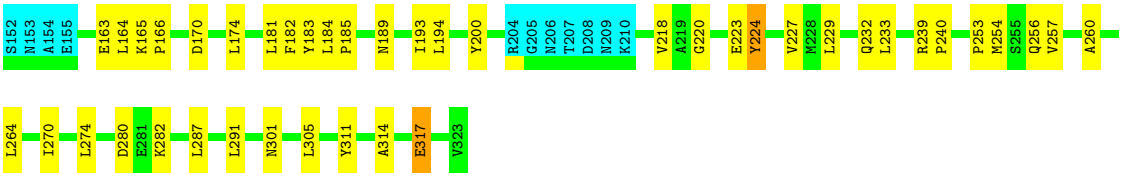
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

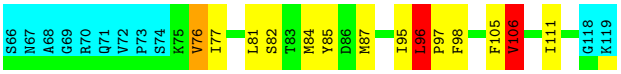
Chain B:



4.2.7 Score per residue for model 7

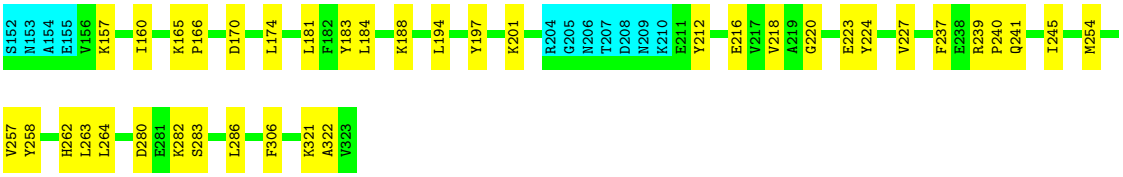
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

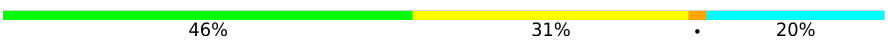
Chain B:

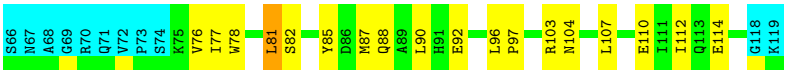


4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: MRG/MORF4L-binding protein

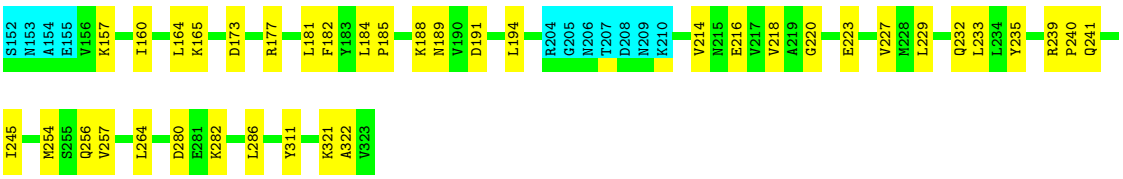
Chain A:





• Molecule 2: Mortality factor 4-like protein 1

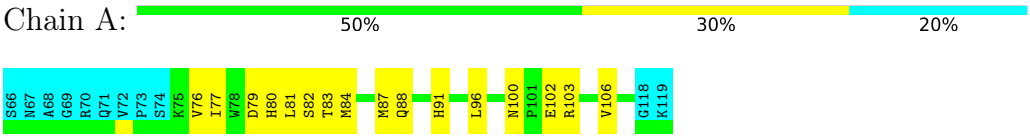
Chain B:



4.2.9 Score per residue for model 9

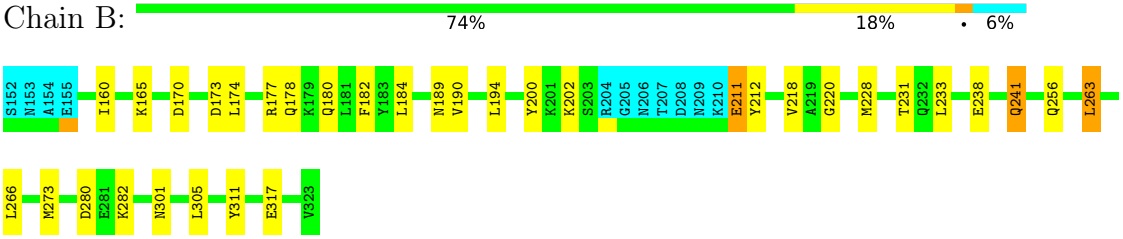
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

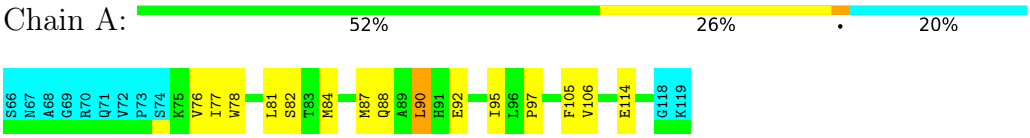
Chain B:



4.2.10 Score per residue for model 10

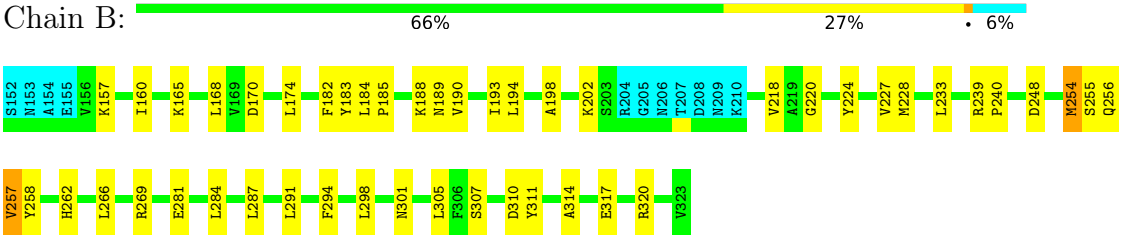
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

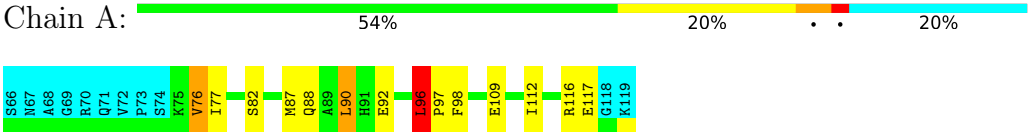
Chain B:



4.2.11 Score per residue for model 11

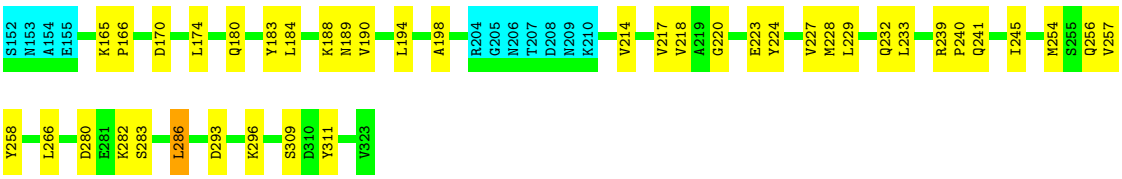
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

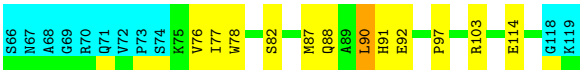
Chain B:



4.2.12 Score per residue for model 12

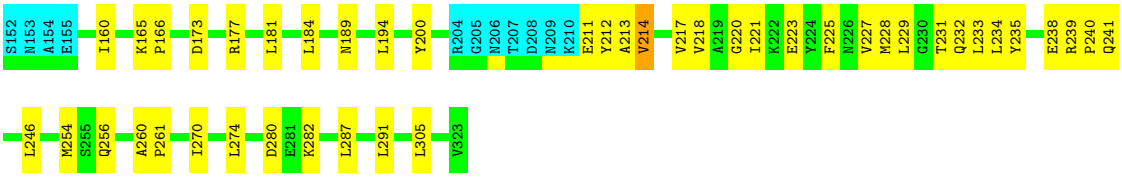
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

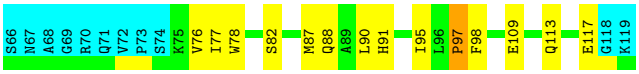
Chain B:



4.2.13 Score per residue for model 13

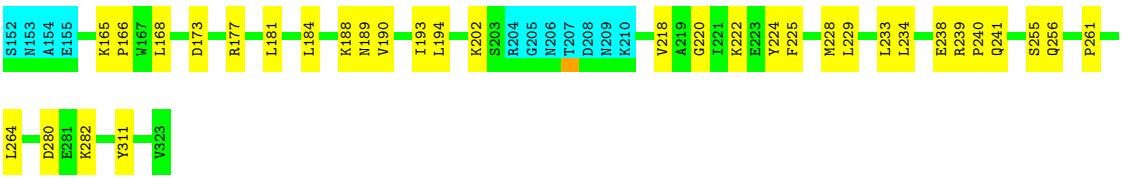
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

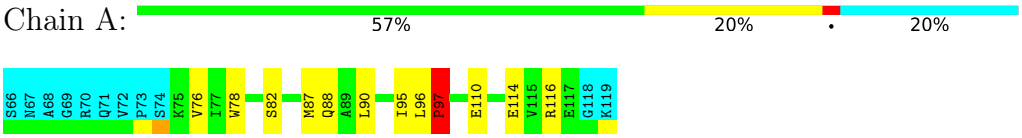
Chain B:



4.2.14 Score per residue for model 14

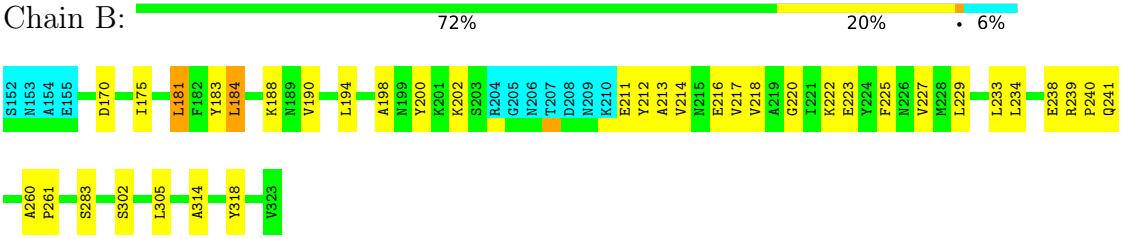
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

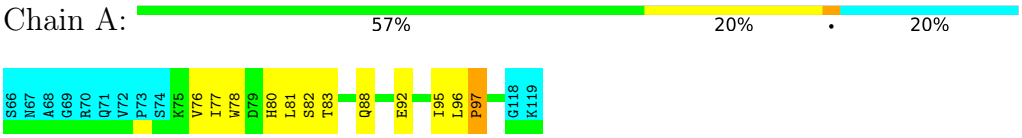
Chain B:



4.2.15 Score per residue for model 15

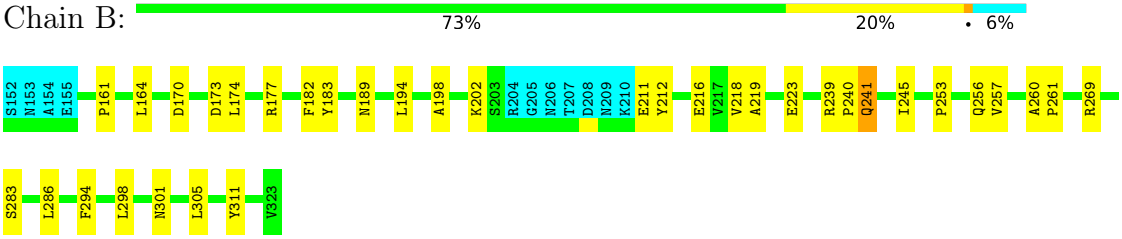
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

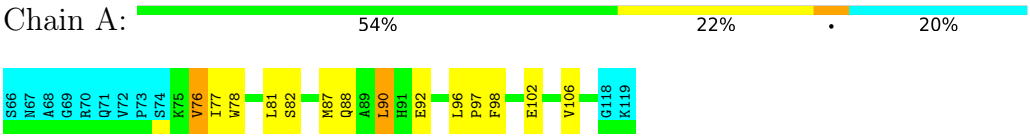
Chain B:



4.2.16 Score per residue for model 16

• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

Chain B:

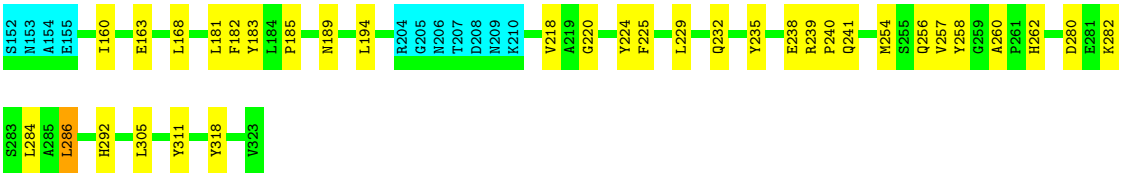
4.2.17 Score per residue for model 17

• Molecule 1: MRG/MORF4L-binding protein

Chain A:

• Molecule 2: Mortality factor 4-like protein 1

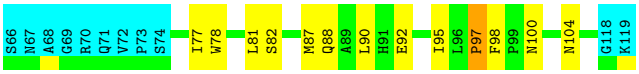
Chain B:



4.2.18 Score per residue for model 18

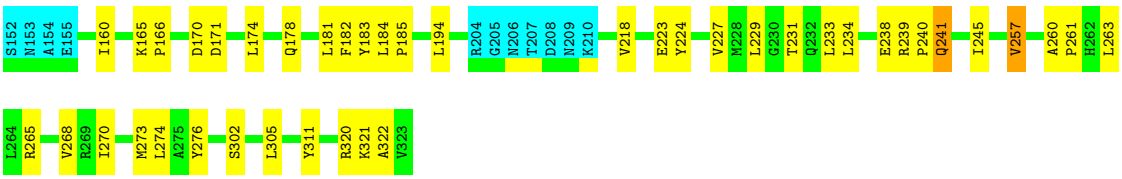
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

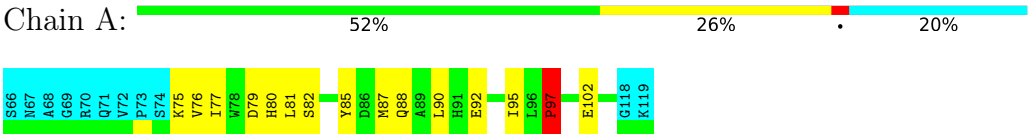
Chain B:



4.2.19 Score per residue for model 19

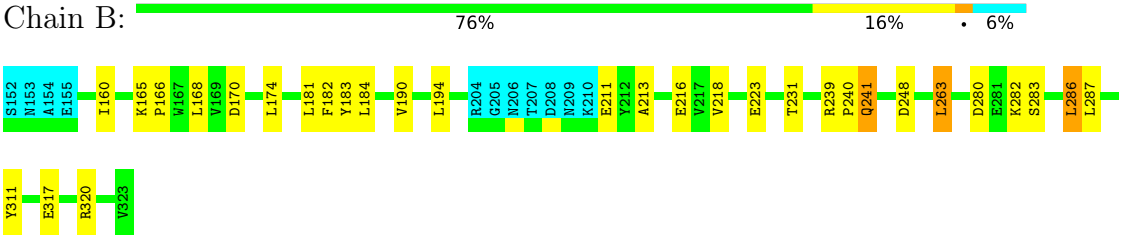
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

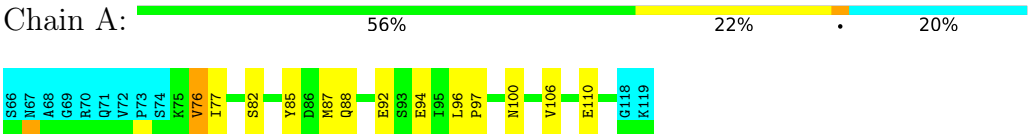
Chain B:



4.2.20 Score per residue for model 20

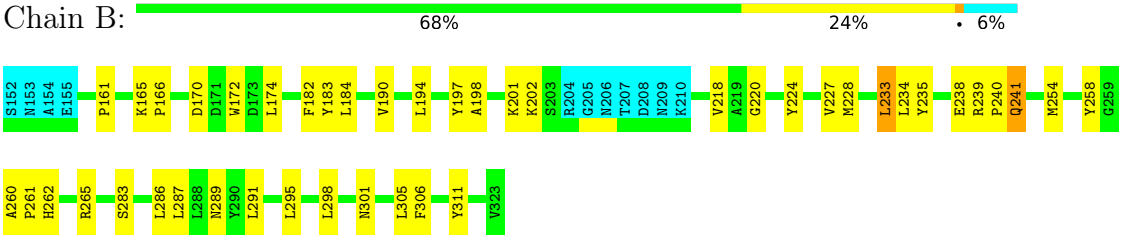
• Molecule 1: MRG/MORF4L-binding protein

Chain A:



• Molecule 2: Mortality factor 4-like protein 1

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy, restraint violations, and RMS deviations from the ideal covalent geometry.*

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

Software name	Classification	Version
ARIA	structure solution	1.2
CNS	refinement	1.1

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	2618
Number of shifts mapped to atoms	2618
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.41±0.01	0±0/376 (0.0± 0.0%)	0.79±0.03	0±0/513 (0.0± 0.0%)
2	B	0.38±0.01	0±0/1356 (0.0± 0.0%)	0.72±0.01	0±0/1842 (0.0± 0.0%)
All	All	0.39	0/34640 (0.0%)	0.73	3/47100 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	314	ALA	CA-C-N	5.08	123.37	119.66	10	1
2	B	314	ALA	C-N-CA	5.08	123.37	119.66	10	1
1	A	77	ILE	CB-CA-C	-5.04	107.42	111.71	17	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	365	353	351	10±3
2	B	1320	1331	1327	22±4
All	All	33700	33680	33560	589

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:293:ASP:HA	2:B:296:LYS:HE2	1.02	1.30	2	1
1:A:77:ILE:HD13	2:B:220:GLY:HA2	0.83	1.50	17	11
2:B:229:LEU:HA	2:B:233:LEU:HB2	0.83	1.50	8	9
2:B:185:PRO:HA	2:B:257:VAL:HA	0.83	1.49	17	7
2:B:194:LEU:HB3	2:B:218:VAL:HG13	0.82	1.50	15	17
2:B:189:ASN:HB2	2:B:256:GLN:HA	0.80	1.51	17	8
1:A:76:VAL:HG13	1:A:77:ILE:HG13	0.77	1.56	10	7
1:A:76:VAL:HG23	1:A:77:ILE:HG13	0.72	1.61	17	6
2:B:188:LYS:HE3	2:B:193:ILE:HG12	0.72	1.60	10	2
1:A:107:LEU:HD22	1:A:112:ILE:HG13	0.71	1.61	8	2
1:A:87:MET:HA	1:A:90:LEU:HG	0.70	1.63	10	3
2:B:235:TYR:HB2	2:B:238:GLU:HG3	0.70	1.64	17	2
1:A:102:GLU:HG3	2:B:231:THR:HG22	0.69	1.63	19	1
2:B:238:GLU:HB3	2:B:241:GLN:HE21	0.69	1.48	14	1
2:B:234:LEU:HG	2:B:238:GLU:HG3	0.68	1.65	13	2
2:B:229:LEU:HA	2:B:233:LEU:HB3	0.68	1.65	3	1
2:B:170:ASP:O	2:B:174:LEU:HG	0.67	1.89	15	13
1:A:103:ARG:HB2	2:B:232:GLN:HG3	0.66	1.64	4	2
2:B:189:ASN:CB	2:B:256:GLN:HA	0.65	2.20	15	7
2:B:258:TYR:HB3	2:B:262:HIS:HB2	0.65	1.69	20	4
2:B:181:LEU:HG	2:B:314:ALA:HB2	0.65	1.69	6	1
2:B:238:GLU:HB3	2:B:241:GLN:NE2	0.64	2.07	14	2
2:B:189:ASN:HB2	2:B:256:GLN:O	0.64	1.90	13	2
2:B:168:LEU:HD21	2:B:264:LEU:HD12	0.63	1.71	16	1
1:A:85:TYR:HB3	1:A:87:MET:HG3	0.63	1.68	8	4
2:B:261:PRO:HD3	2:B:306:PHE:HA	0.63	1.69	20	1
2:B:160:ILE:HB	2:B:165:LYS:HE3	0.63	1.69	7	1
1:A:87:MET:HA	1:A:90:LEU:HD23	0.63	1.71	14	4
1:A:89:ALA:O	1:A:92:GLU:HG2	0.62	1.94	4	1
1:A:95:ILE:O	1:A:97:PRO:HD3	0.62	1.95	19	7
1:A:82:SER:HB3	1:A:88:GLN:N	0.62	2.09	9	2
2:B:181:LEU:HD21	2:B:241:GLN:HB2	0.62	1.71	19	3
2:B:240:PRO:HB3	2:B:322:ALA:HA	0.61	1.71	8	1
1:A:82:SER:HA	1:A:87:MET:HB3	0.61	1.71	3	12
2:B:190:VAL:HG22	2:B:263:LEU:HG	0.61	1.72	9	4
2:B:214:VAL:O	2:B:218:VAL:HG22	0.61	1.95	16	1
2:B:160:ILE:HG21	2:B:168:LEU:HD11	0.61	1.71	19	5
2:B:269:ARG:HA	2:B:269:ARG:HE	0.60	1.56	3	2
2:B:280:ASP:OD2	2:B:282:LYS:HG3	0.60	1.95	17	1
1:A:76:VAL:HG13	1:A:77:ILE:H	0.60	1.56	6	2
1:A:96:LEU:N	1:A:97:PRO:HD3	0.60	2.11	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:GLN:O	1:A:92:GLU:HG2	0.60	1.96	8	8
2:B:228:MET:HA	2:B:231:THR:OG1	0.60	1.95	12	1
2:B:171:ASP:HB2	2:B:265:ARG:NH2	0.60	2.11	2	2
2:B:269:ARG:NE	2:B:269:ARG:HA	0.60	2.12	4	1
2:B:160:ILE:HG13	2:B:268:VAL:HG12	0.60	1.72	18	1
2:B:239:ARG:HG3	2:B:240:PRO:HD3	0.59	1.72	5	1
1:A:87:MET:SD	2:B:283:SER:HB3	0.59	2.38	14	1
1:A:82:SER:HB3	1:A:88:GLN:CA	0.59	2.28	9	2
2:B:270:ILE:O	2:B:274:LEU:HG	0.58	1.97	12	3
1:A:82:SER:HB2	1:A:88:GLN:N	0.58	2.12	17	7
2:B:239:ARG:N	2:B:240:PRO:HD2	0.58	2.11	15	14
2:B:165:LYS:N	2:B:166:PRO:HD2	0.58	2.13	20	7
2:B:254:MET:HA	2:B:254:MET:HE2	0.58	1.74	20	8
2:B:175:ILE:O	2:B:179:LYS:HA	0.57	1.99	16	2
2:B:260:ALA:N	2:B:261:PRO:HD2	0.57	2.15	3	7
2:B:181:LEU:HB3	2:B:183:TYR:CD1	0.57	2.35	14	1
1:A:103:ARG:HB3	2:B:232:GLN:HG3	0.57	1.76	5	1
1:A:85:TYR:CE2	2:B:282:LYS:HB2	0.57	2.34	2	1
2:B:245:ILE:HG21	2:B:257:VAL:HG21	0.57	1.77	8	3
2:B:280:ASP:OD1	2:B:282:LYS:HG2	0.56	2.00	6	5
2:B:241:GLN:HA	2:B:318:TYR:OH	0.56	2.01	17	1
2:B:238:GLU:O	2:B:241:GLN:HG3	0.56	1.99	9	2
2:B:220:GLY:O	2:B:224:TYR:HB2	0.56	2.01	13	6
2:B:301:ASN:O	2:B:305:LEU:HD13	0.56	2.01	20	8
1:A:78:TRP:HE1	2:B:224:TYR:HE2	0.56	1.43	13	1
2:B:317:GLU:HA	2:B:320:ARG:HG2	0.56	1.78	19	1
1:A:78:TRP:CH2	2:B:220:GLY:HA3	0.55	2.36	2	5
1:A:78:TRP:CE3	1:A:81:LEU:HD22	0.55	2.36	3	3
2:B:160:ILE:O	2:B:165:LYS:HE3	0.55	2.01	3	5
1:A:96:LEU:H	1:A:96:LEU:HD13	0.55	1.62	7	1
1:A:78:TRP:CZ3	1:A:81:LEU:HD13	0.55	2.35	18	1
2:B:225:PHE:O	2:B:229:LEU:HB2	0.55	2.02	14	4
1:A:100:ASN:HD21	2:B:232:GLN:HB2	0.55	1.60	1	1
2:B:178:GLN:HB3	2:B:180:GLN:HG3	0.55	1.78	9	1
1:A:82:SER:HA	1:A:87:MET:HB2	0.54	1.79	20	4
2:B:190:VAL:O	2:B:194:LEU:HG	0.54	2.01	11	3
2:B:223:GLU:O	2:B:227:VAL:HG23	0.54	2.02	2	9
1:A:103:ARG:HB3	2:B:232:GLN:HB3	0.54	1.80	12	1
2:B:181:LEU:HD11	2:B:238:GLU:HB3	0.54	1.78	13	1
2:B:181:LEU:HD21	2:B:238:GLU:HG2	0.53	1.79	14	1
1:A:103:ARG:O	2:B:232:GLN:HA	0.53	2.03	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:GLN:O	1:A:92:GLU:HG3	0.53	2.02	20	3
1:A:85:TYR:HE2	2:B:282:LYS:HB2	0.53	1.62	2	2
1:A:96:LEU:HA	1:A:98:PHE:CE2	0.53	2.39	11	1
2:B:184:LEU:HD11	2:B:310:ASP:HB3	0.53	1.80	5	1
2:B:245:ILE:HG21	2:B:257:VAL:HG11	0.53	1.78	5	3
1:A:82:SER:HB3	1:A:88:GLN:HA	0.53	1.79	9	2
2:B:182:PHE:HB2	2:B:311:TYR:CE1	0.52	2.39	19	6
2:B:217:VAL:O	2:B:221:ILE:HG12	0.52	2.05	16	2
2:B:233:LEU:HD11	2:B:265:ARG:HB2	0.52	1.81	3	1
2:B:298:LEU:HD12	2:B:305:LEU:HD23	0.52	1.79	5	2
1:A:76:VAL:HG23	1:A:77:ILE:H	0.52	1.64	9	1
1:A:81:LEU:HD22	1:A:87:MET:CE	0.52	2.35	8	3
2:B:190:VAL:HB	2:B:255:SER:O	0.52	2.05	13	1
2:B:287:LEU:O	2:B:291:LEU:HG	0.51	2.04	6	5
1:A:95:ILE:C	1:A:97:PRO:HD3	0.51	2.31	15	4
2:B:280:ASP:OD2	2:B:282:LYS:HG2	0.51	2.04	8	4
2:B:234:LEU:HD22	2:B:238:GLU:HG3	0.51	1.82	20	1
1:A:113:GLN:O	1:A:117:GLU:HB2	0.51	2.04	13	1
2:B:298:LEU:HD22	2:B:305:LEU:HD21	0.51	1.80	4	1
1:A:105:PHE:O	1:A:106:VAL:HG22	0.51	2.05	7	1
2:B:183:TYR:HB3	2:B:241:GLN:HG3	0.51	1.82	4	1
2:B:185:PRO:HB3	2:B:257:VAL:HG12	0.51	1.82	4	3
2:B:238:GLU:O	2:B:241:GLN:HB3	0.51	2.06	14	1
2:B:246:LEU:HD23	2:B:254:MET:SD	0.50	2.45	12	1
2:B:239:ARG:HB2	2:B:240:PRO:HD3	0.50	1.83	3	1
1:A:96:LEU:HA	1:A:98:PHE:CE1	0.50	2.41	7	1
1:A:82:SER:CA	1:A:87:MET:HB3	0.50	2.37	16	2
2:B:173:ASP:OD2	2:B:177:ARG:HD3	0.50	2.07	12	5
2:B:307:SER:HB2	2:B:310:ASP:OD1	0.50	2.07	10	1
1:A:81:LEU:HA	1:A:84:MET:HE2	0.50	1.83	9	1
2:B:212:TYR:O	2:B:216:GLU:HG2	0.50	2.07	1	3
2:B:291:LEU:O	2:B:295:LEU:HG	0.50	2.07	20	2
2:B:164:LEU:HB3	2:B:264:LEU:HD21	0.50	1.84	6	1
2:B:174:LEU:HD23	2:B:178:GLN:HG3	0.50	1.82	18	1
2:B:165:LYS:HB2	2:B:166:PRO:HD3	0.49	1.83	6	3
1:A:76:VAL:HG23	1:A:77:ILE:N	0.49	2.22	9	1
1:A:75:LYS:O	1:A:79:ASP:HB2	0.49	2.07	19	1
1:A:107:LEU:HD22	1:A:112:ILE:CG1	0.49	2.37	3	1
1:A:80:HIS:HB3	2:B:212:TYR:OH	0.49	2.08	9	1
1:A:82:SER:HB2	1:A:88:GLN:HA	0.49	1.85	18	1
2:B:227:VAL:HG13	2:B:228:MET:HG3	0.49	1.85	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:229:LEU:HA	2:B:233:LEU:CB	0.48	2.37	3	1
2:B:172:TRP:CD1	2:B:235:TYR:HH	0.48	2.26	20	1
2:B:182:PHE:HB2	2:B:311:TYR:CE2	0.48	2.43	1	6
2:B:239:ARG:HA	2:B:239:ARG:HE	0.48	1.68	11	1
2:B:241:GLN:HE22	2:B:258:TYR:HE1	0.48	1.52	2	2
2:B:268:VAL:HG23	2:B:269:ARG:HG2	0.48	1.86	3	1
2:B:269:ARG:HA	2:B:269:ARG:NE	0.48	2.23	3	1
2:B:198:ALA:O	2:B:202:LYS:HG2	0.48	2.09	5	1
1:A:82:SER:CB	1:A:87:MET:HB3	0.48	2.39	16	1
2:B:260:ALA:HB1	2:B:305:LEU:HD13	0.48	1.86	17	1
2:B:265:ARG:N	2:B:265:ARG:HD2	0.48	2.22	2	1
2:B:198:ALA:HB2	2:B:218:VAL:HG21	0.48	1.84	10	4
2:B:189:ASN:ND2	2:B:256:GLN:HG3	0.47	2.24	13	2
2:B:227:VAL:HG13	2:B:228:MET:HG2	0.47	1.86	10	1
1:A:100:ASN:HB2	2:B:231:THR:HG21	0.47	1.86	18	1
1:A:91:HIS:O	1:A:95:ILE:HA	0.47	2.09	6	1
2:B:294:PHE:O	2:B:298:LEU:HG	0.47	2.09	10	4
2:B:181:LEU:HD21	2:B:237:PHE:CE2	0.47	2.44	4	2
2:B:189:ASN:HD22	2:B:256:GLN:HG3	0.47	1.68	11	2
2:B:233:LEU:HD11	2:B:266:LEU:HG	0.47	1.86	2	1
1:A:82:SER:HB2	1:A:87:MET:C	0.47	2.34	17	5
2:B:233:LEU:HD11	2:B:266:LEU:HD23	0.47	1.87	10	2
2:B:181:LEU:HD22	2:B:241:GLN:HE21	0.47	1.69	12	1
1:A:80:HIS:HB2	2:B:216:GLU:OE2	0.47	2.09	1	1
1:A:102:GLU:HB3	2:B:239:ARG:HH22	0.47	1.69	19	1
2:B:280:ASP:OD1	2:B:282:LYS:HG3	0.47	2.10	7	1
2:B:164:LEU:HD23	2:B:264:LEU:HD22	0.47	1.87	8	1
2:B:173:ASP:OD1	2:B:177:ARG:HD3	0.47	2.10	9	1
2:B:234:LEU:HG	2:B:238:GLU:HB2	0.47	1.86	12	3
2:B:283:SER:O	2:B:286:LEU:HG	0.46	2.10	4	6
1:A:79:ASP:O	1:A:83:THR:HG23	0.46	2.11	9	1
1:A:114:GLU:HG2	2:B:165:LYS:HG2	0.46	1.86	10	1
2:B:228:MET:SD	2:B:273:MET:HE2	0.46	2.51	16	1
2:B:233:LEU:HD13	2:B:233:LEU:O	0.46	2.11	20	1
2:B:239:ARG:N	2:B:240:PRO:CD	0.46	2.78	5	1
2:B:180:GLN:HG2	2:B:313:VAL:HA	0.46	1.86	16	1
1:A:78:TRP:CE3	1:A:81:LEU:HD13	0.46	2.45	18	2
1:A:109:GLU:H	1:A:109:GLU:CD	0.46	2.19	11	1
2:B:194:LEU:HB3	2:B:218:VAL:CG1	0.46	2.41	10	2
2:B:168:LEU:HA	2:B:265:ARG:NH2	0.46	2.26	4	1
2:B:190:VAL:HB	2:B:255:SER:HB2	0.46	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:161:PRO:HB2	2:B:164:LEU:HD13	0.46	1.87	15	2
2:B:228:MET:HG3	2:B:233:LEU:HB2	0.46	1.86	3	1
2:B:302:SER:HA	2:B:305:LEU:CB	0.45	2.41	18	4
2:B:245:ILE:CG2	2:B:257:VAL:HG21	0.45	2.41	16	1
2:B:264:LEU:HB3	2:B:265:ARG:NH1	0.45	2.26	2	1
2:B:181:LEU:HB3	2:B:241:GLN:NE2	0.45	2.27	8	1
1:A:102:GLU:O	1:A:103:ARG:HD2	0.45	2.11	9	1
2:B:183:TYR:HB3	2:B:241:GLN:HG2	0.45	1.88	3	1
2:B:240:PRO:HG3	2:B:322:ALA:HB2	0.45	1.88	18	2
2:B:287:LEU:O	2:B:291:LEU:HB2	0.45	2.11	10	1
2:B:181:LEU:HB2	2:B:183:TYR:CE2	0.45	2.47	17	1
1:A:88:GLN:HA	1:A:91:HIS:CD2	0.45	2.47	12	3
1:A:96:LEU:N	1:A:97:PRO:CD	0.45	2.79	7	2
2:B:198:ALA:HA	2:B:214:VAL:HG11	0.45	1.88	16	1
2:B:202:LYS:HG2	2:B:211:GLU:HB2	0.45	1.88	9	1
2:B:242:TYR:HA	2:B:258:TYR:OH	0.44	2.12	1	1
2:B:197:TYR:O	2:B:201:LYS:HG2	0.44	2.13	7	2
1:A:77:ILE:HD13	2:B:220:GLY:CA	0.44	2.39	10	1
1:A:87:MET:O	1:A:90:LEU:HB2	0.44	2.12	13	1
1:A:102:GLU:HG2	2:B:231:THR:HG22	0.44	1.89	16	3
2:B:254:MET:HA	2:B:257:VAL:HG22	0.44	1.87	17	2
2:B:301:ASN:O	2:B:305:LEU:HB2	0.44	2.13	4	2
2:B:264:LEU:HB3	2:B:265:ARG:HH11	0.44	1.72	2	1
2:B:240:PRO:HB3	2:B:321:LYS:HG3	0.44	1.87	7	1
2:B:214:VAL:O	2:B:217:VAL:HG12	0.44	2.13	11	1
2:B:302:SER:HA	2:B:305:LEU:HB3	0.44	1.89	1	2
2:B:264:LEU:HD11	2:B:306:PHE:CZ	0.44	2.47	7	1
2:B:262:HIS:HA	2:B:265:ARG:HG3	0.44	1.89	20	1
2:B:193:ILE:HD11	2:B:260:ALA:HB2	0.44	1.88	2	2
2:B:280:ASP:HB3	2:B:282:LYS:HG2	0.44	1.89	2	1
1:A:77:ILE:HG13	1:A:78:TRP:H	0.44	1.72	15	1
2:B:253:PRO:HD2	2:B:256:GLN:OE1	0.44	2.13	6	1
1:A:111:ILE:HG23	2:B:165:LYS:HD2	0.44	1.90	7	1
1:A:78:TRP:CZ2	2:B:224:TYR:HE2	0.44	2.31	18	1
2:B:189:ASN:ND2	2:B:191:ASP:HB3	0.44	2.28	8	1
2:B:168:LEU:HD21	2:B:264:LEU:HG	0.43	1.90	13	1
2:B:293:ASP:O	2:B:296:LYS:HB3	0.43	2.13	11	1
2:B:219:ALA:O	2:B:223:GLU:HG2	0.43	2.14	15	1
2:B:182:PHE:HE1	2:B:310:ASP:HB2	0.43	1.74	4	1
2:B:241:GLN:OE1	2:B:245:ILE:HG12	0.43	2.13	15	1
1:A:116:ARG:HB3	1:A:117:GLU:OE2	0.43	2.13	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:171:ASP:OD1	2:B:265:ARG:HD2	0.43	2.13	18	1
1:A:104:ASN:OD1	2:B:236:LYS:HB2	0.43	2.14	3	1
2:B:189:ASN:CG	2:B:256:GLN:HG3	0.43	2.39	4	1
2:B:234:LEU:HA	2:B:265:ARG:NH2	0.43	2.28	20	1
1:A:105:PHE:HB2	2:B:232:GLN:O	0.43	2.13	17	1
2:B:161:PRO:O	2:B:165:LYS:HG3	0.43	2.14	20	1
1:A:81:LEU:HD12	1:A:84:MET:HE2	0.43	1.90	7	2
1:A:90:LEU:N	1:A:90:LEU:HD12	0.43	2.29	4	1
2:B:189:ASN:HB3	2:B:256:GLN:HG3	0.43	1.90	15	2
1:A:103:ARG:HG3	2:B:232:GLN:HG3	0.43	1.89	6	1
1:A:90:LEU:HD23	1:A:90:LEU:N	0.42	2.30	16	2
2:B:181:LEU:HD22	2:B:238:GLU:HB3	0.42	1.90	3	1
2:B:180:GLN:HB3	2:B:311:TYR:HB3	0.42	1.91	11	1
1:A:78:TRP:O	1:A:82:SER:HB2	0.42	2.13	5	1
2:B:198:ALA:O	2:B:202:LYS:HG3	0.42	2.14	14	4
2:B:317:GLU:O	2:B:320:ARG:HG2	0.42	2.14	10	1
2:B:184:LEU:N	2:B:184:LEU:HD13	0.42	2.28	14	1
2:B:286:LEU:HG	2:B:287:LEU:N	0.42	2.28	19	1
1:A:105:PHE:CE1	2:B:269:ARG:HB2	0.42	2.48	10	1
2:B:254:MET:HE3	2:B:254:MET:HA	0.42	1.91	10	1
1:A:109:GLU:O	1:A:113:GLN:HG2	0.42	2.14	13	1
2:B:163:GLU:H	2:B:163:GLU:CD	0.42	2.23	5	1
2:B:283:SER:HA	2:B:286:LEU:HD23	0.42	1.90	11	3
2:B:161:PRO:HG3	2:B:295:LEU:HB3	0.42	1.91	1	1
1:A:87:MET:HA	1:A:90:LEU:CG	0.42	2.41	10	1
1:A:96:LEU:O	1:A:96:LEU:HD22	0.42	2.15	11	1
2:B:194:LEU:HB3	2:B:218:VAL:HB	0.42	1.90	5	2
2:B:261:PRO:HB3	2:B:311:TYR:OH	0.42	2.15	13	1
1:A:76:VAL:HG13	1:A:77:ILE:N	0.42	2.27	6	2
2:B:213:ALA:O	2:B:217:VAL:HG23	0.42	2.15	12	2
2:B:175:ILE:HD12	2:B:181:LEU:HG	0.42	1.92	14	1
1:A:82:SER:HB2	1:A:88:GLN:CA	0.42	2.44	18	1
2:B:317:GLU:HA	2:B:320:ARG:CG	0.42	2.43	19	1
2:B:198:ALA:HA	2:B:214:VAL:CG1	0.41	2.45	14	1
2:B:212:TYR:O	2:B:216:GLU:HG3	0.41	2.14	14	1
2:B:314:ALA:HB1	2:B:318:TYR:CD2	0.41	2.50	14	1
1:A:105:PHE:HE1	2:B:269:ARG:HB2	0.41	1.75	10	1
2:B:188:LYS:HB3	2:B:188:LYS:NZ	0.41	2.30	4	1
1:A:96:LEU:H	1:A:96:LEU:CD1	0.41	2.28	7	1
1:A:112:ILE:O	1:A:116:ARG:HG2	0.41	2.16	11	1
2:B:228:MET:HG2	2:B:232:GLN:HB3	0.41	1.92	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:164:LEU:HD13	2:B:264:LEU:HD21	0.41	1.91	1	1
2:B:160:ILE:HB	2:B:165:LYS:CE	0.41	2.42	7	1
2:B:264:LEU:HD23	2:B:306:PHE:CZ	0.41	2.51	16	1
2:B:229:LEU:O	2:B:234:LEU:HB2	0.41	2.15	2	1
1:A:110:GLU:O	1:A:114:GLU:HB2	0.41	2.15	14	1
2:B:253:PRO:HG2	2:B:256:GLN:HB2	0.41	1.92	15	1
1:A:96:LEU:HG	1:A:96:LEU:O	0.41	2.15	8	1
1:A:95:ILE:HG22	1:A:96:LEU:N	0.41	2.31	15	1
2:B:264:LEU:HD13	2:B:264:LEU:O	0.41	2.16	2	1
2:B:273:MET:HA	2:B:276:TYR:CD2	0.41	2.51	18	1
2:B:213:ALA:HA	2:B:216:GLU:OE2	0.41	2.15	19	1
2:B:181:LEU:HG	2:B:241:GLN:NE2	0.41	2.30	4	1
2:B:228:MET:HE2	2:B:273:MET:SD	0.41	2.56	9	1
2:B:189:ASN:O	2:B:193:ILE:HG13	0.41	2.16	2	2
2:B:181:LEU:HD21	2:B:237:PHE:CZ	0.41	2.51	4	1
1:A:81:LEU:HD21	2:B:286:LEU:HD11	0.41	1.93	17	1
1:A:78:TRP:CZ2	2:B:224:TYR:CE2	0.41	3.09	18	1
2:B:240:PRO:HB2	2:B:321:LYS:HE3	0.41	1.92	18	1
1:A:85:TYR:CD1	2:B:286:LEU:HD11	0.41	2.51	8	1
1:A:80:HIS:HA	1:A:83:THR:HG22	0.40	1.92	15	1
2:B:317:GLU:H	2:B:317:GLU:CD	0.40	2.24	6	1
2:B:239:ARG:HA	2:B:239:ARG:NE	0.40	2.31	11	1
2:B:254:MET:N	2:B:254:MET:SD	0.40	2.94	10	1
2:B:213:ALA:HA	2:B:216:GLU:HG2	0.40	1.93	19	1
2:B:184:LEU:HD22	2:B:184:LEU:C	0.40	2.41	5	1
2:B:286:LEU:O	2:B:289:ASN:HB3	0.40	2.17	20	1
1:A:102:GLU:HA	2:B:231:THR:O	0.40	2.16	4	1
1:A:90:LEU:N	1:A:90:LEU:HD23	0.40	2.31	11	1
2:B:229:LEU:HD13	2:B:229:LEU:C	0.40	2.41	11	1
1:A:82:SER:HB2	1:A:87:MET:HB3	0.40	1.93	16	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	43/54 (80%)	37±2 (87±4%)	4±2 (9±5%)	2±1 (4±2%)	4 31
2	B	160/172 (93%)	153±2 (95±1%)	7±2 (4±1%)	0±0 (0±0%)	100 100
All	All	4060/4520 (90%)	3803 (94%)	223 (5%)	34 (1%)	18 68

All 7 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	97	PRO	12
1	A	106	VAL	9
1	A	76	VAL	5
1	A	98	PHE	3
1	A	96	LEU	2
1	A	100	ASN	2
2	B	278	PRO	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	42/50 (84%)	40±1 (96±3%)	2±1 (4±3%)	32 82
2	B	141/150 (94%)	136±2 (96±1%)	5±2 (4±1%)	30 81
All	All	3660/4000 (92%)	3524 (96%)	136 (4%)	31 81

All 51 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)
2	B	184	LEU	17
2	B	183	TYR	11
1	A	90	LEU	9
2	B	188	LYS	8
2	B	241	GLN	7
2	B	224	TYR	7
2	B	263	LEU	5
1	A	97	PRO	4
2	B	157	LYS	4

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Mol	Chain	Res	Type	Models (Total)
2	B	286	LEU	4
1	A	91	HIS	3
1	A	110	GLU	3
2	B	284	LEU	3
2	B	317	GLU	3
2	B	163	GLU	3
2	B	266	LEU	2
2	B	233	LEU	2
2	B	235	TYR	2
2	B	170	ASP	2
1	A	96	LEU	2
1	A	104	ASN	2
2	B	248	ASP	2
2	B	257	VAL	2
2	B	222	LYS	2
2	B	196	ASP	1
2	B	310	ASP	1
1	A	100	ASN	1
2	B	217	VAL	1
2	B	255	SER	1
2	B	273	MET	1
1	A	95	ILE	1
1	A	106	VAL	1
1	A	81	LEU	1
2	B	216	GLU	1
2	B	321	LYS	1
2	B	211	GLU	1
2	B	254	MET	1
2	B	281	GLU	1
2	B	309	SER	1
2	B	200	TYR	1
2	B	214	VAL	1
2	B	305	LEU	1
2	B	228	MET	1
2	B	181	LEU	1
2	B	190	VAL	1
2	B	264	LEU	1
2	B	292	HIS	1
1	A	77	ILE	1
2	B	320	ARG	1
1	A	80	HIS	1
1	A	94	GLU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 82% 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	2618
Number of shifts mapped to atoms	2618
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	225	-0.50 ± 0.07	Should be checked
$^{13}C_{\beta}$	216	0.17 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	215	-0.12 ± 0.07	None needed (< 0.5 ppm)
^{15}N	197	0.55 ± 0.19	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 2418 atoms were assigned a chemical shift out of a possible 2932. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	971/996 (97%)	391/398 (98%)	399/408 (98%)	181/190 (95%)
Sidechain	1356/1646 (82%)	906/1075 (84%)	437/520 (84%)	13/51 (25%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	91/290 (31%)	75/138 (54%)	13/137 (9%)	3/15 (20%)
Overall	2418/2932 (82%)	1372/1611 (85%)	849/1065 (80%)	197/256 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 2617 atoms were assigned a chemical shift out of a possible 3196. 0 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1065/1107 (96%)	428/444 (96%)	440/452 (97%)	197/211 (93%)
Sidechain	1461/1799 (81%)	972/1170 (83%)	472/565 (84%)	17/64 (27%)
Aromatic	91/290 (31%)	75/138 (54%)	13/137 (9%)	3/15 (20%)
Overall	2617/3196 (82%)	1475/1752 (84%)	925/1154 (80%)	217/290 (75%)

7.1.4 Statistically unusual chemical shifts (i)

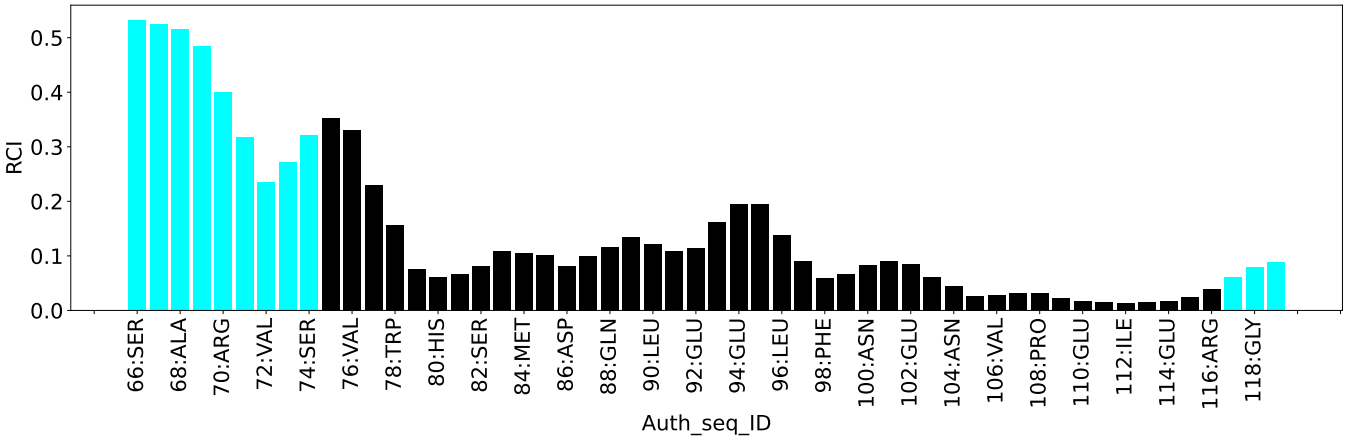
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	176	THR	HG1	2.75	0.08 – 2.19	7.6

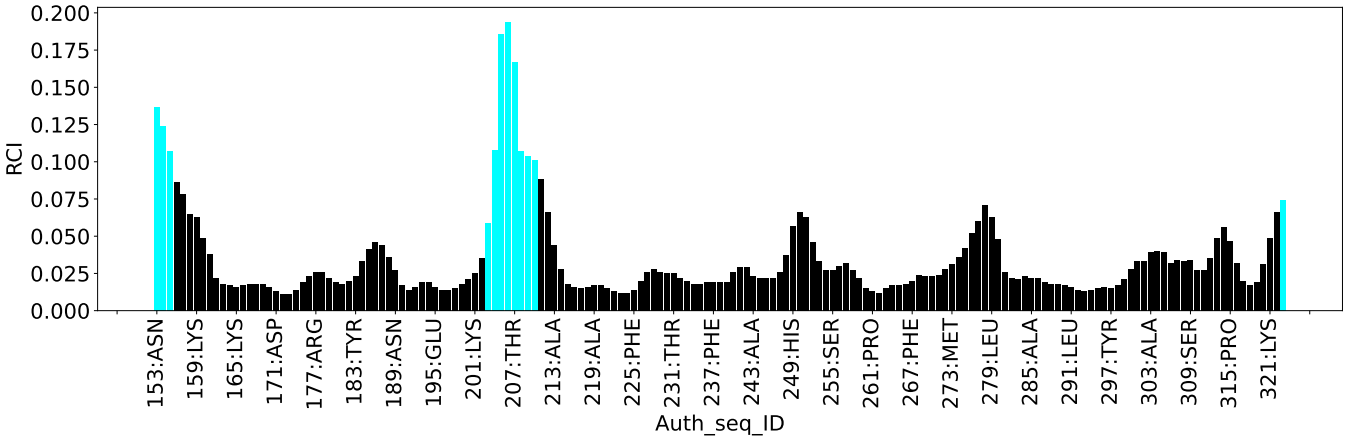
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:



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	5091
Intra-residue (|i-j|=0)	2181
Sequential (|i-j|=1)	949
Medium range (|i-j|>1 and |i-j|<5)	793
Long range (|i-j|≥5)	576
Inter-chain	470
Hydrogen bond restraints	122
Disulfide bond restraints	0
Total dihedral-angle restraints	348
Number of unmapped restraints	0
Number of restraints per residue	24.1
Number of long range restraints per residue[1]	2.5

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	48.2	0.2
0.2-0.5 (Medium)	72.8	0.5
>0.5 (Large)	101.0	4.39

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	5.5	3.6
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

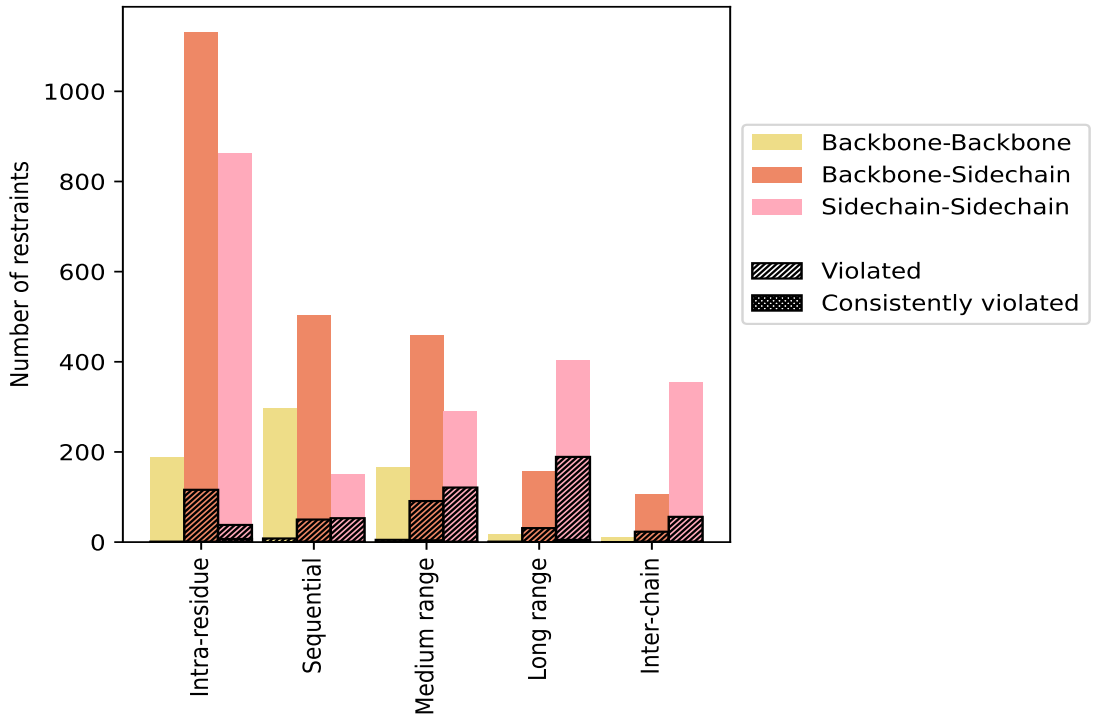
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	2181	42.8	155	7.1	3.0	8	0.4	0.2
Backbone-Backbone	188	3.7	1	0.5	0.0	0	0.0	0.0
Backbone-Sidechain	1131	22.2	116	10.3	2.3	1	0.1	0.0
Sidechain-Sidechain	862	16.9	38	4.4	0.7	7	0.8	0.1
Sequential (|i-j|=1)	949	18.6	111	11.7	2.2	2	0.2	0.0
Backbone-Backbone	297	5.8	8	2.7	0.2	0	0.0	0.0
Backbone-Sidechain	502	9.9	50	10.0	1.0	1	0.2	0.0
Sidechain-Sidechain	150	2.9	53	35.3	1.0	1	0.7	0.0
Medium range (|i-j|>1 & |i-j|<5)	793	15.6	202	25.5	4.0	5	0.6	0.1
Backbone-Backbone	165	3.2	5	3.0	0.1	0	0.0	0.0
Backbone-Sidechain	337	6.6	76	22.6	1.5	4	1.2	0.1
Sidechain-Sidechain	291	5.7	121	41.6	2.4	1	0.3	0.0
Long range (|i-j|≥5)	576	11.3	221	38.4	4.3	5	0.9	0.1
Backbone-Backbone	16	0.3	1	6.2	0.0	0	0.0	0.0
Backbone-Sidechain	157	3.1	31	19.7	0.6	0	0.0	0.0
Sidechain-Sidechain	403	7.9	189	46.9	3.7	5	1.2	0.1
Inter-chain	470	9.2	79	16.8	1.6	2	0.4	0.0
Backbone-Backbone	10	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	105	2.1	23	21.9	0.5	1	1.0	0.0
Sidechain-Sidechain	355	7.0	56	15.8	1.1	1	0.3	0.0
Hydrogen bond	122	2.4	15	12.3	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	5091	100.0	783	15.4	15.4	22	0.4	0.4
Backbone-Backbone	676	13.3	15	2.2	0.3	0	0.0	0.0
Backbone-Sidechain	2354	46.2	311	13.2	6.1	7	0.3	0.1
Sidechain-Sidechain	2061	40.5	457	22.2	9.0	15	0.7	0.3

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	42	33	57	69	23	224	0.59	2.6	0.49	0.43
2	39	36	65	65	26	231	0.61	3.19	0.59	0.43
3	38	44	62	62	25	231	0.61	3.31	0.57	0.4
4	31	39	64	56	27	217	0.65	3.13	0.56	0.48
5	36	37	65	62	28	228	0.68	3.45	0.6	0.47
6	42	34	64	61	31	232	0.66	3.73	0.62	0.42
7	37	31	61	50	33	212	0.62	4.18	0.56	0.47
8	42	34	81	62	23	242	0.62	3.24	0.57	0.42
9	36	36	64	58	25	219	0.64	3.57	0.61	0.43
10	37	34	72	65	27	235	0.68	4.01	0.65	0.46

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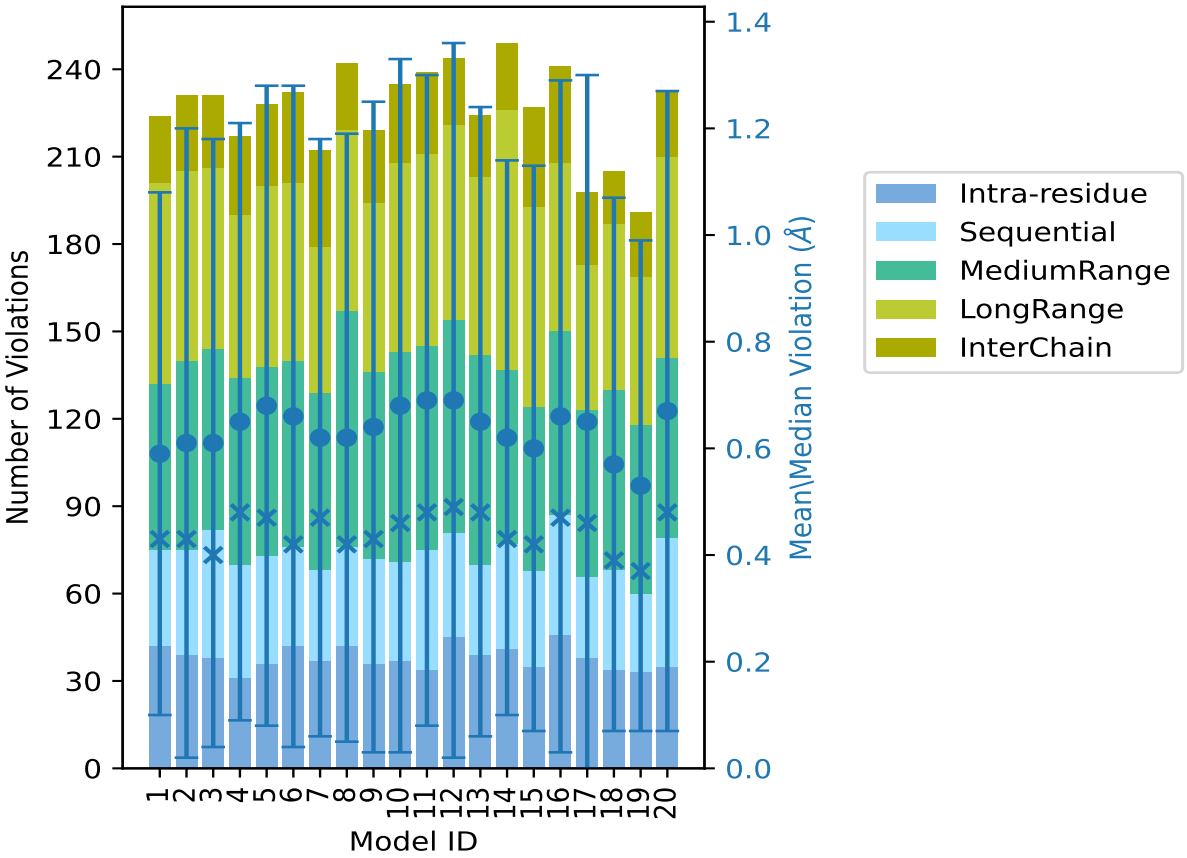
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	34	41	70	66	28	239	0.69	3.23	0.61	0.48
12	45	36	73	67	23	244	0.69	4.29	0.67	0.49
13	39	31	72	61	21	224	0.65	3.08	0.59	0.48
14	41	36	60	89	23	249	0.62	2.56	0.52	0.43
15	35	33	56	69	34	227	0.6	2.96	0.53	0.42
16	46	41	63	58	33	241	0.66	4.39	0.63	0.47
17	38	28	57	50	25	198	0.65	4.31	0.65	0.46
18	34	34	62	57	18	205	0.57	3.02	0.5	0.39
19	33	27	58	51	22	191	0.53	2.99	0.46	0.37
20	35	44	62	69	22	232	0.67	3.2	0.6	0.48

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

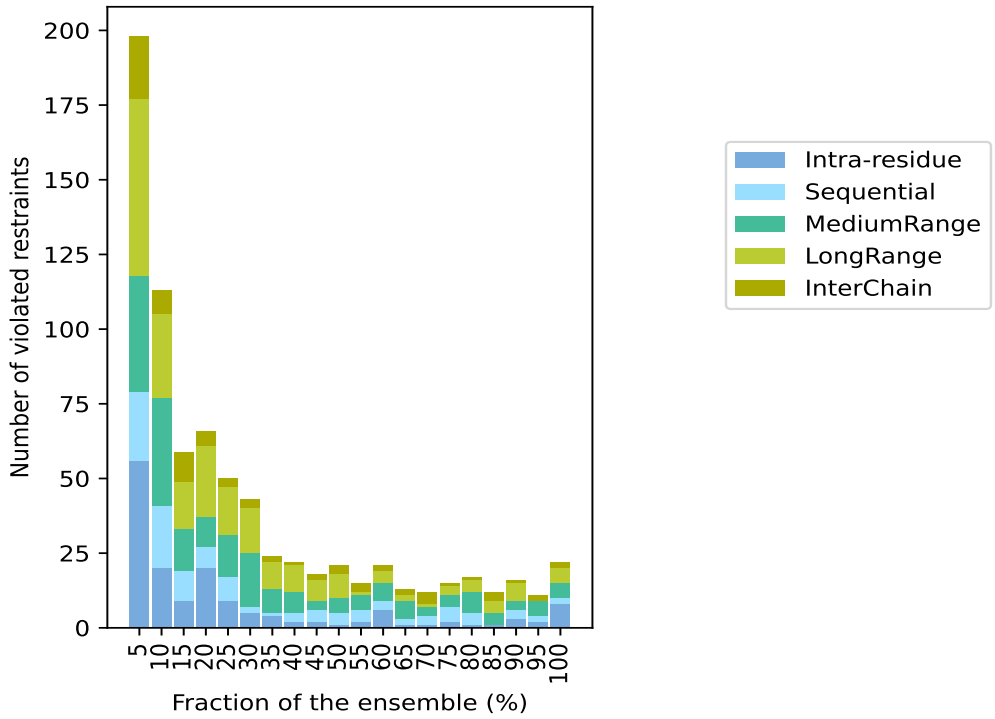
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 4201(IR:2026, SQ:838, MR:591, LR:355, IC:391) 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]	%
56	23	39	59	21	198	1	5.0
20	21	36	28	8	113	2	10.0
9	10	14	16	10	59	3	15.0
20	7	10	24	5	66	4	20.0
9	8	14	16	3	50	5	25.0
5	2	18	15	3	43	6	30.0
4	1	8	9	2	24	7	35.0
2	3	7	9	1	22	8	40.0
2	4	3	7	2	18	9	45.0
1	4	5	8	3	21	10	50.0
2	4	5	1	3	15	11	55.0
6	3	6	4	2	21	12	60.0
1	2	6	2	2	13	13	65.0
1	3	3	1	4	12	14	70.0
2	5	4	3	1	15	15	75.0
1	4	7	4	1	17	16	80.0
1	0	4	4	3	12	17	85.0
3	3	3	6	1	16	18	90.0
2	2	5	0	2	11	19	95.0
8	2	5	5	2	22	20	100.0

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

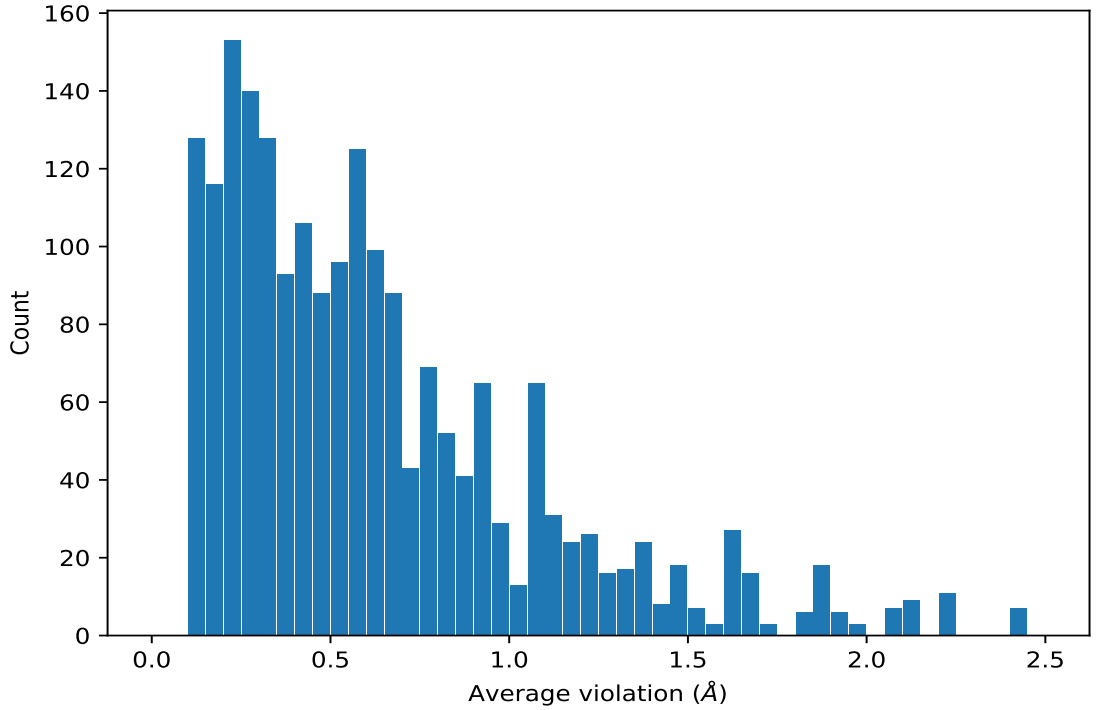
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4269)	1:76:A:VAL:HG23	1:79:A:ASP:HA	20	1.9	0.37	1.76
(1,4269)	1:81:A:LEU:HD13	1:79:A:ASP:HA	20	1.9	0.37	1.76
(1,4269)	1:81:A:LEU:HD11	1:79:A:ASP:HA	20	1.9	0.37	1.76
(1,4269)	1:81:A:LEU:HD12	1:79:A:ASP:HA	20	1.9	0.37	1.76
(1,4269)	1:76:A:VAL:HG21	1:79:A:ASP:HA	20	1.9	0.37	1.76
(1,4269)	1:76:A:VAL:HG22	1:79:A:ASP:HA	20	1.9	0.37	1.76
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG11	20	1.86	0.13	1.9
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG22	20	1.86	0.13	1.9
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG13	20	1.86	0.13	1.9
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG21	20	1.86	0.13	1.9
(2,59)	1:78:A:TRP:HH2	1:76:A:VAL:HG13	20	1.86	0.13	1.9
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG12	20	1.86	0.13	1.9
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG23	20	1.86	0.13	1.9
(1,4333)	1:95:A:ILE:HG23	1:93:A:SER:HA	20	1.7	0.46	1.84
(1,4333)	1:90:A:LEU:HD11	1:93:A:SER:HA	20	1.7	0.46	1.84
(1,4333)	1:90:A:LEU:HD21	1:93:A:SER:HA	20	1.7	0.46	1.84

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4333)	2:279:B:LEU:HD22	1:93:A:SER:HA	20	1.7	0.46	1.84
(1,4333)	1:90:A:LEU:HD13	1:93:A:SER:HA	20	1.7	0.46	1.84
(1,4333)	1:90:A:LEU:HD12	1:93:A:SER:HA	20	1.7	0.46	1.84
(1,4333)	1:95:A:ILE:HG21	1:93:A:SER:HA	20	1.7	0.46	1.84
(1,4333)	2:279:B:LEU:HD21	1:93:A:SER:HA	20	1.7	0.46	1.84
(1,4333)	1:95:A:ILE:HG22	1:93:A:SER:HA	20	1.7	0.46	1.84
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB3	20	1.42	0.2	1.4
(1,4421)	1:111:A:ILE:HD11	1:110:A:GLU:HB2	20	1.42	0.2	1.4
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB2	20	1.42	0.2	1.4
(1,4421)	1:111:A:ILE:HD12	1:110:A:GLU:HB2	20	1.42	0.2	1.4
(1,4505)	2:311:B:TYR:HD2	2:181:B:LEU:HD22	20	1.34	0.46	1.23
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	20	1.34	0.46	1.23
(1,4505)	2:311:B:TYR:HD1	2:181:B:LEU:HD21	20	1.34	0.46	1.23
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	20	1.34	0.46	1.23
(1,4505)	2:311:B:TYR:HD1	2:181:B:LEU:HD22	20	1.34	0.46	1.23
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD21	20	1.34	0.46	1.23
(1,4505)	2:311:B:TYR:HD2	2:181:B:LEU:HD21	20	1.34	0.46	1.23
(1,4505)	2:311:B:TYR:HD1	2:181:B:LEU:HD23	20	1.34	0.46	1.23
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	20	1.24	0.89	1.65
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	20	1.24	0.89	1.65
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	20	1.24	0.89	1.65
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	20	1.24	0.89	1.65
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	20	1.24	0.89	1.65
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	20	1.24	0.89	1.65
(1,158)	2:311:B:TYR:HD1	2:174:B:LEU:HD23	20	1.22	0.46	1.37
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	20	1.22	0.46	1.37
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	20	1.22	0.46	1.37
(1,158)	2:311:B:TYR:HD1	2:174:B:LEU:HD21	20	1.22	0.46	1.37
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD21	20	1.22	0.46	1.37
(1,158)	2:311:B:TYR:HD1	2:174:B:LEU:HD22	20	1.22	0.46	1.37
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG11	20	0.93	0.23	0.96
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	20	0.93	0.23	0.96
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG12	20	0.93	0.23	0.96
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE3	20	0.79	0.38	0.78
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	20	0.79	0.38	0.78
(1,3824)	2:214:B:VAL:HG23	2:202:B:LYS:HE2	20	0.79	0.38	0.78
(1,3824)	2:214:B:VAL:HG23	2:202:B:LYS:HE3	20	0.79	0.38	0.78
(1,3824)	2:214:B:VAL:HG22	2:202:B:LYS:HE3	20	0.79	0.38	0.78
(1,3824)	2:214:B:VAL:HG22	2:202:B:LYS:HE2	20	0.79	0.38	0.78
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	20	0.69	0.59	0.47
(1,4534)	2:183:B:TYR:HD1	2:238:B:GLU:HB2	20	0.69	0.59	0.47
(1,4534)	2:183:B:TYR:HD2	2:238:B:GLU:HB2	20	0.69	0.59	0.47

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3921)	2:221:B:ILE:HG22	2:263:B:LEU:HD23	20	0.63	0.3	0.67
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD22	20	0.63	0.3	0.67
(1,3921)	2:194:B:LEU:HD22	2:263:B:LEU:HD22	20	0.63	0.3	0.67
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	20	0.63	0.3	0.67
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD23	20	0.63	0.3	0.67
(1,3921)	2:221:B:ILE:HG21	2:263:B:LEU:HD23	20	0.63	0.3	0.67
(1,3921)	2:194:B:LEU:HD23	2:263:B:LEU:HD22	20	0.63	0.3	0.67
(1,3921)	2:274:B:LEU:HD21	2:156:B:VAL:HG23	20	0.63	0.3	0.67
(1,3921)	2:194:B:LEU:HD21	2:263:B:LEU:HD21	20	0.63	0.3	0.67
(1,3921)	2:221:B:ILE:HG21	2:263:B:LEU:HD22	20	0.63	0.3	0.67
(1,3921)	2:221:B:ILE:HG21	2:263:B:LEU:HD21	20	0.63	0.3	0.67
(1,3921)	2:221:B:ILE:HG22	2:263:B:LEU:HD21	20	0.63	0.3	0.67
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	20	0.57	0.12	0.57
(1,4390)	1:115:A:VAL:HG23	1:111:A:ILE:HA	20	0.57	0.12	0.57
(1,4390)	1:115:A:VAL:HG22	1:111:A:ILE:HA	20	0.57	0.12	0.57
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	20	0.55	0.08	0.56
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	20	0.51	0.13	0.52
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	20	0.51	0.13	0.52
(1,3846)	2:219:B:ALA:HA	2:219:B:ALA:HB1	20	0.23	0.01	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB2	20	0.23	0.01	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	20	0.23	0.01	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB1	20	0.23	0.01	0.23
(1,3961)	2:282:B:LYS:HG2	2:282:B:LYS:HD3	20	0.22	0.04	0.22
(1,3961)	2:282:B:LYS:HG2	2:282:B:LYS:HD2	20	0.22	0.04	0.22
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	20	0.22	0.04	0.22
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD3	20	0.22	0.04	0.22
(1,3835)	2:156:B:VAL:HG21	2:156:B:VAL:HB	20	0.22	0.02	0.22
(1,3835)	2:214:B:VAL:HG21	2:214:B:VAL:HB	20	0.22	0.02	0.22
(1,3835)	2:214:B:VAL:HG23	2:214:B:VAL:HB	20	0.22	0.02	0.22
(1,3835)	2:156:B:VAL:HG23	2:156:B:VAL:HB	20	0.22	0.02	0.22
(1,3835)	2:156:B:VAL:HG12	2:156:B:VAL:HB	20	0.22	0.02	0.22
(1,3835)	2:214:B:VAL:HG22	2:214:B:VAL:HB	20	0.22	0.02	0.22
(1,3835)	2:156:B:VAL:HG13	2:156:B:VAL:HB	20	0.22	0.02	0.22
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	20	0.21	0.04	0.2
(1,3998)	2:300:B:LYS:HG2	2:300:B:LYS:HD3	20	0.21	0.04	0.2
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	20	0.21	0.03	0.22
(1,3959)	2:210:B:LYS:HD3	2:210:B:LYS:HG2	20	0.21	0.03	0.22
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG2	20	0.21	0.03	0.22
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG3	20	0.2	0.04	0.2
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	20	0.2	0.04	0.2
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	20	0.2	0.04	0.2
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	20	0.2	0.03	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	20	0.2	0.03	0.19
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	20	0.19	0.04	0.19
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	20	0.19	0.04	0.19
(1,4296)	1:90:A:LEU:HD11	1:87:A:MET:HE3	19	1.19	0.75	1.03
(1,4296)	1:90:A:LEU:HD21	1:87:A:MET:HE3	19	1.19	0.75	1.03
(1,4296)	1:90:A:LEU:HD12	1:87:A:MET:HE1	19	1.19	0.75	1.03
(1,4296)	2:279:B:LEU:HD11	1:87:A:MET:HE1	19	1.19	0.75	1.03
(1,4296)	2:279:B:LEU:HD13	1:87:A:MET:HE1	19	1.19	0.75	1.03
(1,4296)	2:279:B:LEU:HD13	1:87:A:MET:HE2	19	1.19	0.75	1.03
(1,4296)	1:90:A:LEU:HD13	1:87:A:MET:HE1	19	1.19	0.75	1.03
(1,4296)	1:90:A:LEU:HD11	1:87:A:MET:HE1	19	1.19	0.75	1.03
(1,4296)	1:90:A:LEU:HD12	1:87:A:MET:HE2	19	1.19	0.75	1.03
(1,4296)	2:279:B:LEU:HD12	1:87:A:MET:HE2	19	1.19	0.75	1.03
(1,4296)	2:279:B:LEU:HD11	1:87:A:MET:HE2	19	1.19	0.75	1.03
(1,4296)	1:90:A:LEU:HD22	1:87:A:MET:HE2	19	1.19	0.75	1.03
(1,4296)	1:90:A:LEU:HD13	1:87:A:MET:HE3	19	1.19	0.75	1.03
(1,4296)	2:279:B:LEU:HD12	1:87:A:MET:HE3	19	1.19	0.75	1.03
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD12	19	1.13	0.4	1.09
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	19	1.13	0.4	1.09
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD13	19	1.13	0.4	1.09
(1,4316)	1:87:A:MET:HE3	1:90:A:LEU:HD21	19	1.13	0.33	1.13
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD22	19	1.13	0.33	1.13
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD21	19	1.13	0.33	1.13
(1,4316)	1:87:A:MET:HE1	1:90:A:LEU:HD21	19	1.13	0.33	1.13
(1,4316)	1:87:A:MET:HE1	1:90:A:LEU:HD22	19	1.13	0.33	1.13
(1,4316)	1:87:A:MET:HE1	1:90:A:LEU:HD23	19	1.13	0.33	1.13
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD23	19	1.13	0.33	1.13
(1,4316)	1:87:A:MET:HE3	1:90:A:LEU:HD23	19	1.13	0.33	1.13
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD21	19	1.07	0.81	0.62
(1,3950)	2:279:B:LEU:HD21	2:274:B:LEU:HD23	19	1.07	0.81	0.62
(1,3950)	2:270:B:ILE:HG22	2:274:B:LEU:HD23	19	1.07	0.81	0.62
(1,3950)	2:270:B:ILE:HG22	2:274:B:LEU:HD21	19	1.07	0.81	0.62
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD23	19	1.07	0.81	0.62
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD22	19	1.07	0.81	0.62
(1,3950)	2:270:B:ILE:HG21	2:274:B:LEU:HD21	19	1.07	0.81	0.62
(1,3950)	2:279:B:LEU:HD22	2:274:B:LEU:HD22	19	1.07	0.81	0.62
(1,3950)	2:270:B:ILE:HG21	2:274:B:LEU:HD23	19	1.07	0.81	0.62
(1,3950)	2:270:B:ILE:HG21	2:274:B:LEU:HD22	19	1.07	0.81	0.62
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	19	1.02	1.06	0.39
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD11	19	1.02	1.06	0.39
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD12	19	1.02	1.06	0.39
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	19	0.64	0.12	0.66

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	19	0.64	0.12	0.66
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	19	0.64	0.12	0.66
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD3	19	0.64	0.12	0.66
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD3	19	0.64	0.12	0.66
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD3	19	0.64	0.12	0.66
(1,4611)	2:290:B:TYR:HD1	2:210:B:LYS:HD2	19	0.61	0.25	0.6
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	19	0.61	0.25	0.6
(1,4611)	2:290:B:TYR:HD2	2:286:B:LEU:HG	19	0.61	0.25	0.6
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	19	0.61	0.25	0.64
(1,4382)	2:168:B:LEU:HD13	1:108:A:PRO:HD3	19	0.61	0.25	0.64
(1,4382)	2:168:B:LEU:HD12	1:108:A:PRO:HD3	19	0.61	0.25	0.64
(1,4382)	1:111:A:ILE:HG12	1:108:A:PRO:HD3	19	0.61	0.25	0.64
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	19	0.52	0.05	0.53
(1,2693)	1:92:A:GLU:HG3	1:93:A:SER:HA	19	0.52	0.05	0.53
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	19	0.22	0.01	0.22
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD2	19	0.22	0.01	0.22
(1,4436)	1:119:A:LYS:HD3	1:119:A:LYS:HG2	19	0.2	0.03	0.19
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	19	0.2	0.03	0.19
(1,4436)	1:119:A:LYS:HD2	1:119:A:LYS:HG3	19	0.2	0.03	0.19
(1,4436)	1:75:A:LYS:HD2	1:75:A:LYS:HG3	19	0.2	0.03	0.19
(1,4282)	1:87:A:MET:HE1	1:83:A:THR:HG22	18	1.61	0.29	1.74
(1,4282)	1:87:A:MET:HE3	1:83:A:THR:HG21	18	1.61	0.29	1.74
(1,4282)	1:87:A:MET:HE3	1:83:A:THR:HG22	18	1.61	0.29	1.74
(1,4282)	1:88:A:GLN:HB2	1:83:A:THR:HG23	18	1.61	0.29	1.74
(1,4282)	1:87:A:MET:HE2	1:83:A:THR:HG23	18	1.61	0.29	1.74
(1,4282)	1:87:A:MET:HE1	1:83:A:THR:HG23	18	1.61	0.29	1.74
(1,4282)	1:87:A:MET:HE3	1:83:A:THR:HG23	18	1.61	0.29	1.74
(1,4282)	1:87:A:MET:HE1	1:83:A:THR:HG21	18	1.61	0.29	1.74
(1,4282)	1:87:A:MET:HE2	1:83:A:THR:HG22	18	1.61	0.29	1.74
(1,4282)	1:88:A:GLN:HB2	1:83:A:THR:HG22	18	1.61	0.29	1.74
(1,4282)	1:88:A:GLN:HB2	1:83:A:THR:HG21	18	1.61	0.29	1.74
(1,4054)	2:313:B:VAL:HG12	2:180:B:GLN:HE22	18	1.36	0.62	1.46
(1,4054)	2:313:B:VAL:HG13	2:180:B:GLN:HE22	18	1.36	0.62	1.46
(1,4054)	2:313:B:VAL:HG11	2:180:B:GLN:HE22	18	1.36	0.62	1.46
(1,4313)	1:87:A:MET:HE3	1:90:A:LEU:HD11	18	1.12	0.86	1.03
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD11	18	1.12	0.86	1.03
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD12	18	1.12	0.86	1.03
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD11	18	1.12	0.86	1.03
(1,4313)	1:87:A:MET:HE2	1:90:A:LEU:HD11	18	1.12	0.86	1.03
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD13	18	1.12	0.86	1.03
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD13	18	1.12	0.86	1.03
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	18	1.12	0.86	1.03

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4313)	1:87:A:MET:HE3	1:90:A:LEU:HD13	18	1.12	0.86	1.03
(1,4555)	2:294:B:PHE:HD1	2:214:B:VAL:HG13	18	0.92	0.42	0.83
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG12	18	0.92	0.42	0.83
(1,4555)	2:294:B:PHE:HD2	2:217:B:VAL:HG11	18	0.92	0.42	0.83
(1,4555)	2:294:B:PHE:HD2	2:217:B:VAL:HG12	18	0.92	0.42	0.83
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG11	18	0.92	0.42	0.83
(1,4555)	2:294:B:PHE:HD2	2:264:B:LEU:HD11	18	0.92	0.42	0.83
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG13	18	0.92	0.42	0.83
(1,4555)	2:294:B:PHE:HD2	2:264:B:LEU:HD13	18	0.92	0.42	0.83
(1,4555)	2:294:B:PHE:HD2	2:217:B:VAL:HG13	18	0.92	0.42	0.83
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE3	18	0.81	0.31	0.88
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	18	0.81	0.31	0.88
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE1	18	0.81	0.31	0.88
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	18	0.7	0.09	0.72
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	18	0.64	0.18	0.66
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	18	0.64	0.18	0.66
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	18	0.64	0.18	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	18	0.64	0.18	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	18	0.64	0.18	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	18	0.64	0.18	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	18	0.64	0.18	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	18	0.64	0.18	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	18	0.64	0.18	0.66
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB2	18	0.64	0.14	0.65
(1,3832)	2:214:B:VAL:HG11	2:213:B:ALA:HB2	18	0.64	0.14	0.65
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB3	18	0.64	0.14	0.65
(1,3832)	2:217:B:VAL:HG13	2:213:B:ALA:HB2	18	0.64	0.14	0.65
(1,3832)	2:214:B:VAL:HG11	2:213:B:ALA:HB3	18	0.64	0.14	0.65
(1,3832)	2:214:B:VAL:HG12	2:213:B:ALA:HB1	18	0.64	0.14	0.65
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB1	18	0.64	0.14	0.65
(1,3832)	2:217:B:VAL:HG12	2:213:B:ALA:HB1	18	0.64	0.14	0.65
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	18	0.56	0.22	0.52
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	18	0.56	0.22	0.52
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	18	0.56	0.22	0.52
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	18	0.55	0.23	0.53
(1,4533)	2:183:B:TYR:HE2	2:321:B:LYS:HE3	18	0.55	0.23	0.53
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	18	0.3	0.09	0.28
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	18	0.26	0.09	0.26
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	18	0.21	0.03	0.22
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	18	0.21	0.03	0.22
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	18	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	18	0.18	0.05	0.18
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	18	0.18	0.05	0.18
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	18	0.18	0.05	0.18
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	18	0.18	0.05	0.18
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB3	18	0.18	0.05	0.18
(1,453)	2:211:B:GLU:HG3	2:211:B:GLU:HB2	18	0.16	0.04	0.15
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB2	18	0.16	0.04	0.15
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	18	0.16	0.04	0.15
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG12	17	1.61	0.46	1.57
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG13	17	1.61	0.46	1.57
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG13	17	1.61	0.46	1.57
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG11	17	1.61	0.46	1.57
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG11	17	1.61	0.46	1.57
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG12	17	1.61	0.46	1.57
(1,3945)	2:274:B:LEU:HD21	2:271:B:GLY:HA3	17	1.6	1.03	2.03
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	17	1.6	1.03	2.03
(1,3945)	2:274:B:LEU:HD22	2:271:B:GLY:HA3	17	1.6	1.03	2.03
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	17	1.13	0.24	1.11
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	17	1.13	0.24	1.11
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	17	1.13	0.24	1.11
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD11	17	1.08	0.45	0.96
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD12	17	1.08	0.45	0.96
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD13	17	1.08	0.45	0.96
(1,4497)	2:292:B:HIS:HE1	2:158:B:VAL:HG21	17	0.92	0.42	0.9
(1,4497)	2:292:B:HIS:HE1	2:295:B:LEU:HD12	17	0.92	0.42	0.9
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD23	17	0.92	0.42	0.9
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD21	17	0.92	0.42	0.9
(1,4497)	2:292:B:HIS:HE1	2:158:B:VAL:HG23	17	0.92	0.42	0.9
(1,4497)	2:292:B:HIS:HE1	2:158:B:VAL:HG22	17	0.92	0.42	0.9
(1,4497)	2:292:B:HIS:HE1	2:295:B:LEU:HD13	17	0.92	0.42	0.9
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD22	17	0.92	0.42	0.9
(1,4497)	2:292:B:HIS:HE1	2:295:B:LEU:HD11	17	0.92	0.42	0.9
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD23	17	0.81	0.42	0.92
(1,3745)	2:294:B:PHE:HA	2:298:B:LEU:HD23	17	0.81	0.42	0.92

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3745)	2:165:B:LYS:HA	2:164:B:LEU:HD23	17	0.81	0.42	0.92
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD22	17	0.81	0.42	0.92
(1,3745)	2:302:B:SER:HA	2:298:B:LEU:HD21	17	0.81	0.42	0.92
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD21	17	0.81	0.42	0.92
(1,3745)	2:294:B:PHE:HA	2:298:B:LEU:HD21	17	0.81	0.42	0.92
(1,3745)	2:165:B:LYS:HA	2:164:B:LEU:HD21	17	0.81	0.42	0.92
(1,3745)	2:302:B:SER:HA	2:298:B:LEU:HD23	17	0.81	0.42	0.92
(1,3745)	2:165:B:LYS:HA	2:164:B:LEU:HD22	17	0.81	0.42	0.92
(1,4237)	2:218:B:VAL:HG12	2:198:B:ALA:H	17	0.67	0.41	0.44
(1,4237)	2:218:B:VAL:HG13	2:198:B:ALA:H	17	0.67	0.41	0.44
(1,4237)	2:218:B:VAL:HG11	2:198:B:ALA:H	17	0.67	0.41	0.44
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	17	0.58	0.34	0.46
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD11	17	0.58	0.34	0.46
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD13	17	0.58	0.34	0.46
(1,4511)	2:182:B:PHE:HD1	2:175:B:ILE:HD12	17	0.54	0.22	0.5
(1,4511)	2:182:B:PHE:HD2	2:181:B:LEU:HG	17	0.54	0.22	0.5
(1,4511)	2:182:B:PHE:HD1	2:184:B:LEU:HB3	17	0.54	0.22	0.5
(1,4511)	2:182:B:PHE:HD1	2:175:B:ILE:HD13	17	0.54	0.22	0.5
(1,4511)	2:182:B:PHE:HD2	2:184:B:LEU:HB3	17	0.54	0.22	0.5
(1,4511)	2:182:B:PHE:HD1	2:175:B:ILE:HD11	17	0.54	0.22	0.5
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	17	0.31	0.12	0.29
(1,1061)	2:296:B:LYS:HE3	2:294:B:PHE:HA	17	0.31	0.12	0.29
(1,3740)	2:317:B:GLU:HB2	2:317:B:GLU:HG3	17	0.21	0.04	0.22
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG2	17	0.21	0.04	0.22
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG3	17	0.21	0.04	0.22
(1,3740)	2:317:B:GLU:HB3	2:317:B:GLU:HG3	17	0.21	0.04	0.22
(1,3740)	2:281:B:GLU:HB3	2:281:B:GLU:HG3	17	0.21	0.04	0.22
(1,4413)	2:169:B:VAL:HG21	1:112:A:ILE:HB	17	0.18	0.07	0.16
(1,4413)	2:169:B:VAL:HG22	1:112:A:ILE:HB	17	0.18	0.07	0.16
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	17	0.18	0.07	0.16
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	16	1.56	0.6	1.62
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	16	1.56	0.6	1.62
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	16	1.56	0.6	1.62
(1,3942)	2:274:B:LEU:HD21	2:270:B:ILE:HG21	16	1.39	1.1	1.72
(1,3942)	2:274:B:LEU:HD21	2:270:B:ILE:HG22	16	1.39	1.1	1.72
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG23	16	1.39	1.1	1.72
(1,3942)	2:274:B:LEU:HD22	2:270:B:ILE:HG23	16	1.39	1.1	1.72
(1,3942)	2:233:B:LEU:HD22	2:270:B:ILE:HG21	16	1.39	1.1	1.72
(1,3942)	2:274:B:LEU:HD21	2:270:B:ILE:HG23	16	1.39	1.1	1.72
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG21	16	1.39	1.1	1.72
(1,3942)	2:274:B:LEU:HD22	2:270:B:ILE:HG21	16	1.39	1.1	1.72
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG22	16	1.39	1.1	1.72

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3949)	2:302:B:SER:HB2	2:305:B:LEU:HD11	16	0.97	0.33	1.09
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD13	16	0.97	0.33	1.09
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD11	16	0.97	0.33	1.09
(1,3949)	2:272:B:ALA:HA	2:274:B:LEU:HD13	16	0.97	0.33	1.09
(1,3949)	2:302:B:SER:HB2	2:305:B:LEU:HD12	16	0.97	0.33	1.09
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD12	16	0.97	0.33	1.09
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE2	16	0.95	0.35	0.94
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE3	16	0.95	0.35	0.94
(1,4520)	2:212:B:TYR:HD1	2:215:B:ASN:HB2	16	0.95	0.35	0.94
(1,4520)	2:237:B:PHE:HE1	2:179:B:LYS:HE2	16	0.95	0.35	0.94
(1,4520)	2:212:B:TYR:HD2	2:215:B:ASN:HB2	16	0.95	0.35	0.94
(1,4520)	2:237:B:PHE:HE1	2:179:B:LYS:HE3	16	0.95	0.35	0.94
(1,4609)	2:224:B:TYR:HD2	2:223:B:GLU:HB3	16	0.88	0.33	0.82
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HE3	16	0.88	0.33	0.82
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HB3	16	0.88	0.33	0.82
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HE2	16	0.88	0.33	0.82
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HE1	16	0.88	0.33	0.82
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	16	0.87	0.18	0.82
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	16	0.87	0.18	0.82
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	16	0.87	0.18	0.82
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	16	0.86	0.29	0.92
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	16	0.86	0.29	0.92
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	16	0.86	0.29	0.92
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	16	0.78	0.29	0.88
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	16	0.78	0.29	0.88
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	16	0.78	0.29	0.88
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	16	0.78	0.29	0.88
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	16	0.78	0.29	0.88
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	16	0.78	0.29	0.88
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	16	0.69	0.45	0.64
(1,4589)	2:182:B:PHE:HD2	2:259:B:GLY:HA2	16	0.69	0.45	0.64
(1,4589)	2:182:B:PHE:HD2	2:261:B:PRO:HD3	16	0.69	0.45	0.64
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	16	0.65	0.51	0.48
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	16	0.65	0.51	0.48
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	16	0.65	0.51	0.48
(1,2775)	1:96:A:LEU:HD11	1:100:A:ASN:HB3	16	0.65	0.51	0.48
(1,2775)	1:96:A:LEU:HD12	1:100:A:ASN:HB3	16	0.65	0.51	0.48
(1,2775)	1:96:A:LEU:HD13	1:100:A:ASN:HB3	16	0.65	0.51	0.48
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	16	0.61	0.27	0.55
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	16	0.61	0.27	0.55
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	16	0.61	0.27	0.55
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	16	0.56	0.12	0.6

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	16	0.56	0.12	0.6
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	16	0.56	0.12	0.6
(1,4384)	2:169:B:VAL:HG21	1:109:A:GLU:HA	16	0.48	0.19	0.46
(1,4384)	2:169:B:VAL:HG22	1:109:A:GLU:HA	16	0.48	0.19	0.46
(1,4384)	1:106:A:VAL:HG12	1:109:A:GLU:HA	16	0.48	0.19	0.46
(1,4384)	2:169:B:VAL:HG23	1:109:A:GLU:HA	16	0.48	0.19	0.46
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	16	0.36	0.14	0.3
(1,4460)	1:87:A:MET:HG3	1:87:A:MET:H	16	0.36	0.14	0.3
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	16	0.34	0.5	0.14
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	16	0.34	0.5	0.14
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	16	0.34	0.5	0.14
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	16	0.3	0.17	0.26
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	16	0.3	0.17	0.26
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	16	0.3	0.17	0.26
(1,2206)	2:286:B:LEU:HD21	2:289:B:ASN:HD22	16	0.3	0.17	0.26
(1,2206)	2:286:B:LEU:HD22	2:289:B:ASN:HD22	16	0.3	0.17	0.26
(1,2206)	2:286:B:LEU:HD23	2:289:B:ASN:HD22	16	0.3	0.17	0.26
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	16	0.13	0.01	0.13
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	15	2.24	1.01	2.72
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD12	15	2.24	1.01	2.72
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD11	15	2.24	1.01	2.72
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	15	1.39	0.02	1.39
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	15	1.39	0.02	1.39
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	15	1.39	0.02	1.39
(1,4243)	1:115:A:VAL:HG23	1:114:A:GLU:HB2	15	1.21	0.42	1.36
(1,4243)	1:72:A:VAL:HG21	1:71:A:GLN:HB2	15	1.21	0.42	1.36
(1,4243)	1:115:A:VAL:HG22	1:114:A:GLU:HB2	15	1.21	0.42	1.36
(1,4243)	1:72:A:VAL:HG23	1:71:A:GLN:HB2	15	1.21	0.42	1.36
(1,4243)	1:72:A:VAL:HG22	1:71:A:GLN:HB2	15	1.21	0.42	1.36
(1,4243)	1:115:A:VAL:HG21	1:114:A:GLU:HB2	15	1.21	0.42	1.36
(1,4011)	2:314:B:ALA:HB3	2:313:B:VAL:HG21	15	0.95	0.09	0.95
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG23	15	0.95	0.09	0.95
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG22	15	0.95	0.09	0.95
(1,4011)	2:314:B:ALA:HB1	2:313:B:VAL:HG23	15	0.95	0.09	0.95
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG21	15	0.95	0.09	0.95
(1,4011)	2:314:B:ALA:HB1	2:313:B:VAL:HG22	15	0.95	0.09	0.95
(1,4011)	2:314:B:ALA:HB1	2:313:B:VAL:HG21	15	0.95	0.09	0.95
(1,4011)	2:314:B:ALA:HB3	2:313:B:VAL:HG23	15	0.95	0.09	0.95
(1,3774)	2:245:B:ILE:HG12	2:184:B:LEU:HD22	15	0.86	0.46	0.69
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD22	15	0.86	0.46	0.69
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD21	15	0.86	0.46	0.69
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD23	15	0.86	0.46	0.69

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3774)	2:245:B:ILE:HG12	2:184:B:LEU:HD23	15	0.86	0.46	0.69
(1,3774)	2:245:B:ILE:HG12	2:184:B:LEU:HD21	15	0.86	0.46	0.69
(1,3852)	2:218:B:VAL:HG21	2:202:B:LYS:HE3	15	0.79	0.36	0.92
(1,3852)	2:218:B:VAL:HG22	2:202:B:LYS:HE2	15	0.79	0.36	0.92
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE3	15	0.79	0.36	0.92
(1,3852)	2:218:B:VAL:HG22	2:222:B:LYS:HE2	15	0.79	0.36	0.92
(1,3852)	2:218:B:VAL:HG22	2:202:B:LYS:HE3	15	0.79	0.36	0.92
(1,3852)	2:218:B:VAL:HG21	2:202:B:LYS:HE2	15	0.79	0.36	0.92
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE2	15	0.79	0.36	0.92
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	15	0.79	0.45	0.65
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	15	0.79	0.45	0.65
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	15	0.79	0.45	0.65
(1,4324)	1:81:A:LEU:HD11	1:80:A:HIS:HB2	15	0.7	0.25	0.73
(1,4324)	1:81:A:LEU:HD13	1:80:A:HIS:HB2	15	0.7	0.25	0.73
(1,4324)	1:95:A:ILE:HG22	1:91:A:HIS:HB2	15	0.7	0.25	0.73
(1,4324)	1:81:A:LEU:HD12	1:80:A:HIS:HB2	15	0.7	0.25	0.73
(1,4324)	1:95:A:ILE:HG21	1:91:A:HIS:HB2	15	0.7	0.25	0.73
(1,4324)	1:95:A:ILE:HG23	1:91:A:HIS:HB2	15	0.7	0.25	0.73
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	15	0.62	0.18	0.61
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	15	0.62	0.18	0.61
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	15	0.62	0.18	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	15	0.62	0.18	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	15	0.62	0.18	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	15	0.62	0.18	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	15	0.62	0.18	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	15	0.62	0.18	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	15	0.62	0.18	0.61
(1,3947)	2:269:B:ARG:HB3	2:273:B:MET:HE1	15	0.6	0.2	0.59
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE3	15	0.6	0.2	0.59
(1,3947)	2:272:B:ALA:HB2	2:273:B:MET:HE2	15	0.6	0.2	0.59
(1,3947)	2:272:B:ALA:HB1	2:273:B:MET:HE2	15	0.6	0.2	0.59
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE1	15	0.6	0.2	0.59
(1,3947)	2:269:B:ARG:HB3	2:273:B:MET:HE2	15	0.6	0.2	0.59
(1,3947)	2:272:B:ALA:HB2	2:273:B:MET:HE3	15	0.6	0.2	0.59
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE2	15	0.6	0.2	0.59
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	15	0.41	0.15	0.43
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	15	0.41	0.15	0.43
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	15	0.41	0.15	0.43
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	15	0.41	0.15	0.43
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	15	0.41	0.15	0.43
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	15	0.41	0.15	0.43
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	15	0.41	0.15	0.43

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	15	0.41	0.15	0.43
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	15	0.41	0.15	0.43
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	15	0.32	0.1	0.31
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	15	0.32	0.1	0.31
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	15	0.32	0.1	0.31
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	15	0.15	0.02	0.15
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	15	0.14	0.03	0.14
(1,40)	2:159:B:LYS:HD3	2:159:B:LYS:HG2	15	0.14	0.03	0.14
(1,40)	2:159:B:LYS:HB2	2:159:B:LYS:HG2	15	0.14	0.03	0.14
(1,40)	2:159:B:LYS:HD2	2:159:B:LYS:HG2	15	0.14	0.03	0.14
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	15	0.12	0.01	0.12
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	15	0.12	0.01	0.12
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	15	0.12	0.01	0.12
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	14	1.72	0.42	1.81
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	14	1.72	0.42	1.81
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	14	1.72	0.42	1.81
(1,3936)	2:268:B:VAL:HG23	2:269:B:ARG:HD2	14	1.54	0.69	1.5
(1,3936)	2:268:B:VAL:HG21	2:269:B:ARG:HD2	14	1.54	0.69	1.5
(1,3936)	2:265:B:ARG:HB2	2:269:B:ARG:HD2	14	1.54	0.69	1.5
(1,3936)	2:268:B:VAL:HG22	2:269:B:ARG:HD2	14	1.54	0.69	1.5
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG23	14	1.28	0.35	1.28
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG21	14	1.28	0.35	1.28
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG22	14	1.28	0.35	1.28
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	14	1.18	0.3	1.19
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	14	1.18	0.3	1.19
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	14	1.18	0.3	1.19
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD21	14	0.79	0.34	0.66
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD23	14	0.79	0.34	0.66
(1,4280)	2:290:B:TYR:HE2	1:81:A:LEU:HD21	14	0.79	0.34	0.66
(1,4280)	2:290:B:TYR:HE2	1:81:A:LEU:HD23	14	0.79	0.34	0.66
(1,4280)	2:290:B:TYR:HE1	1:81:A:LEU:HD23	14	0.79	0.34	0.66
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD22	14	0.79	0.34	0.66
(1,4280)	2:290:B:TYR:HE2	1:81:A:LEU:HD22	14	0.79	0.34	0.66
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	14	0.61	0.28	0.62
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	14	0.61	0.28	0.62
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG21	14	0.59	0.23	0.56
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG23	14	0.59	0.23	0.56
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG22	14	0.59	0.23	0.56
(1,4407)	2:162:B:GLU:HG2	1:111:A:ILE:HG21	14	0.59	0.23	0.56
(1,3795)	2:194:B:LEU:HD23	2:190:B:VAL:HG11	14	0.56	0.57	0.32
(1,3795)	2:194:B:LEU:HD22	2:190:B:VAL:HG12	14	0.56	0.57	0.32
(1,3795)	2:221:B:ILE:HG22	2:190:B:VAL:HG13	14	0.56	0.57	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3795)	2:194:B:LEU:HD22	2:190:B:VAL:HG11	14	0.56	0.57	0.32
(1,3795)	2:194:B:LEU:HD21	2:190:B:VAL:HG12	14	0.56	0.57	0.32
(1,3795)	2:194:B:LEU:HD23	2:190:B:VAL:HG12	14	0.56	0.57	0.32
(1,3795)	2:194:B:LEU:HD23	2:190:B:VAL:HG13	14	0.56	0.57	0.32
(1,3795)	2:221:B:ILE:HG22	2:190:B:VAL:HG12	14	0.56	0.57	0.32
(1,3795)	2:194:B:LEU:HD21	2:190:B:VAL:HG13	14	0.56	0.57	0.32
(1,3795)	2:194:B:LEU:HD22	2:190:B:VAL:HG13	14	0.56	0.57	0.32
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG12	14	0.53	0.23	0.58
(1,4008)	2:178:B:GLN:HB2	2:313:B:VAL:HG13	14	0.53	0.23	0.58
(1,4008)	2:170:B:ASP:HB3	2:169:B:VAL:HG13	14	0.53	0.23	0.58
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG13	14	0.53	0.23	0.58
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG11	14	0.53	0.23	0.58
(1,4008)	2:170:B:ASP:HB3	2:169:B:VAL:HG11	14	0.53	0.23	0.58
(1,4008)	2:170:B:ASP:HB3	2:169:B:VAL:HG12	14	0.53	0.23	0.58
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	14	0.48	0.23	0.48
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	14	0.48	0.23	0.48
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	14	0.48	0.23	0.48
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	14	0.16	0.05	0.15
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	14	0.14	0.02	0.14
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG2	14	0.14	0.02	0.14
(1,3842)	2:214:B:VAL:HG22	2:207:B:THR:HG21	13	2.22	1.32	1.93
(1,3842)	2:214:B:VAL:HG21	2:207:B:THR:HG23	13	2.22	1.32	1.93
(1,3842)	2:214:B:VAL:HG23	2:218:B:VAL:HG13	13	2.22	1.32	1.93
(1,3842)	2:214:B:VAL:HG23	2:207:B:THR:HG21	13	2.22	1.32	1.93
(1,3842)	2:214:B:VAL:HG22	2:218:B:VAL:HG13	13	2.22	1.32	1.93
(1,3842)	2:214:B:VAL:HG22	2:218:B:VAL:HG11	13	2.22	1.32	1.93
(1,3842)	2:214:B:VAL:HG21	2:218:B:VAL:HG12	13	2.22	1.32	1.93
(1,3842)	2:214:B:VAL:HG23	2:218:B:VAL:HG11	13	2.22	1.32	1.93
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG22	13	1.9	0.96	1.82
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG23	13	1.9	0.96	1.82
(1,4442)	1:74:A:SER:HB3	1:76:A:VAL:HG21	13	1.9	0.96	1.82
(1,4442)	1:74:A:SER:HB3	1:76:A:VAL:HG23	13	1.9	0.96	1.82
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG21	13	1.9	0.96	1.82
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	13	1.61	0.5	1.81
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	13	1.61	0.5	1.81
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	13	1.61	0.5	1.81
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	13	1.25	0.42	1.14
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	13	1.25	0.42	1.14
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	13	1.25	0.42	1.14
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG22	13	0.97	0.55	0.98
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG23	13	0.97	0.55	0.98
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG23	13	0.97	0.55	0.98

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG22	13	0.97	0.55	0.98
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG21	13	0.97	0.55	0.98
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG21	13	0.97	0.55	0.98
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	13	0.92	0.32	0.87
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	13	0.92	0.32	0.87
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	13	0.92	0.32	0.87
(1,4492)	2:212:B:TYR:HE1	1:81:A:LEU:H	13	0.71	0.33	0.73
(1,4492)	1:85:A:TYR:HE2	1:86:A:ASP:H	13	0.71	0.33	0.73
(1,4492)	2:212:B:TYR:HE2	1:81:A:LEU:H	13	0.71	0.33	0.73
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD12	13	0.56	0.25	0.5
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD11	13	0.56	0.25	0.5
(1,4644)	2:182:B:PHE:HD1	2:184:B:LEU:HB2	13	0.56	0.25	0.5
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD13	13	0.56	0.25	0.5
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD12	13	0.51	0.31	0.44
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	13	0.51	0.31	0.44
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD13	13	0.51	0.31	0.44
(1,3250)	1:103:A:ARG:HD3	1:102:A:GLU:H	13	0.44	0.2	0.49
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	13	0.44	0.2	0.49
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD3	13	0.4	0.2	0.31
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	13	0.4	0.2	0.31
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	13	0.36	0.17	0.33
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	13	0.29	0.03	0.28
(1,3989)	2:295:B:LEU:HD21	2:298:B:LEU:HD12	12	2.41	0.87	2.14
(1,3989)	2:295:B:LEU:HD22	2:298:B:LEU:HD11	12	2.41	0.87	2.14
(1,3989)	2:295:B:LEU:HD23	2:298:B:LEU:HD12	12	2.41	0.87	2.14
(1,3989)	2:190:B:VAL:HG21	2:298:B:LEU:HD12	12	2.41	0.87	2.14
(1,3989)	2:190:B:VAL:HG22	2:298:B:LEU:HD13	12	2.41	0.87	2.14
(1,3989)	2:295:B:LEU:HD23	2:298:B:LEU:HD11	12	2.41	0.87	2.14
(1,3989)	2:190:B:VAL:HG22	2:298:B:LEU:HD12	12	2.41	0.87	2.14
(1,3935)	2:265:B:ARG:HB2	2:269:B:ARG:HD3	12	1.68	0.44	1.81
(1,3935)	2:268:B:VAL:HG23	2:269:B:ARG:HD3	12	1.68	0.44	1.81
(1,3935)	2:268:B:VAL:HG21	2:269:B:ARG:HD3	12	1.68	0.44	1.81
(1,3935)	2:268:B:VAL:HG22	2:269:B:ARG:HD3	12	1.68	0.44	1.81
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD23	12	1.66	1.44	1.5
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD21	12	1.66	1.44	1.5
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD22	12	1.66	1.44	1.5
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	12	1.47	0.87	1.27
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	12	1.47	0.87	1.27
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	12	1.47	0.87	1.27
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	12	1.47	0.87	1.27
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	12	1.47	0.87	1.27
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	12	1.47	0.87	1.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	12	1.47	0.87	1.27
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	12	1.47	0.87	1.27
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	12	1.47	0.87	1.27
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD11	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD12	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD13	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD11	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD12	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD13	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD11	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD12	12	0.92	0.26	0.96
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD13	12	0.92	0.26	0.96
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	12	0.78	0.16	0.82
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	12	0.78	0.16	0.82
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	12	0.78	0.16	0.82
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE1	12	0.74	0.36	0.79
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE3	12	0.74	0.36	0.79
(1,3859)	2:266:B:LEU:HD12	2:228:B:MET:HE2	12	0.74	0.36	0.79
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE2	12	0.74	0.36	0.79
(1,3859)	2:266:B:LEU:HD11	2:228:B:MET:HE2	12	0.74	0.36	0.79
(1,3859)	2:266:B:LEU:HD13	2:228:B:MET:HE3	12	0.74	0.36	0.79
(1,3859)	2:266:B:LEU:HD12	2:228:B:MET:HE1	12	0.74	0.36	0.79
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD22	12	0.66	0.38	0.64
(1,4279)	1:84:A:MET:HG3	1:81:A:LEU:HD22	12	0.66	0.38	0.64
(1,4279)	1:88:A:GLN:HG3	1:90:A:LEU:HD22	12	0.66	0.38	0.64
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD21	12	0.66	0.38	0.64
(1,4279)	1:88:A:GLN:HG2	1:90:A:LEU:HD22	12	0.66	0.38	0.64
(1,4030)	2:192:B:SER:HB2	2:188:B:LYS:HG2	12	0.6	0.31	0.67
(1,4030)	2:192:B:SER:HB3	2:188:B:LYS:HG2	12	0.6	0.31	0.67
(1,4030)	2:187:B:LYS:HA	2:188:B:LYS:HG2	12	0.6	0.31	0.67
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG23	12	0.55	0.24	0.56
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG21	12	0.55	0.24	0.56
(1,3934)	2:173:B:ASP:HA	2:169:B:VAL:HG13	12	0.55	0.24	0.56

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG22	12	0.55	0.24	0.56
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	12	0.42	0.2	0.4
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	12	0.42	0.2	0.4
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE3	12	0.42	0.2	0.4
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE3	12	0.42	0.2	0.4
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	12	0.41	0.09	0.4
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	12	0.41	0.09	0.4
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	12	0.41	0.09	0.4
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	12	0.37	0.16	0.36
(1,4310)	1:85:A:TYR:HD2	1:90:A:LEU:HB3	12	0.37	0.16	0.36
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	12	0.37	0.27	0.22
(1,4418)	2:169:B:VAL:HG21	1:112:A:ILE:HG21	12	0.37	0.15	0.36
(1,4418)	2:169:B:VAL:HG22	1:112:A:ILE:HG22	12	0.37	0.15	0.36
(1,4418)	2:169:B:VAL:HG22	1:112:A:ILE:HG23	12	0.37	0.15	0.36
(1,4418)	2:169:B:VAL:HG21	1:112:A:ILE:HG22	12	0.37	0.15	0.36
(1,4418)	2:169:B:VAL:HG23	1:112:A:ILE:HG22	12	0.37	0.15	0.36
(1,4418)	2:169:B:VAL:HG23	1:112:A:ILE:HG21	12	0.37	0.15	0.36
(1,4418)	2:169:B:VAL:HG22	1:112:A:ILE:HG21	12	0.37	0.15	0.36
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	12	0.27	0.02	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	12	0.27	0.02	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	12	0.27	0.02	0.27
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	12	0.23	0.07	0.23
(1,4451)	1:71:A:GLN:HA	1:72:A:VAL:H	12	0.23	0.07	0.23
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	12	0.23	0.07	0.25
(1,2374)	2:312:B:GLU:HG2	2:312:B:GLU:H	12	0.23	0.07	0.25
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	12	0.18	0.01	0.18
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	12	0.18	0.01	0.18
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	12	0.18	0.01	0.18
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	12	0.12	0.03	0.11
(1,4340)	1:92:A:GLU:HG2	1:92:A:GLU:HB2	12	0.12	0.01	0.12
(1,4340)	1:94:A:GLU:HG2	1:94:A:GLU:HB2	12	0.12	0.01	0.12
(1,4340)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	12	0.12	0.01	0.12
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	12	0.12	0.02	0.11
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	12	0.12	0.02	0.11
(1,4328)	2:279:B:LEU:HD21	1:94:A:GLU:HB2	11	1.08	0.82	1.05
(1,4328)	2:279:B:LEU:HD22	1:94:A:GLU:HB2	11	1.08	0.82	1.05
(1,4328)	2:279:B:LEU:HD23	1:94:A:GLU:HB2	11	1.08	0.82	1.05
(1,4328)	1:95:A:ILE:HD12	1:92:A:GLU:HB2	11	1.08	0.82	1.05
(1,4328)	1:95:A:ILE:HD13	1:92:A:GLU:HB2	11	1.08	0.82	1.05
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD22	11	1.07	0.07	1.05
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD21	11	1.07	0.07	1.05
(1,3896)	2:246:B:LEU:HA	2:246:B:LEU:HD22	11	1.07	0.07	1.05

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3896)	2:246:B:LEU:HA	2:246:B:LEU:HD23	11	1.07	0.07	1.05
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD23	11	1.07	0.07	1.05
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	11	0.83	0.5	1.03
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	11	0.83	0.5	1.03
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	11	0.83	0.5	1.03
(1,4363)	2:235:B:TYR:HD1	1:106:A:VAL:HG23	11	0.79	0.57	0.58
(1,4363)	2:235:B:TYR:HD1	1:106:A:VAL:HG22	11	0.79	0.57	0.58
(1,4363)	2:172:B:TRP:HD1	1:106:A:VAL:HG22	11	0.79	0.57	0.58
(1,4363)	2:172:B:TRP:HD1	1:106:A:VAL:HG21	11	0.79	0.57	0.58
(1,4363)	2:235:B:TYR:HD2	1:106:A:VAL:HG23	11	0.79	0.57	0.58
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	11	0.75	0.67	0.49
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	11	0.75	0.67	0.49
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	11	0.75	0.67	0.49
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB3	11	0.56	0.15	0.59
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB3	11	0.56	0.15	0.59
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB3	11	0.56	0.15	0.59
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB2	11	0.56	0.15	0.59
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB2	11	0.56	0.15	0.59
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB2	11	0.56	0.15	0.59
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG21	11	0.55	0.3	0.54
(1,3845)	2:202:B:LYS:HE2	2:218:B:VAL:HG22	11	0.55	0.3	0.54
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG23	11	0.55	0.3	0.54
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG22	11	0.55	0.3	0.54
(1,3845)	2:202:B:LYS:HE2	2:218:B:VAL:HG21	11	0.55	0.3	0.54
(1,3845)	2:202:B:LYS:HE2	2:218:B:VAL:HG23	11	0.55	0.3	0.54
(1,4575)	2:167:B:TRP:HD1	2:164:B:LEU:HD22	11	0.55	0.38	0.43
(1,4575)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	11	0.55	0.38	0.43
(1,4575)	2:167:B:TRP:HD1	2:164:B:LEU:HD21	11	0.55	0.38	0.43
(1,4575)	2:242:B:TYR:HE2	2:246:B:LEU:HD11	11	0.55	0.38	0.43
(1,4575)	2:242:B:TYR:HE1	2:234:B:LEU:HD13	11	0.55	0.38	0.43
(1,4575)	2:242:B:TYR:HE1	2:246:B:LEU:HD12	11	0.55	0.38	0.43
(1,4575)	2:242:B:TYR:HE2	2:246:B:LEU:HD13	11	0.55	0.38	0.43
(1,4575)	2:167:B:TRP:HD1	2:164:B:LEU:HD23	11	0.55	0.38	0.43
(1,4575)	2:242:B:TYR:HE1	2:234:B:LEU:HD12	11	0.55	0.38	0.43
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	11	0.53	0.14	0.54
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	11	0.53	0.14	0.54
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	11	0.53	0.14	0.54
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG2	11	0.49	0.36	0.35
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG2	11	0.49	0.36	0.35
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG2	11	0.49	0.36	0.35
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG3	11	0.49	0.36	0.35
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG3	11	0.49	0.36	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG3	11	0.49	0.36	0.35
(1,4364)	1:111:A:ILE:HD12	1:107:A:LEU:HA	11	0.39	0.15	0.37
(1,4364)	1:111:A:ILE:HD11	1:107:A:LEU:HA	11	0.39	0.15	0.37
(1,4364)	1:111:A:ILE:HD13	1:107:A:LEU:HA	11	0.39	0.15	0.37
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD11	11	0.37	0.27	0.29
(1,4623)	2:306:B:PHE:HE2	2:298:B:LEU:HD12	11	0.37	0.27	0.29
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD13	11	0.37	0.27	0.29
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD12	11	0.37	0.27	0.29
(1,4623)	2:306:B:PHE:HE2	2:305:B:LEU:HD12	11	0.37	0.27	0.29
(1,4623)	2:306:B:PHE:HE2	2:298:B:LEU:HD13	11	0.37	0.27	0.29
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG21	11	0.31	0.13	0.32
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG23	11	0.31	0.13	0.32
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG22	11	0.31	0.13	0.32
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	11	0.16	0.03	0.15
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	11	0.16	0.03	0.15
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	11	0.16	0.03	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	11	0.16	0.03	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	11	0.16	0.03	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	11	0.16	0.03	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	11	0.16	0.03	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	11	0.16	0.03	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	11	0.16	0.03	0.15
(1,4326)	1:94:A:GLU:HG2	1:94:A:GLU:HB3	11	0.12	0.02	0.12
(1,4326)	1:94:A:GLU:HG3	1:94:A:GLU:HB3	11	0.12	0.02	0.12
(1,4326)	1:92:A:GLU:HG3	1:92:A:GLU:HB3	11	0.12	0.02	0.12
(1,3980)	2:298:B:LEU:HD12	2:295:B:LEU:HD21	10	2.09	1.39	1.84
(1,3980)	2:298:B:LEU:HD11	2:295:B:LEU:HD22	10	2.09	1.39	1.84
(1,3980)	2:164:B:LEU:HD22	2:295:B:LEU:HD21	10	2.09	1.39	1.84
(1,3980)	2:164:B:LEU:HD21	2:295:B:LEU:HD22	10	2.09	1.39	1.84
(1,3980)	2:164:B:LEU:HD23	2:295:B:LEU:HD22	10	2.09	1.39	1.84
(1,3980)	2:164:B:LEU:HD22	2:295:B:LEU:HD22	10	2.09	1.39	1.84
(1,3980)	2:164:B:LEU:HD23	2:295:B:LEU:HD23	10	2.09	1.39	1.84
(1,4343)	1:74:A:SER:HB3	1:95:A:ILE:HD12	10	1.06	0.59	1.14
(1,4343)	1:93:A:SER:HB3	1:95:A:ILE:HD12	10	1.06	0.59	1.14
(1,4343)	1:93:A:SER:HB2	1:95:A:ILE:HD12	10	1.06	0.59	1.14
(1,4343)	1:74:A:SER:HB2	1:95:A:ILE:HD12	10	1.06	0.59	1.14
(1,4343)	1:93:A:SER:HB2	1:95:A:ILE:HD11	10	1.06	0.59	1.14
(1,4343)	1:74:A:SER:HB3	1:95:A:ILE:HD11	10	1.06	0.59	1.14
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD13	10	0.99	0.35	1.04
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD12	10	0.99	0.35	1.04
(1,3962)	2:156:B:VAL:HA	2:284:B:LEU:HD13	10	0.99	0.35	1.04
(1,3962)	2:156:B:VAL:HA	2:284:B:LEU:HD11	10	0.99	0.35	1.04

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD11	10	0.99	0.35	1.04
(1,3837)	2:198:B:ALA:HB1	2:214:B:VAL:HG23	10	0.89	0.44	0.97
(1,3837)	2:198:B:ALA:HB3	2:214:B:VAL:HG21	10	0.89	0.44	0.97
(1,3837)	2:210:B:LYS:HG3	2:214:B:VAL:HG21	10	0.89	0.44	0.97
(1,3837)	2:198:B:ALA:HB2	2:214:B:VAL:HG22	10	0.89	0.44	0.97
(1,3837)	2:198:B:ALA:HB1	2:214:B:VAL:HG21	10	0.89	0.44	0.97
(1,3837)	2:198:B:ALA:HB3	2:214:B:VAL:HG23	10	0.89	0.44	0.97
(1,3837)	2:198:B:ALA:HB2	2:214:B:VAL:HG21	10	0.89	0.44	0.97
(1,3837)	2:210:B:LYS:HG3	2:214:B:VAL:HG22	10	0.89	0.44	0.97
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD12	10	0.82	0.34	0.73
(1,4001)	2:273:B:MET:HB3	2:274:B:LEU:HD13	10	0.82	0.34	0.73
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD13	10	0.82	0.34	0.73
(1,4001)	2:273:B:MET:HB3	2:274:B:LEU:HD12	10	0.82	0.34	0.73
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD11	10	0.82	0.34	0.73
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	10	0.76	0.63	0.5
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	10	0.76	0.63	0.5
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	10	0.76	0.63	0.5
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	10	0.76	0.63	0.5
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	10	0.76	0.63	0.5
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	10	0.76	0.63	0.5
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	10	0.76	0.63	0.5
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	10	0.76	0.63	0.5
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	10	0.76	0.63	0.5
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD13	10	0.74	0.31	0.77
(1,4031)	2:298:B:LEU:HB2	2:193:B:ILE:HD13	10	0.74	0.31	0.77
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD12	10	0.74	0.31	0.77
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD11	10	0.74	0.31	0.77
(1,4031)	2:298:B:LEU:HB2	2:193:B:ILE:HD12	10	0.74	0.31	0.77
(1,4327)	1:95:A:ILE:HD12	1:92:A:GLU:HB3	10	0.73	0.35	0.68
(1,4327)	2:279:B:LEU:HD22	1:94:A:GLU:HB3	10	0.73	0.35	0.68
(1,4327)	1:95:A:ILE:HD11	1:92:A:GLU:HB3	10	0.73	0.35	0.68
(1,4327)	2:279:B:LEU:HD21	1:94:A:GLU:HB3	10	0.73	0.35	0.68
(1,4327)	1:95:A:ILE:HD13	1:92:A:GLU:HB3	10	0.73	0.35	0.68
(1,4444)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	10	0.71	0.45	0.58
(1,4444)	1:97:A:PRO:HG3	1:96:A:LEU:HD11	10	0.71	0.45	0.58
(1,4444)	2:273:B:MET:HB3	1:96:A:LEU:HD13	10	0.71	0.45	0.58
(1,4444)	1:97:A:PRO:HG3	1:96:A:LEU:HD13	10	0.71	0.45	0.58
(1,4444)	1:97:A:PRO:HG3	1:96:A:LEU:HD12	10	0.71	0.45	0.58
(1,4444)	2:273:B:MET:HB3	1:96:A:LEU:HD11	10	0.71	0.45	0.58
(1,815)	2:253:B:PRO:HB2	2:256:B:GLN:HG2	10	0.67	0.21	0.67
(1,815)	2:253:B:PRO:HG2	2:256:B:GLN:HG3	10	0.67	0.21	0.67
(1,815)	2:253:B:PRO:HG2	2:256:B:GLN:HG2	10	0.67	0.21	0.67

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,815)	2:253:B:PRO:HB2	2:256:B:GLN:HG3	10	0.67	0.21	0.67
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD21	10	0.65	0.46	0.51
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD23	10	0.65	0.46	0.51
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD22	10	0.65	0.46	0.51
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD23	10	0.56	0.6	0.34
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD22	10	0.56	0.6	0.34
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD21	10	0.56	0.6	0.34
(1,3920)	2:194:B:LEU:HD22	2:263:B:LEU:HD12	10	0.56	0.27	0.55
(1,3920)	2:194:B:LEU:HD21	2:263:B:LEU:HD13	10	0.56	0.27	0.55
(1,3920)	2:194:B:LEU:HD23	2:263:B:LEU:HD12	10	0.56	0.27	0.55
(1,3920)	2:194:B:LEU:HD23	2:263:B:LEU:HD13	10	0.56	0.27	0.55
(1,3920)	2:194:B:LEU:HD21	2:263:B:LEU:HD11	10	0.56	0.27	0.55
(1,3920)	2:194:B:LEU:HD22	2:263:B:LEU:HD13	10	0.56	0.27	0.55
(1,3776)	2:257:B:VAL:HG22	2:185:B:PRO:HB3	10	0.49	0.18	0.5
(1,3776)	2:257:B:VAL:HG23	2:185:B:PRO:HB3	10	0.49	0.18	0.5
(1,3776)	2:257:B:VAL:HG21	2:185:B:PRO:HB3	10	0.49	0.18	0.5
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG11	10	0.44	0.22	0.47
(1,4429)	1:73:A:PRO:HB2	1:76:A:VAL:HG12	10	0.44	0.22	0.47
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG12	10	0.44	0.22	0.47
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG13	10	0.44	0.22	0.47
(1,4429)	1:73:A:PRO:HB2	1:76:A:VAL:HG11	10	0.44	0.22	0.47
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD3	10	0.36	0.1	0.37
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD2	10	0.36	0.1	0.37
(1,3990)	2:263:B:LEU:HD13	2:298:B:LEU:HD22	10	0.35	0.24	0.24
(1,3990)	2:263:B:LEU:HD11	2:298:B:LEU:HD23	10	0.35	0.24	0.24
(1,3990)	2:263:B:LEU:HD12	2:194:B:LEU:HD22	10	0.35	0.24	0.24
(1,3990)	2:263:B:LEU:HD11	2:298:B:LEU:HD21	10	0.35	0.24	0.24
(1,3990)	2:263:B:LEU:HD12	2:194:B:LEU:HD23	10	0.35	0.24	0.24
(1,3990)	2:263:B:LEU:HD12	2:194:B:LEU:HD21	10	0.35	0.24	0.24
(1,3990)	2:263:B:LEU:HD12	2:298:B:LEU:HD21	10	0.35	0.24	0.24
(1,3990)	2:263:B:LEU:HD13	2:194:B:LEU:HD23	10	0.35	0.24	0.24
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	10	0.34	0.11	0.35
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	10	0.34	0.11	0.35
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG3	10	0.34	0.11	0.35
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG3	10	0.34	0.11	0.35
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	10	0.31	0.03	0.3
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG3	10	0.31	0.03	0.3
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	10	0.31	0.03	0.3
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG3	10	0.31	0.03	0.3
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	10	0.25	0.1	0.21
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB3	10	0.25	0.1	0.21
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	9	2.1	0.29	2.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	9	2.1	0.29	2.17
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	9	2.1	0.29	2.17
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	9	2.1	0.29	2.17
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	9	2.1	0.29	2.17
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	9	2.1	0.29	2.17
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	9	1.4	0.68	1.07
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	9	1.4	0.68	1.07
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	9	1.4	0.68	1.07
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	9	1.3	0.19	1.28
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	9	1.3	0.19	1.28
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	9	1.3	0.19	1.28
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	9	1.3	0.19	1.28
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	9	1.3	0.19	1.28
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	9	1.3	0.19	1.28
(1,4312)	1:73:A:PRO:HB3	1:96:A:LEU:HD12	9	1.24	0.56	1.32
(1,4312)	1:94:A:GLU:HG2	1:90:A:LEU:HD11	9	1.24	0.56	1.32
(1,4312)	1:94:A:GLU:HG2	1:90:A:LEU:HD12	9	1.24	0.56	1.32
(1,4312)	1:94:A:GLU:HG3	1:90:A:LEU:HD11	9	1.24	0.56	1.32
(1,4312)	1:94:A:GLU:HG3	1:90:A:LEU:HD12	9	1.24	0.56	1.32
(1,4312)	2:223:B:GLU:HG3	1:96:A:LEU:HD11	9	1.24	0.56	1.32
(1,4312)	1:73:A:PRO:HB3	1:96:A:LEU:HD11	9	1.24	0.56	1.32
(1,4312)	1:73:A:PRO:HB3	1:96:A:LEU:HD13	9	1.24	0.56	1.32
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	9	1.09	0.36	1.05
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	9	1.09	0.36	1.05
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	9	1.09	0.36	1.05
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	9	1.09	0.36	1.05
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	9	1.09	0.36	1.05
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	9	1.09	0.36	1.05
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	9	1.09	0.36	1.05
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	9	1.09	0.36	1.05
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	9	1.09	0.36	1.05
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	9	1.0	0.48	0.79
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	9	1.0	0.48	0.79
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	9	1.0	0.48	0.79
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	9	1.0	0.48	0.79
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	9	1.0	0.48	0.79
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	9	1.0	0.48	0.79
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	9	1.0	0.48	0.79
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	9	1.0	0.48	0.79
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	9	1.0	0.48	0.79
(1,3803)	2:194:B:LEU:HD22	2:193:B:ILE:HG23	9	0.97	0.23	1.06
(1,3803)	2:194:B:LEU:HD23	2:193:B:ILE:HG21	9	0.97	0.23	1.06

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3803)	2:194:B:LEU:HD21	2:193:B:ILE:HG23	9	0.97	0.23	1.06
(1,3803)	2:298:B:LEU:HD22	2:193:B:ILE:HG22	9	0.97	0.23	1.06
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	9	0.89	0.55	1.23
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	9	0.89	0.55	1.23
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	9	0.89	0.55	1.23
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	9	0.7	0.5	0.61
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	9	0.7	0.5	0.61
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	9	0.7	0.5	0.61
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	9	0.7	0.5	0.61
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	9	0.7	0.5	0.61
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	9	0.7	0.5	0.61
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	9	0.7	0.5	0.61
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	9	0.7	0.5	0.61
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	9	0.7	0.5	0.61
(1,4560)	2:225:B:PHE:HD1	2:233:B:LEU:HD12	9	0.65	0.36	0.66
(1,4560)	2:225:B:PHE:HD1	2:221:B:ILE:HG21	9	0.65	0.36	0.66
(1,4560)	2:225:B:PHE:HD1	2:221:B:ILE:HG22	9	0.65	0.36	0.66
(1,4560)	2:225:B:PHE:HD1	2:233:B:LEU:HD11	9	0.65	0.36	0.66
(1,3901)	2:257:B:VAL:HG21	2:252:B:ALA:HB2	9	0.64	0.46	0.46
(1,3901)	2:246:B:LEU:HD12	2:252:B:ALA:HB1	9	0.64	0.46	0.46
(1,3901)	2:246:B:LEU:HD12	2:252:B:ALA:HB2	9	0.64	0.46	0.46
(1,3901)	2:257:B:VAL:HG23	2:252:B:ALA:HB2	9	0.64	0.46	0.46
(1,3901)	2:246:B:LEU:HD12	2:252:B:ALA:HB3	9	0.64	0.46	0.46
(1,3901)	2:257:B:VAL:HG22	2:252:B:ALA:HB2	9	0.64	0.46	0.46
(1,3901)	2:257:B:VAL:HG23	2:252:B:ALA:HB1	9	0.64	0.46	0.46
(1,3901)	2:257:B:VAL:HG22	2:252:B:ALA:HB1	9	0.64	0.46	0.46
(1,3901)	2:257:B:VAL:HG21	2:252:B:ALA:HB1	9	0.64	0.46	0.46
(1,4357)	2:273:B:MET:HE3	1:100:A:ASN:HA	9	0.5	0.28	0.36
(1,4357)	2:273:B:MET:HE2	1:100:A:ASN:HA	9	0.5	0.28	0.36
(1,4357)	2:273:B:MET:HE1	1:100:A:ASN:HA	9	0.5	0.28	0.36
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	9	0.42	0.13	0.43
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	9	0.42	0.13	0.43
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	9	0.42	0.13	0.43
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	9	0.4	0.31	0.29
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	9	0.4	0.31	0.29
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	9	0.4	0.31	0.29
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	9	0.36	0.02	0.36
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	9	0.36	0.02	0.36
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	9	0.36	0.02	0.36
(1,4198)	2:164:B:LEU:HD23	2:299:B:ALA:H	9	0.35	0.16	0.31
(1,4198)	2:164:B:LEU:HD21	2:299:B:ALA:H	9	0.35	0.16	0.31
(1,4198)	2:164:B:LEU:HD22	2:299:B:ALA:H	9	0.35	0.16	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	9	0.17	0.02	0.17
(1,3953)	2:317:B:GLU:HB3	2:317:B:GLU:HG2	9	0.15	0.03	0.15
(1,3953)	2:281:B:GLU:HB3	2:281:B:GLU:HG2	9	0.15	0.03	0.15
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	8	2.12	0.26	2.12
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	8	2.12	0.26	2.12
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	8	2.12	0.26	2.12
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	8	1.07	0.41	0.94
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	8	1.07	0.41	0.94
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	8	1.07	0.41	0.94
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	8	1.07	0.41	0.94
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	8	1.07	0.41	0.94
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	8	1.07	0.41	0.94
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	8	1.07	0.41	0.94
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	8	1.07	0.41	0.94
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	8	1.07	0.41	0.94
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	8	0.98	0.19	0.88
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	8	0.98	0.19	0.88
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	8	0.98	0.19	0.88
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	8	0.76	0.09	0.72
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	8	0.76	0.09	0.72
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	8	0.76	0.09	0.72
(1,4385)	1:112:A:ILE:HG22	1:109:A:GLU:HB3	8	0.74	0.46	0.82
(1,4385)	1:112:A:ILE:HG21	1:109:A:GLU:HB3	8	0.74	0.46	0.82
(1,4385)	1:112:A:ILE:HG23	1:109:A:GLU:HB3	8	0.74	0.46	0.82
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	8	0.7	0.45	0.73
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	8	0.7	0.45	0.73
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	8	0.7	0.45	0.73
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	8	0.7	0.45	0.73
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	8	0.7	0.45	0.73
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	8	0.7	0.45	0.73
(1,3843)	1:96:A:LEU:HD21	2:227:B:VAL:HG11	8	0.68	0.28	0.62
(1,3843)	2:194:B:LEU:HD13	2:218:B:VAL:HG22	8	0.68	0.28	0.62
(1,3843)	2:194:B:LEU:HD12	2:218:B:VAL:HG21	8	0.68	0.28	0.62
(1,3843)	1:96:A:LEU:HD21	2:227:B:VAL:HG12	8	0.68	0.28	0.62
(1,3843)	1:96:A:LEU:HD22	2:227:B:VAL:HG13	8	0.68	0.28	0.62
(1,3843)	2:194:B:LEU:HD12	2:218:B:VAL:HG23	8	0.68	0.28	0.62
(1,4140)	2:185:B:PRO:HB3	2:252:B:ALA:H	8	0.63	0.35	0.57
(1,4140)	2:254:B:MET:HE1	2:252:B:ALA:H	8	0.63	0.35	0.57
(1,4140)	2:254:B:MET:HE3	2:252:B:ALA:H	8	0.63	0.35	0.57
(1,4140)	2:254:B:MET:HE2	2:252:B:ALA:H	8	0.63	0.35	0.57
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE3	8	0.55	0.21	0.54
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE3	8	0.55	0.21	0.54

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE2	8	0.55	0.21	0.54
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE2	8	0.55	0.21	0.54
(1,4167)	2:279:B:LEU:HD11	2:280:B:ASP:H	8	0.5	0.25	0.52
(1,4167)	1:90:A:LEU:HD11	2:280:B:ASP:H	8	0.5	0.25	0.52
(1,4167)	2:279:B:LEU:HD13	2:280:B:ASP:H	8	0.5	0.25	0.52
(1,4167)	1:90:A:LEU:HD13	2:280:B:ASP:H	8	0.5	0.25	0.52
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	8	0.49	0.15	0.55
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	8	0.49	0.15	0.55
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	8	0.49	0.15	0.55
(1,3750)	2:160:B:ILE:HG23	2:165:B:LYS:HE2	8	0.45	0.18	0.44
(1,3750)	1:111:A:ILE:HD11	2:165:B:LYS:HE2	8	0.45	0.18	0.44
(1,3750)	2:160:B:ILE:HG21	2:165:B:LYS:HE2	8	0.45	0.18	0.44
(1,3750)	1:111:A:ILE:HD13	2:165:B:LYS:HE2	8	0.45	0.18	0.44
(1,3749)	2:160:B:ILE:HG21	2:165:B:LYS:HE3	8	0.44	0.27	0.34
(1,3749)	2:160:B:ILE:HG23	2:165:B:LYS:HE3	8	0.44	0.27	0.34
(1,3749)	2:160:B:ILE:HG22	2:165:B:LYS:HE3	8	0.44	0.27	0.34
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	8	0.42	0.1	0.42
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	8	0.42	0.1	0.42
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	8	0.42	0.1	0.42
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB1	8	0.37	0.15	0.33
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB2	8	0.37	0.15	0.33
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB3	8	0.37	0.15	0.33
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB1	8	0.37	0.15	0.33
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB2	8	0.37	0.15	0.33
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB3	8	0.37	0.15	0.33
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	8	0.36	0.15	0.41
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	8	0.36	0.15	0.41
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	8	0.36	0.15	0.41
(1,4564)	2:290:B:TYR:HE1	2:210:B:LYS:HG3	8	0.33	0.21	0.24
(1,4564)	2:197:B:TYR:HE2	2:198:B:ALA:HB3	8	0.33	0.21	0.24
(1,4564)	2:197:B:TYR:HE2	2:198:B:ALA:HB2	8	0.33	0.21	0.24
(1,4564)	2:197:B:TYR:HE2	2:198:B:ALA:HB1	8	0.33	0.21	0.24
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	8	0.31	0.16	0.3
(1,1904)	2:241:B:GLN:HG2	2:241:B:GLN:H	8	0.2	0.04	0.21
(1,1904)	2:241:B:GLN:HG3	2:241:B:GLN:H	8	0.2	0.04	0.21
(1,2138)	2:279:B:LEU:HB3	2:279:B:LEU:H	8	0.18	0.04	0.2
(1,2138)	2:279:B:LEU:HG	2:279:B:LEU:H	8	0.18	0.04	0.2
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	8	0.18	0.1	0.14
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	8	0.18	0.1	0.14
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	8	0.18	0.1	0.14
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	8	0.18	0.1	0.14
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	8	0.18	0.1	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	8	0.18	0.1	0.14
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	8	0.14	0.02	0.13
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	7	1.95	1.23	2.11
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD11	7	1.95	1.23	2.11
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	7	1.95	1.23	2.11
(1,4640)	2:267:B:PHE:HD1	2:168:B:LEU:HD23	7	1.65	0.52	1.47
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD23	7	1.65	0.52	1.47
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD22	7	1.65	0.52	1.47
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD21	7	1.65	0.52	1.47
(1,3988)	2:263:B:LEU:HD12	2:298:B:LEU:HD12	7	1.07	0.91	0.6
(1,3988)	2:263:B:LEU:HD13	2:298:B:LEU:HD11	7	1.07	0.91	0.6
(1,3988)	2:295:B:LEU:HG	2:298:B:LEU:HD12	7	1.07	0.91	0.6
(1,3988)	2:263:B:LEU:HD12	2:298:B:LEU:HD11	7	1.07	0.91	0.6
(1,3988)	2:263:B:LEU:HD13	2:298:B:LEU:HD13	7	1.07	0.91	0.6
(1,4604)	2:225:B:PHE:HE1	2:266:B:LEU:HD11	7	0.86	0.44	0.71
(1,4604)	2:225:B:PHE:HE1	2:266:B:LEU:HD12	7	0.86	0.44	0.71
(1,4604)	2:167:B:TRP:HD1	2:164:B:LEU:HD11	7	0.86	0.44	0.71
(1,4604)	2:225:B:PHE:HE2	2:229:B:LEU:HG	7	0.86	0.44	0.71
(1,4604)	2:225:B:PHE:HE1	2:266:B:LEU:HD13	7	0.86	0.44	0.71
(1,2812)	1:106:A:VAL:HG11	1:104:A:ASN:HB2	7	0.82	0.54	0.9
(1,2812)	1:106:A:VAL:HG12	1:104:A:ASN:HB2	7	0.82	0.54	0.9
(1,2812)	1:106:A:VAL:HG13	1:104:A:ASN:HB2	7	0.82	0.54	0.9
(1,3857)	1:98:A:PHE:HE2	2:227:B:VAL:HG11	7	0.8	0.37	0.84
(1,3857)	2:224:B:TYR:HD1	2:227:B:VAL:HG13	7	0.8	0.37	0.84
(1,3857)	2:224:B:TYR:HD1	2:227:B:VAL:HG12	7	0.8	0.37	0.84
(1,3857)	1:98:A:PHE:HE2	2:227:B:VAL:HG12	7	0.8	0.37	0.84
(1,3812)	2:218:B:VAL:HG23	2:194:B:LEU:HD23	7	0.74	0.24	0.76
(1,3812)	2:193:B:ILE:HG23	2:194:B:LEU:HD22	7	0.74	0.24	0.76
(1,3812)	2:218:B:VAL:HG21	2:194:B:LEU:HD21	7	0.74	0.24	0.76
(1,3812)	2:218:B:VAL:HG23	2:194:B:LEU:HD22	7	0.74	0.24	0.76
(1,3812)	2:218:B:VAL:HG22	2:194:B:LEU:HD22	7	0.74	0.24	0.76
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD11	7	0.7	0.27	0.62
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD12	7	0.7	0.27	0.62
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD13	7	0.7	0.27	0.62
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD11	7	0.7	0.27	0.62
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD12	7	0.7	0.27	0.62
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD13	7	0.7	0.27	0.62
(1,4153)	2:298:B:LEU:HD11	2:264:B:LEU:H	7	0.6	0.36	0.75
(1,4153)	2:298:B:LEU:HD13	2:264:B:LEU:H	7	0.6	0.36	0.75
(1,4153)	2:298:B:LEU:HD12	2:264:B:LEU:H	7	0.6	0.36	0.75
(1,4612)	2:290:B:TYR:HE2	2:286:B:LEU:HG	7	0.59	0.17	0.57
(1,4612)	2:262:B:HIS:HD2	2:265:B:ARG:HG3	7	0.59	0.17	0.57

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4612)	2:290:B:TYR:HE1	2:210:B:LYS:HD2	7	0.59	0.17	0.57
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD21	7	0.54	0.29	0.44
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD22	7	0.54	0.29	0.44
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD23	7	0.54	0.29	0.44
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD21	7	0.54	0.29	0.44
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD22	7	0.54	0.29	0.44
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD23	7	0.54	0.29	0.44
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD21	7	0.54	0.29	0.44
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD22	7	0.54	0.29	0.44
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD23	7	0.54	0.29	0.44
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD11	7	0.54	0.02	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD12	7	0.54	0.02	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD13	7	0.54	0.02	0.53
(1,4014)	2:181:B:LEU:HD12	2:314:B:ALA:HB3	7	0.5	0.2	0.35
(1,4014)	2:181:B:LEU:HD13	2:314:B:ALA:HB3	7	0.5	0.2	0.35
(1,4014)	2:179:B:LYS:HD2	2:314:B:ALA:HB1	7	0.5	0.2	0.35
(1,4014)	2:181:B:LEU:HD13	2:314:B:ALA:HB2	7	0.5	0.2	0.35
(1,4014)	2:181:B:LEU:HD12	2:314:B:ALA:HB2	7	0.5	0.2	0.35
(1,4014)	2:179:B:LYS:HD2	2:314:B:ALA:HB3	7	0.5	0.2	0.35
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG23	7	0.5	0.08	0.44
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG22	7	0.5	0.08	0.44
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB1	7	0.49	0.35	0.39
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB2	7	0.49	0.35	0.39
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB3	7	0.49	0.35	0.39
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB1	7	0.49	0.35	0.39
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB2	7	0.49	0.35	0.39
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB3	7	0.49	0.35	0.39
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB1	7	0.49	0.35	0.39
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB2	7	0.49	0.35	0.39
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB3	7	0.49	0.35	0.39
(1,3893)	2:246:B:LEU:HB2	2:245:B:ILE:HG22	7	0.48	0.22	0.43
(1,3893)	2:252:B:ALA:HB3	2:245:B:ILE:HG23	7	0.48	0.22	0.43
(1,3893)	2:252:B:ALA:HB2	2:245:B:ILE:HG23	7	0.48	0.22	0.43
(1,3893)	2:252:B:ALA:HB2	2:245:B:ILE:HG21	7	0.48	0.22	0.43
(1,3893)	2:252:B:ALA:HB1	2:245:B:ILE:HG22	7	0.48	0.22	0.43
(1,3893)	2:246:B:LEU:HB2	2:245:B:ILE:HG21	7	0.48	0.22	0.43
(1,4447)	2:232:B:GLN:HG3	1:103:A:ARG:HG2	7	0.44	0.28	0.42
(1,4447)	2:232:B:GLN:HG2	1:103:A:ARG:HG2	7	0.44	0.28	0.42
(1,4496)	2:267:B:PHE:HD2	2:263:B:LEU:HD21	7	0.4	0.25	0.28
(1,4496)	2:267:B:PHE:HD2	2:263:B:LEU:HD23	7	0.4	0.25	0.28
(1,4496)	2:267:B:PHE:HD1	2:158:B:VAL:HG13	7	0.4	0.25	0.28
(1,432)	2:204:B:ARG:HA	2:204:B:ARG:HD3	7	0.38	0.18	0.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4435)	1:119:A:LYS:HE3	1:119:A:LYS:HA	7	0.34	0.12	0.36
(1,4435)	1:75:A:LYS:HE3	1:92:A:GLU:HA	7	0.34	0.12	0.36
(1,4435)	1:119:A:LYS:HE2	1:119:A:LYS:HA	7	0.34	0.12	0.36
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE1	7	0.3	0.1	0.32
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE2	7	0.3	0.1	0.32
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE3	7	0.3	0.1	0.32
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE1	7	0.3	0.1	0.32
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE2	7	0.3	0.1	0.32
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE3	7	0.3	0.1	0.32
(1,4527)	2:242:B:TYR:HE2	2:243:B:ALA:HB3	7	0.29	0.2	0.21
(1,4527)	2:242:B:TYR:HE2	2:243:B:ALA:HB1	7	0.29	0.2	0.21
(1,4527)	2:306:B:PHE:HD1	2:305:B:LEU:HG	7	0.29	0.2	0.21
(1,3395)	1:117:A:GLU:HG2	1:117:A:GLU:H	7	0.22	0.07	0.19
(1,3395)	1:117:A:GLU:HG3	1:117:A:GLU:H	7	0.22	0.07	0.19
(1,2581)	1:86:A:ASP:HB3	1:83:A:THR:HA	7	0.12	0.02	0.11
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD11	6	1.4	0.37	1.28
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD12	6	1.4	0.37	1.28
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD13	6	1.4	0.37	1.28
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD21	6	1.28	0.21	1.28
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD22	6	1.28	0.21	1.28
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD23	6	1.28	0.21	1.28
(1,3918)	2:298:B:LEU:HD12	2:263:B:LEU:HD12	6	1.28	0.72	1.46
(1,3918)	2:298:B:LEU:HD13	2:263:B:LEU:HD12	6	1.28	0.72	1.46
(1,3918)	2:193:B:ILE:HD13	2:263:B:LEU:HD13	6	1.28	0.72	1.46
(1,3918)	2:298:B:LEU:HD13	2:263:B:LEU:HD13	6	1.28	0.72	1.46
(1,3918)	2:298:B:LEU:HD12	2:263:B:LEU:HD11	6	1.28	0.72	1.46
(1,4346)	1:94:A:GLU:HB3	1:95:A:ILE:HG21	6	1.19	0.17	1.22
(1,4346)	1:92:A:GLU:HB3	1:95:A:ILE:HG23	6	1.19	0.17	1.22
(1,4346)	1:72:A:VAL:HB	1:95:A:ILE:HG22	6	1.19	0.17	1.22
(1,4346)	1:72:A:VAL:HB	1:95:A:ILE:HG21	6	1.19	0.17	1.22
(1,4346)	1:72:A:VAL:HB	1:95:A:ILE:HG23	6	1.19	0.17	1.22
(1,4028)	1:96:A:LEU:HD13	2:277:B:THR:HB	6	0.88	0.75	0.56
(1,4028)	1:96:A:LEU:HD12	2:277:B:THR:HB	6	0.88	0.75	0.56
(1,4028)	1:96:A:LEU:HD11	2:277:B:THR:HB	6	0.88	0.75	0.56
(1,4028)	2:279:B:LEU:HD22	2:277:B:THR:HB	6	0.88	0.75	0.56
(1,4028)	2:279:B:LEU:HD23	2:277:B:THR:HB	6	0.88	0.75	0.56
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD11	6	0.8	0.11	0.78
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD12	6	0.8	0.11	0.78
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD13	6	0.8	0.11	0.78
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD21	6	0.75	0.28	0.78
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD22	6	0.75	0.28	0.78
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD23	6	0.75	0.28	0.78

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3979)	2:160:B:ILE:HG22	2:295:B:LEU:HD21	6	0.68	0.41	0.63
(1,3979)	2:160:B:ILE:HG22	2:295:B:LEU:HD22	6	0.68	0.41	0.63
(1,3979)	2:160:B:ILE:HG23	2:295:B:LEU:HD23	6	0.68	0.41	0.63
(1,3979)	2:164:B:LEU:HD11	2:295:B:LEU:HD23	6	0.68	0.41	0.63
(1,3979)	2:160:B:ILE:HG23	2:295:B:LEU:HD21	6	0.68	0.41	0.63
(1,3768)	2:235:B:TYR:HE1	2:176:B:THR:HG21	6	0.64	0.3	0.56
(1,3768)	2:235:B:TYR:HE2	2:176:B:THR:HG23	6	0.64	0.3	0.56
(1,3768)	2:235:B:TYR:HE1	2:176:B:THR:HG23	6	0.64	0.3	0.56
(1,3768)	2:235:B:TYR:HE2	2:176:B:THR:HG22	6	0.64	0.3	0.56
(1,4513)	2:235:B:TYR:HE2	2:175:B:ILE:HD11	6	0.61	0.27	0.53
(1,4513)	2:235:B:TYR:HE2	2:175:B:ILE:HD13	6	0.61	0.27	0.53
(1,4513)	2:235:B:TYR:HE1	2:175:B:ILE:HD13	6	0.61	0.27	0.53
(1,1112)	2:300:B:LYS:HB2	2:300:B:LYS:HG3	6	0.61	0.0	0.61
(1,1054)	2:295:B:LEU:HD11	2:292:B:HIS:HA	6	0.59	0.07	0.58
(1,1054)	2:295:B:LEU:HD12	2:292:B:HIS:HA	6	0.59	0.07	0.58
(1,1054)	2:295:B:LEU:HD13	2:292:B:HIS:HA	6	0.59	0.07	0.58
(1,4271)	2:212:B:TYR:HD1	1:81:A:LEU:HA	6	0.56	0.31	0.5
(1,4271)	2:212:B:TYR:HD2	1:81:A:LEU:HA	6	0.56	0.31	0.5
(1,1558)	2:189:B:ASN:HD21	2:191:B:ASP:H	6	0.54	0.07	0.54
(1,4547)	2:200:B:TYR:HD1	2:204:B:ARG:HD3	6	0.54	0.25	0.49
(1,4547)	2:200:B:TYR:HD1	2:204:B:ARG:HD2	6	0.54	0.25	0.49
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD11	6	0.48	0.2	0.5
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD12	6	0.48	0.2	0.5
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD13	6	0.48	0.2	0.5
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD11	6	0.48	0.2	0.5
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	6	0.48	0.2	0.5
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD13	6	0.48	0.2	0.5
(1,3766)	2:235:B:TYR:HD2	2:175:B:ILE:HD13	6	0.47	0.19	0.49
(1,3766)	2:235:B:TYR:HD2	2:175:B:ILE:HD11	6	0.47	0.19	0.49
(1,3766)	2:235:B:TYR:HD1	2:175:B:ILE:HD12	6	0.47	0.19	0.49
(1,3766)	2:235:B:TYR:HD1	2:175:B:ILE:HD13	6	0.47	0.19	0.49
(1,4639)	2:212:B:TYR:HD1	2:213:B:ALA:HB1	6	0.45	0.17	0.47
(1,4639)	2:237:B:PHE:HE1	2:322:B:ALA:HB1	6	0.45	0.17	0.47
(1,4639)	2:212:B:TYR:HD1	2:213:B:ALA:HB2	6	0.45	0.17	0.47
(1,4639)	2:237:B:PHE:HE1	2:322:B:ALA:HB3	6	0.45	0.17	0.47
(1,4639)	2:237:B:PHE:HE1	2:322:B:ALA:HB2	6	0.45	0.17	0.47
(1,3915)	2:305:B:LEU:HD21	2:260:B:ALA:HB3	6	0.45	0.31	0.27
(1,3915)	2:305:B:LEU:HD21	2:260:B:ALA:HB1	6	0.45	0.31	0.27
(1,3915)	2:305:B:LEU:HD21	2:260:B:ALA:HB2	6	0.45	0.31	0.27
(1,3915)	2:305:B:LEU:HD22	2:260:B:ALA:HB1	6	0.45	0.31	0.27
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD21	6	0.44	0.22	0.4
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD22	6	0.44	0.22	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD23	6	0.44	0.22	0.4
(1,2803)	2:232:B:GLN:HA	1:103:A:ARG:HD2	6	0.43	0.14	0.46
(1,2803)	2:232:B:GLN:HA	1:103:A:ARG:HD3	6	0.43	0.14	0.46
(1,3039)	2:231:B:THR:HA	1:102:A:GLU:HG3	6	0.4	0.15	0.38
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD11	6	0.38	0.09	0.36
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD12	6	0.38	0.09	0.36
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD13	6	0.38	0.09	0.36
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD11	6	0.38	0.09	0.36
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD12	6	0.38	0.09	0.36
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD13	6	0.38	0.09	0.36
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD11	6	0.35	0.22	0.26
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD12	6	0.35	0.22	0.26
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD13	6	0.35	0.22	0.26
(1,3817)	2:198:B:ALA:HB3	2:195:B:GLU:HG2	6	0.32	0.07	0.34
(1,3817)	2:198:B:ALA:HB1	2:195:B:GLU:HG3	6	0.32	0.07	0.34
(1,3817)	2:198:B:ALA:HB3	2:195:B:GLU:HG3	6	0.32	0.07	0.34
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD21	6	0.32	0.13	0.35
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD22	6	0.32	0.13	0.35
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD23	6	0.32	0.13	0.35
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD21	6	0.32	0.13	0.35
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD22	6	0.32	0.13	0.35
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD23	6	0.32	0.13	0.35
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD21	6	0.32	0.13	0.35
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD22	6	0.32	0.13	0.35
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD23	6	0.32	0.13	0.35
(1,4036)	2:164:B:LEU:HD13	2:164:B:LEU:H	6	0.32	0.09	0.31
(1,4036)	2:160:B:ILE:HG23	2:164:B:LEU:H	6	0.32	0.09	0.31
(1,4036)	2:164:B:LEU:HD11	2:164:B:LEU:H	6	0.32	0.09	0.31
(1,4036)	2:160:B:ILE:HG22	2:164:B:LEU:H	6	0.32	0.09	0.31
(1,4036)	2:160:B:ILE:HG21	2:164:B:LEU:H	6	0.32	0.09	0.31
(1,1703)	2:211:B:GLU:HG3	2:212:B:TYR:H	6	0.31	0.13	0.37
(1,1703)	2:211:B:GLU:HG2	2:212:B:TYR:H	6	0.31	0.13	0.37
(1,4562)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	6	0.31	0.07	0.31
(1,4562)	2:242:B:TYR:HE2	2:246:B:LEU:HD12	6	0.31	0.07	0.31
(1,4562)	2:225:B:PHE:HE1	2:233:B:LEU:HD13	6	0.31	0.07	0.31
(1,4597)	2:267:B:PHE:HE2	2:263:B:LEU:HG	6	0.31	0.19	0.24
(1,4597)	2:267:B:PHE:HE1	2:295:B:LEU:HB2	6	0.31	0.19	0.24
(1,342)	2:188:B:LYS:HG2	2:192:B:SER:HB2	6	0.28	0.1	0.24
(1,1310)	2:157:B:LYS:HG2	2:157:B:LYS:H	6	0.28	0.07	0.28
(1,1310)	2:157:B:LYS:HG3	2:157:B:LYS:H	6	0.28	0.07	0.28
(1,45)	2:159:B:LYS:HA	2:159:B:LYS:HD3	6	0.27	0.1	0.32
(1,4055)	2:175:B:ILE:HG22	2:180:B:GLN:H	6	0.27	0.09	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4055)	2:175:B:ILE:HG21	2:180:B:GLN:H	6	0.27	0.09	0.24
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE1	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE2	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE3	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE1	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE2	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE3	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE1	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE2	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE3	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE1	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE2	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE3	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE1	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE2	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE3	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE1	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE2	6	0.24	0.08	0.26
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE3	6	0.24	0.08	0.26
(1,1115)	2:297:B:TYR:HA	2:300:B:LYS:HD3	6	0.24	0.1	0.23
(1,4574)	2:242:B:TYR:HD1	2:246:B:LEU:HD11	6	0.22	0.11	0.19
(1,4574)	2:242:B:TYR:HD1	2:234:B:LEU:HD13	6	0.22	0.11	0.19
(1,4574)	2:242:B:TYR:HD1	2:246:B:LEU:HD13	6	0.22	0.11	0.19
(1,2440)	2:253:B:PRO:HG2	2:256:B:GLN:H	6	0.2	0.04	0.17
(1,2440)	2:253:B:PRO:HB2	2:256:B:GLN:H	6	0.2	0.04	0.17
(1,2900)	1:112:A:ILE:HD11	1:109:A:GLU:HB3	6	0.2	0.06	0.22
(1,2900)	1:112:A:ILE:HD12	1:109:A:GLU:HB3	6	0.2	0.06	0.22
(1,2900)	1:112:A:ILE:HD13	1:109:A:GLU:HB3	6	0.2	0.06	0.22
(1,1505)	2:184:B:LEU:HD11	2:186:B:ALA:H	6	0.19	0.07	0.19
(1,1505)	2:184:B:LEU:HD12	2:186:B:ALA:H	6	0.19	0.07	0.19
(1,1505)	2:184:B:LEU:HD13	2:186:B:ALA:H	6	0.19	0.07	0.19
(1,2623)	1:90:A:LEU:HD11	1:87:A:MET:HA	6	0.18	0.02	0.18
(1,2623)	1:90:A:LEU:HD12	1:87:A:MET:HA	6	0.18	0.02	0.18
(1,2623)	1:90:A:LEU:HD13	1:87:A:MET:HA	6	0.18	0.02	0.18
(1,2246)	2:295:B:LEU:HG	2:295:B:LEU:H	6	0.16	0.02	0.16
(1,2147)	2:280:B:ASP:HB3	2:281:B:GLU:H	6	0.13	0.02	0.14
(3,13)	1:89:A:ALA:O	1:93:A:SER:H	6	0.12	0.02	0.11
(3,7)	1:80:A:HIS:O	1:84:A:MET:H	6	0.11	0.01	0.11
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD11	5	1.96	0.53	1.93
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	5	1.96	0.53	1.93
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	5	1.96	0.53	1.93
(1,2287)	2:305:B:LEU:HD21	2:301:B:ASN:H	5	1.84	0.29	1.73

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2287)	2:305:B:LEU:HD22	2:301:B:ASN:H	5	1.84	0.29	1.73
(1,2287)	2:305:B:LEU:HD23	2:301:B:ASN:H	5	1.84	0.29	1.73
(1,2293)	2:305:B:LEU:HD21	2:302:B:SER:H	5	1.53	0.27	1.6
(1,2293)	2:305:B:LEU:HD22	2:302:B:SER:H	5	1.53	0.27	1.6
(1,2293)	2:305:B:LEU:HD23	2:302:B:SER:H	5	1.53	0.27	1.6
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG21	5	1.47	0.18	1.41
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG22	5	1.47	0.18	1.41
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG23	5	1.47	0.18	1.41
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG21	5	1.47	0.18	1.41
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG22	5	1.47	0.18	1.41
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG23	5	1.47	0.18	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG21	5	1.47	0.18	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG22	5	1.47	0.18	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG23	5	1.47	0.18	1.41
(1,4027)	2:321:B:LYS:HA	2:323:B:VAL:HG22	5	1.42	0.8	1.51
(1,4027)	2:320:B:ARG:HA	2:323:B:VAL:HG22	5	1.42	0.8	1.51
(1,4027)	2:321:B:LYS:HA	2:323:B:VAL:HG21	5	1.42	0.8	1.51
(1,4027)	2:320:B:ARG:HA	2:323:B:VAL:HG23	5	1.42	0.8	1.51
(1,3967)	2:224:B:TYR:HA	2:266:B:LEU:HD11	5	1.15	0.39	1.08
(1,3967)	2:224:B:TYR:HA	2:266:B:LEU:HD13	5	1.15	0.39	1.08
(1,3967)	2:285:B:ALA:HA	2:288:B:LEU:HD11	5	1.15	0.39	1.08
(1,3967)	2:224:B:TYR:HA	2:266:B:LEU:HD12	5	1.15	0.39	1.08
(1,2811)	1:106:A:VAL:HG11	1:104:A:ASN:HB3	5	1.05	0.65	0.65
(1,2811)	1:106:A:VAL:HG12	1:104:A:ASN:HB3	5	1.05	0.65	0.65
(1,2811)	1:106:A:VAL:HG13	1:104:A:ASN:HB3	5	1.05	0.65	0.65
(1,3724)	2:271:B:GLY:HA3	2:156:B:VAL:HG12	5	0.99	0.63	1.15
(1,3724)	2:271:B:GLY:HA3	2:156:B:VAL:HG11	5	0.99	0.63	1.15
(1,3184)	1:90:A:LEU:HD21	1:89:A:ALA:H	5	0.96	0.27	0.94
(1,3184)	1:90:A:LEU:HD22	1:89:A:ALA:H	5	0.96	0.27	0.94
(1,3184)	1:90:A:LEU:HD23	1:89:A:ALA:H	5	0.96	0.27	0.94
(1,2007)	2:226:B:ASN:HD21	2:255:B:SER:H	5	0.83	0.43	0.7
(1,298)	2:192:B:SER:HB2	2:188:B:LYS:HD3	5	0.77	0.38	0.86
(1,671)	2:234:B:LEU:HD21	2:239:B:ARG:HD2	5	0.77	0.33	0.8
(1,671)	2:234:B:LEU:HD22	2:239:B:ARG:HD2	5	0.77	0.33	0.8
(1,671)	2:234:B:LEU:HD23	2:239:B:ARG:HD2	5	0.77	0.33	0.8
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD11	5	0.72	0.25	0.71
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD12	5	0.72	0.25	0.71
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD13	5	0.72	0.25	0.71
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD11	5	0.72	0.25	0.71
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD12	5	0.72	0.25	0.71
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD13	5	0.72	0.25	0.71
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD11	5	0.72	0.25	0.71

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD12	5	0.72	0.25	0.71
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD13	5	0.72	0.25	0.71
(1,4361)	1:105:A:PHE:HD2	1:106:A:VAL:HG12	5	0.7	0.27	0.72
(1,4361)	2:235:B:TYR:HE1	1:106:A:VAL:HG11	5	0.7	0.27	0.72
(1,4361)	2:235:B:TYR:HE1	1:106:A:VAL:HG12	5	0.7	0.27	0.72
(1,4361)	2:235:B:TYR:HE1	1:106:A:VAL:HG13	5	0.7	0.27	0.72
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD21	5	0.67	0.07	0.69
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD22	5	0.67	0.07	0.69
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD23	5	0.67	0.07	0.69
(1,454)	2:202:B:LYS:HD3	2:211:B:GLU:HG3	5	0.66	0.42	0.65
(1,454)	2:202:B:LYS:HD3	2:211:B:GLU:HG2	5	0.66	0.42	0.65
(1,1120)	2:305:B:LEU:HD21	2:301:B:ASN:HB2	5	0.62	0.11	0.59
(1,1120)	2:305:B:LEU:HD22	2:301:B:ASN:HB2	5	0.62	0.11	0.59
(1,1120)	2:305:B:LEU:HD23	2:301:B:ASN:HB2	5	0.62	0.11	0.59
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD21	5	0.6	0.37	0.38
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD22	5	0.6	0.37	0.38
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD23	5	0.6	0.37	0.38
(1,4462)	1:88:A:GLN:HB2	1:88:A:GLN:H	5	0.57	0.01	0.57
(1,2653)	1:90:A:LEU:HD21	1:89:A:ALA:HA	5	0.54	0.03	0.54
(1,2653)	1:90:A:LEU:HD22	1:89:A:ALA:HA	5	0.54	0.03	0.54
(1,2653)	1:90:A:LEU:HD23	1:89:A:ALA:HA	5	0.54	0.03	0.54
(1,4472)	1:93:A:SER:HB3	1:90:A:LEU:H	5	0.5	0.24	0.56
(1,4472)	1:93:A:SER:HB2	1:95:A:ILE:H	5	0.5	0.24	0.56
(1,4634)	2:237:B:PHE:HE2	2:314:B:ALA:HB3	5	0.5	0.3	0.33
(1,4634)	2:237:B:PHE:HE2	2:181:B:LEU:HG	5	0.5	0.3	0.33
(1,4634)	2:237:B:PHE:HE2	2:314:B:ALA:HB1	5	0.5	0.3	0.33
(1,3869)	2:232:B:GLN:HB3	2:233:B:LEU:HD21	5	0.5	0.1	0.47
(1,3869)	2:232:B:GLN:HB2	2:233:B:LEU:HD23	5	0.5	0.1	0.47
(1,3869)	2:228:B:MET:HE1	2:233:B:LEU:HD22	5	0.5	0.1	0.47
(1,3789)	2:305:B:LEU:HD12	2:188:B:LYS:HE2	5	0.47	0.3	0.45
(1,3789)	2:193:B:ILE:HD11	2:188:B:LYS:HE2	5	0.47	0.3	0.45
(1,3789)	2:193:B:ILE:HD12	2:188:B:LYS:HE2	5	0.47	0.3	0.45
(1,1702)	2:211:B:GLU:HB2	2:212:B:TYR:H	5	0.45	0.14	0.45
(1,1702)	2:211:B:GLU:HB3	2:212:B:TYR:H	5	0.45	0.14	0.45
(1,3894)	2:254:B:MET:HE3	2:245:B:ILE:HG23	5	0.38	0.18	0.47
(1,3894)	2:254:B:MET:HE2	2:245:B:ILE:HG23	5	0.38	0.18	0.47
(1,3894)	2:254:B:MET:HE1	2:245:B:ILE:HG23	5	0.38	0.18	0.47
(1,3894)	2:254:B:MET:HE1	2:245:B:ILE:HG21	5	0.38	0.18	0.47
(1,3894)	2:254:B:MET:HE3	2:245:B:ILE:HG21	5	0.38	0.18	0.47
(1,455)	2:211:B:GLU:HA	2:211:B:GLU:HG3	5	0.37	0.05	0.35
(1,455)	2:211:B:GLU:HA	2:211:B:GLU:HG2	5	0.37	0.05	0.35
(1,4024)	2:323:B:VAL:HG23	2:320:B:ARG:HA	5	0.36	0.2	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4024)	2:323:B:VAL:HG11	2:320:B:ARG:HA	5	0.36	0.2	0.22
(1,4599)	2:294:B:PHE:HZ	2:263:B:LEU:HD12	5	0.35	0.12	0.38
(1,4599)	2:292:B:HIS:HD2	2:295:B:LEU:HG	5	0.35	0.12	0.38
(1,4599)	2:294:B:PHE:HZ	2:263:B:LEU:HD13	5	0.35	0.12	0.38
(1,1542)	2:188:B:LYS:HG2	2:189:B:ASN:H	5	0.33	0.09	0.31
(1,3976)	2:264:B:LEU:HA	2:295:B:LEU:HD13	5	0.31	0.12	0.27
(1,3976)	2:264:B:LEU:HA	2:295:B:LEU:HD11	5	0.31	0.12	0.27
(1,3976)	2:292:B:HIS:HA	2:295:B:LEU:HD13	5	0.31	0.12	0.27
(1,3732)	2:168:B:LEU:HD13	2:160:B:ILE:HD12	5	0.28	0.14	0.33
(1,3732)	2:168:B:LEU:HD12	2:160:B:ILE:HD11	5	0.28	0.14	0.33
(1,3732)	2:168:B:LEU:HD13	2:160:B:ILE:HD13	5	0.28	0.14	0.33
(1,3732)	2:168:B:LEU:HD11	2:160:B:ILE:HD13	5	0.28	0.14	0.33
(1,3732)	2:168:B:LEU:HD11	2:160:B:ILE:HD12	5	0.28	0.14	0.33
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE1	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE2	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE3	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE1	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE2	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE3	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE1	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE2	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE3	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE1	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE2	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE3	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE1	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE2	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE3	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE1	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE2	5	0.27	0.11	0.23
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE3	5	0.27	0.11	0.23
(1,2210)	2:288:B:LEU:HB2	2:289:B:ASN:H	5	0.25	0.06	0.25
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD21	5	0.25	0.09	0.24
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD22	5	0.25	0.09	0.24
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD23	5	0.25	0.09	0.24
(1,4087)	2:202:B:LYS:HG2	2:202:B:LYS:H	5	0.25	0.08	0.26
(1,2902)	1:112:A:ILE:HD11	1:109:A:GLU:HG3	5	0.24	0.07	0.23
(1,2902)	1:112:A:ILE:HD12	1:109:A:GLU:HG3	5	0.24	0.07	0.23
(1,2902)	1:112:A:ILE:HD13	1:109:A:GLU:HG3	5	0.24	0.07	0.23
(1,2902)	1:112:A:ILE:HD11	1:109:A:GLU:HG2	5	0.24	0.07	0.23
(1,2902)	1:112:A:ILE:HD12	1:109:A:GLU:HG2	5	0.24	0.07	0.23
(1,2902)	1:112:A:ILE:HD13	1:109:A:GLU:HG2	5	0.24	0.07	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4283)	1:82:A:SER:HA	1:84:A:MET:HE2	5	0.23	0.07	0.24
(1,4283)	1:82:A:SER:HA	1:84:A:MET:HE1	5	0.23	0.07	0.24
(1,4009)	2:180:B:GLN:HG3	2:313:B:VAL:HG13	5	0.2	0.09	0.15
(1,4009)	2:180:B:GLN:HG3	2:313:B:VAL:HG12	5	0.2	0.09	0.15
(1,4009)	2:264:B:LEU:HB3	2:268:B:VAL:HG22	5	0.2	0.09	0.15
(1,4179)	2:288:B:LEU:HG	2:288:B:LEU:H	5	0.19	0.03	0.19
(1,4179)	2:286:B:LEU:HG	2:288:B:LEU:H	5	0.19	0.03	0.19
(1,4304)	1:86:A:ASP:HB2	1:89:A:ALA:HB1	5	0.19	0.12	0.13
(1,4304)	1:86:A:ASP:HB2	1:89:A:ALA:HB3	5	0.19	0.12	0.13
(1,4304)	1:86:A:ASP:HB2	1:89:A:ALA:HB2	5	0.19	0.12	0.13
(1,3541)	2:200:B:TYR:HE1	2:204:B:ARG:HD2	5	0.19	0.03	0.18
(1,3541)	2:200:B:TYR:HE2	2:204:B:ARG:HD2	5	0.19	0.03	0.18
(1,3541)	2:200:B:TYR:HE1	2:204:B:ARG:HD3	5	0.19	0.03	0.18
(1,3541)	2:200:B:TYR:HE2	2:204:B:ARG:HD3	5	0.19	0.03	0.18
(1,4499)	2:306:B:PHE:HE1	2:298:B:LEU:HD21	5	0.18	0.05	0.19
(1,4499)	2:306:B:PHE:HE2	2:298:B:LEU:HD21	5	0.18	0.05	0.19
(1,4499)	2:306:B:PHE:HE1	2:298:B:LEU:HD23	5	0.18	0.05	0.19
(1,4499)	2:306:B:PHE:HE2	2:298:B:LEU:HD23	5	0.18	0.05	0.19
(1,427)	2:204:B:ARG:HG2	2:204:B:ARG:HA	5	0.17	0.04	0.17
(1,427)	2:204:B:ARG:HG3	2:204:B:ARG:HA	5	0.17	0.04	0.17
(1,3399)	1:117:A:GLU:HB3	1:118:A:GLY:H	5	0.16	0.04	0.17
(1,3399)	1:117:A:GLU:HB2	1:118:A:GLY:H	5	0.16	0.04	0.17
(1,3172)	1:88:A:GLN:HB2	1:88:A:GLN:HE21	5	0.16	0.04	0.16
(2,45)	1:85:A:TYR:HD1	1:81:A:LEU:HG	5	0.15	0.04	0.13
(2,45)	1:85:A:TYR:HD2	1:81:A:LEU:HG	5	0.15	0.04	0.13
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG21	5	0.14	0.01	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG22	5	0.14	0.01	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG23	5	0.14	0.01	0.15
(1,3956)	2:282:B:LYS:HE2	2:282:B:LYS:HA	5	0.14	0.03	0.14
(3,2)	1:77:A:ILE:O	1:81:A:LEU:N	5	0.13	0.04	0.12
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD11	5	0.13	0.02	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD12	5	0.13	0.02	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD13	5	0.13	0.02	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD11	5	0.13	0.02	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD12	5	0.13	0.02	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD13	5	0.13	0.02	0.11
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD21	4	1.81	0.91	2.08
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD22	4	1.81	0.91	2.08
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD23	4	1.81	0.91	2.08
(1,3875)	2:242:B:TYR:HB3	2:234:B:LEU:HD21	4	1.39	0.35	1.5
(1,3875)	2:242:B:TYR:HB3	2:234:B:LEU:HD23	4	1.39	0.35	1.5
(1,3875)	2:242:B:TYR:HB3	2:234:B:LEU:HD22	4	1.39	0.35	1.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3911)	2:252:B:ALA:HB3	2:257:B:VAL:HG13	4	1.34	0.7	1.16
(1,3911)	2:252:B:ALA:HB3	2:257:B:VAL:HG11	4	1.34	0.7	1.16
(1,3911)	2:252:B:ALA:HB2	2:257:B:VAL:HG13	4	1.34	0.7	1.16
(1,4314)	2:283:B:SER:HB2	1:90:A:LEU:HD22	4	1.09	0.49	1.2
(1,4314)	2:283:B:SER:HB2	1:90:A:LEU:HD21	4	1.09	0.49	1.2
(1,4314)	1:74:A:SER:HB3	1:96:A:LEU:HD23	4	1.09	0.49	1.2
(1,4314)	1:74:A:SER:HB3	1:96:A:LEU:HD21	4	1.09	0.49	1.2
(1,3742)	2:164:B:LEU:HA	2:164:B:LEU:HD21	4	1.07	0.02	1.08
(1,3742)	2:164:B:LEU:HA	2:164:B:LEU:HD23	4	1.07	0.02	1.08
(1,3742)	2:234:B:LEU:HA	2:234:B:LEU:HD13	4	1.07	0.02	1.08
(1,3742)	2:164:B:LEU:HA	2:164:B:LEU:HD22	4	1.07	0.02	1.08
(1,3419)	2:236:B:LYS:HD3	1:104:A:ASN:HD22	4	1.05	0.62	1.08
(1,3419)	2:236:B:LYS:HD2	1:104:A:ASN:HD22	4	1.05	0.62	1.08
(1,4337)	1:73:A:PRO:HB3	1:74:A:SER:HB2	4	1.04	0.32	1.08
(1,3443)	2:227:B:VAL:HG21	1:100:A:ASN:HD22	4	0.95	0.79	0.66
(1,3443)	2:227:B:VAL:HG22	1:100:A:ASN:HD22	4	0.95	0.79	0.66
(1,3443)	2:227:B:VAL:HG23	1:100:A:ASN:HD22	4	0.95	0.79	0.66
(1,677)	2:234:B:LEU:HD21	2:239:B:ARG:HG3	4	0.94	0.5	0.91
(1,677)	2:234:B:LEU:HD22	2:239:B:ARG:HG3	4	0.94	0.5	0.91
(1,677)	2:234:B:LEU:HD23	2:239:B:ARG:HG3	4	0.94	0.5	0.91
(1,3441)	2:227:B:VAL:HG21	1:100:A:ASN:HD21	4	0.78	0.13	0.76
(1,3441)	2:227:B:VAL:HG22	1:100:A:ASN:HD21	4	0.78	0.13	0.76
(1,3441)	2:227:B:VAL:HG23	1:100:A:ASN:HD21	4	0.78	0.13	0.76
(1,4622)	2:267:B:PHE:HZ	2:298:B:LEU:HD13	4	0.75	0.3	0.7
(1,4622)	2:267:B:PHE:HZ	2:298:B:LEU:HD12	4	0.75	0.3	0.7
(1,4622)	2:267:B:PHE:HZ	2:298:B:LEU:HD11	4	0.75	0.3	0.7
(1,4622)	2:267:B:PHE:HZ	2:221:B:ILE:HG12	4	0.75	0.3	0.7
(1,2160)	2:282:B:LYS:HB3	2:282:B:LYS:H	4	0.66	0.31	0.83
(1,3420)	2:236:B:LYS:HG2	1:104:A:ASN:HD22	4	0.65	0.32	0.68
(1,3796)	2:260:B:ALA:HA	2:190:B:VAL:HG13	4	0.63	0.12	0.63
(1,3796)	2:255:B:SER:HB3	2:190:B:VAL:HG11	4	0.63	0.12	0.63
(1,3796)	2:255:B:SER:HB3	2:190:B:VAL:HG12	4	0.63	0.12	0.63
(1,3796)	2:255:B:SER:HB3	2:190:B:VAL:HG13	4	0.63	0.12	0.63
(1,4621)	2:267:B:PHE:HE2	2:298:B:LEU:HD13	4	0.61	0.31	0.7
(1,4621)	2:267:B:PHE:HE2	2:221:B:ILE:HG12	4	0.61	0.31	0.7
(1,4621)	2:267:B:PHE:HE2	2:298:B:LEU:HD11	4	0.61	0.31	0.7
(1,4621)	2:267:B:PHE:HE2	2:298:B:LEU:HD12	4	0.61	0.31	0.7
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD21	4	0.6	0.26	0.56
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD22	4	0.6	0.26	0.56
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD23	4	0.6	0.26	0.56
(1,4317)	1:87:A:MET:HB2	1:90:A:LEU:HD22	4	0.58	0.27	0.57
(1,4317)	1:87:A:MET:HB2	1:90:A:LEU:HD23	4	0.58	0.27	0.57

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2420)	2:321:B:LYS:HB3	2:321:B:LYS:H	4	0.56	0.03	0.56
(1,4433)	2:169:B:VAL:HG21	1:116:A:ARG:HG3	4	0.53	0.37	0.46
(1,4433)	2:169:B:VAL:HG23	1:116:A:ARG:HG3	4	0.53	0.37	0.46
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD21	4	0.51	0.29	0.48
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD22	4	0.51	0.29	0.48
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD23	4	0.51	0.29	0.48
(1,1344)	2:163:B:GLU:HB2	2:163:B:GLU:H	4	0.51	0.04	0.5
(1,3966)	2:288:B:LEU:HD22	2:288:B:LEU:HA	4	0.5	0.03	0.51
(1,4334)	1:95:A:ILE:HG22	1:74:A:SER:HB3	4	0.45	0.22	0.48
(1,4334)	1:96:A:LEU:HD12	1:74:A:SER:HB3	4	0.45	0.22	0.48
(1,4334)	1:96:A:LEU:HD13	1:74:A:SER:HB3	4	0.45	0.22	0.48
(1,4334)	1:95:A:ILE:HG21	1:74:A:SER:HB3	4	0.45	0.22	0.48
(1,4579)	2:306:B:PHE:HD1	2:261:B:PRO:HG3	4	0.44	0.21	0.4
(1,4579)	2:242:B:TYR:HE1	2:254:B:MET:HE3	4	0.44	0.21	0.4
(1,4579)	2:306:B:PHE:HD2	2:261:B:PRO:HG3	4	0.44	0.21	0.4
(1,4579)	2:242:B:TYR:HE1	2:254:B:MET:HE1	4	0.44	0.21	0.4
(1,1450)	2:179:B:LYS:HD3	2:179:B:LYS:H	4	0.43	0.05	0.45
(1,309)	2:192:B:SER:HB2	2:188:B:LYS:HE2	4	0.43	0.11	0.39
(1,3734)	2:161:B:PRO:HB2	2:160:B:ILE:HG23	4	0.41	0.2	0.35
(1,3734)	2:161:B:PRO:HB2	2:160:B:ILE:HG21	4	0.41	0.2	0.35
(1,3734)	2:164:B:LEU:HB3	2:160:B:ILE:HG22	4	0.41	0.2	0.35
(1,4318)	2:279:B:LEU:HD23	1:91:A:HIS:HA	4	0.4	0.11	0.44
(1,4318)	2:279:B:LEU:HD22	1:91:A:HIS:HA	4	0.4	0.11	0.44
(1,4318)	2:279:B:LEU:HD11	1:91:A:HIS:HA	4	0.4	0.11	0.44
(1,4318)	1:95:A:ILE:HG22	1:91:A:HIS:HA	4	0.4	0.11	0.44
(1,4591)	2:182:B:PHE:HD1	2:261:B:PRO:HD2	4	0.4	0.31	0.24
(1,4591)	2:258:B:TYR:HE2	2:230:B:GLY:HA3	4	0.4	0.31	0.24
(1,4591)	2:182:B:PHE:HD2	2:261:B:PRO:HD2	4	0.4	0.31	0.24
(2,12)	2:288:B:LEU:HD21	2:157:B:LYS:H	4	0.39	0.21	0.39
(2,12)	2:288:B:LEU:HD22	2:157:B:LYS:H	4	0.39	0.21	0.39
(2,12)	2:288:B:LEU:HD23	2:157:B:LYS:H	4	0.39	0.21	0.39
(1,3409)	1:119:A:LYS:HG2	1:119:A:LYS:H	4	0.38	0.07	0.36
(1,3409)	1:119:A:LYS:HG3	1:119:A:LYS:H	4	0.38	0.07	0.36
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD21	4	0.38	0.17	0.38
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD22	4	0.38	0.17	0.38
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD23	4	0.38	0.17	0.38
(1,1249)	2:321:B:LYS:HG2	2:321:B:LYS:HE2	4	0.38	0.02	0.38
(1,1249)	2:321:B:LYS:HG3	2:321:B:LYS:HE2	4	0.38	0.02	0.38
(1,4278)	1:84:A:MET:HE2	1:81:A:LEU:HD22	4	0.37	0.15	0.31
(1,4278)	1:84:A:MET:HE1	1:81:A:LEU:HD23	4	0.37	0.15	0.31
(1,4278)	1:84:A:MET:HE2	1:81:A:LEU:HD21	4	0.37	0.15	0.31
(1,3689)	2:318:B:TYR:HE1	2:241:B:GLN:HG2	4	0.36	0.23	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3689)	2:318:B:TYR:HE2	2:241:B:GLN:HG2	4	0.36	0.23	0.29
(1,4620)	2:182:B:PHE:HZ	2:184:B:LEU:HB2	4	0.33	0.12	0.3
(1,4620)	2:267:B:PHE:HD2	2:298:B:LEU:HD13	4	0.33	0.12	0.3
(1,4620)	2:267:B:PHE:HD1	2:266:B:LEU:HD23	4	0.33	0.12	0.3
(1,3219)	1:94:A:GLU:HG3	1:94:A:GLU:H	4	0.33	0.08	0.36
(1,3219)	1:94:A:GLU:HG2	1:94:A:GLU:H	4	0.33	0.08	0.36
(1,4515)	2:172:B:TRP:HZ3	2:169:B:VAL:HG12	4	0.33	0.16	0.36
(1,4515)	2:172:B:TRP:HZ3	2:169:B:VAL:HG13	4	0.33	0.16	0.36
(1,4515)	2:172:B:TRP:HZ3	2:169:B:VAL:HG11	4	0.33	0.16	0.36
(1,4182)	2:291:B:LEU:HD21	2:292:B:HIS:H	4	0.32	0.07	0.36
(1,4182)	2:291:B:LEU:HD23	2:292:B:HIS:H	4	0.32	0.07	0.36
(1,4603)	2:224:B:TYR:HD1	2:266:B:LEU:HD11	4	0.32	0.18	0.26
(1,4603)	2:225:B:PHE:HD1	2:266:B:LEU:HD13	4	0.32	0.18	0.26
(1,4603)	2:225:B:PHE:HD1	2:266:B:LEU:HD12	4	0.32	0.18	0.26
(1,4548)	2:200:B:TYR:HE2	2:201:B:LYS:HD2	4	0.31	0.13	0.29
(1,4548)	2:200:B:TYR:HE2	2:204:B:ARG:HG3	4	0.31	0.13	0.29
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD21	4	0.31	0.01	0.31
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD22	4	0.31	0.01	0.31
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD23	4	0.31	0.01	0.31
(1,4613)	2:197:B:TYR:HE2	2:214:B:VAL:HG11	4	0.3	0.13	0.32
(1,4613)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	4	0.3	0.13	0.32
(1,4613)	2:197:B:TYR:HE2	2:214:B:VAL:HG13	4	0.3	0.13	0.32
(1,285)	2:187:B:LYS:HG3	2:187:B:LYS:HE2	4	0.3	0.03	0.3
(1,3851)	2:211:B:GLU:HA	2:202:B:LYS:HE2	4	0.3	0.11	0.34
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD21	4	0.3	0.01	0.3
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD22	4	0.3	0.01	0.3
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD23	4	0.3	0.01	0.3
(1,4450)	1:71:A:GLN:HB3	1:72:A:VAL:H	4	0.28	0.13	0.26
(1,4450)	1:72:A:VAL:HB	1:72:A:VAL:H	4	0.28	0.13	0.26
(1,1270)	2:193:B:ILE:HD11	2:188:B:LYS:HE3	4	0.27	0.12	0.23
(1,1270)	2:193:B:ILE:HD12	2:188:B:LYS:HE3	4	0.27	0.12	0.23
(1,1270)	2:193:B:ILE:HD13	2:188:B:LYS:HE3	4	0.27	0.12	0.23
(1,1228)	2:320:B:ARG:HG3	2:320:B:ARG:HA	4	0.26	0.17	0.18
(1,1228)	2:320:B:ARG:HG2	2:320:B:ARG:HA	4	0.26	0.17	0.18
(1,923)	2:155:B:GLU:HG2	2:272:B:ALA:HA	4	0.25	0.09	0.24
(1,923)	2:155:B:GLU:HG3	2:272:B:ALA:HA	4	0.25	0.09	0.24
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD11	4	0.24	0.08	0.22
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD12	4	0.24	0.08	0.22
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD13	4	0.24	0.08	0.22
(1,2261)	2:164:B:LEU:HD11	2:298:B:LEU:H	4	0.23	0.16	0.15
(1,2261)	2:164:B:LEU:HD12	2:298:B:LEU:H	4	0.23	0.16	0.15
(1,2261)	2:164:B:LEU:HD13	2:298:B:LEU:H	4	0.23	0.16	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,547)	2:194:B:LEU:HD11	2:222:B:LYS:HE3	4	0.23	0.02	0.23
(1,547)	2:194:B:LEU:HD12	2:222:B:LYS:HE3	4	0.23	0.02	0.23
(1,547)	2:194:B:LEU:HD13	2:222:B:LYS:HE3	4	0.23	0.02	0.23
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG21	4	0.22	0.15	0.16
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG22	4	0.22	0.15	0.16
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG23	4	0.22	0.15	0.16
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG21	4	0.22	0.15	0.16
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG22	4	0.22	0.15	0.16
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG23	4	0.22	0.15	0.16
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG21	4	0.22	0.15	0.16
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG22	4	0.22	0.15	0.16
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG23	4	0.22	0.15	0.16
(1,1676)	2:204:B:ARG:HG3	2:204:B:ARG:H	4	0.21	0.04	0.2
(1,4490)	1:116:A:ARG:HG2	1:115:A:VAL:H	4	0.21	0.09	0.17
(1,4490)	2:165:B:LYS:HB2	1:115:A:VAL:H	4	0.21	0.09	0.17
(1,1539)	2:188:B:LYS:HD3	2:189:B:ASN:H	4	0.2	0.08	0.2
(1,4063)	2:186:B:ALA:HB2	2:188:B:LYS:H	4	0.19	0.06	0.18
(1,4063)	2:186:B:ALA:HB3	2:188:B:LYS:H	4	0.19	0.06	0.18
(1,3380)	1:116:A:ARG:HG3	1:116:A:ARG:H	4	0.19	0.09	0.16
(1,3960)	2:282:B:LYS:HB3	2:282:B:LYS:HD3	4	0.18	0.04	0.19
(1,1985)	2:251:B:ASP:HB2	2:251:B:ASP:H	4	0.14	0.01	0.15
(1,4624)	2:267:B:PHE:HE1	2:221:B:ILE:HG21	4	0.14	0.01	0.14
(1,4624)	2:267:B:PHE:HE2	2:298:B:LEU:HD22	4	0.14	0.01	0.14
(1,4624)	2:267:B:PHE:HE1	2:221:B:ILE:HG22	4	0.14	0.01	0.14
(1,437)	2:201:B:LYS:HA	2:204:B:ARG:HG3	4	0.14	0.03	0.14
(1,437)	2:201:B:LYS:HA	2:204:B:ARG:HG2	4	0.14	0.03	0.14
(1,386)	2:195:B:GLU:HA	2:195:B:GLU:HG3	4	0.14	0.02	0.14
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD21	4	0.13	0.02	0.12
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD22	4	0.13	0.02	0.12
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD23	4	0.13	0.02	0.12
(1,3564)	2:235:B:TYR:HE1	2:235:B:TYR:HA	4	0.12	0.01	0.12
(1,3564)	2:235:B:TYR:HE2	2:235:B:TYR:HA	4	0.12	0.01	0.12
(1,3421)	2:236:B:LYS:HE2	1:104:A:ASN:HD22	3	1.2	0.58	1.18
(1,3421)	2:236:B:LYS:HE3	1:104:A:ASN:HD22	3	1.2	0.58	1.18
(2,259)	2:227:B:VAL:HG22	1:98:A:PHE:HD1	3	1.14	0.67	1.34
(2,259)	2:227:B:VAL:HG11	1:98:A:PHE:HE2	3	1.14	0.67	1.34
(2,261)	2:227:B:VAL:HG22	1:98:A:PHE:HD1	3	1.14	0.67	1.34
(2,261)	2:227:B:VAL:HG11	1:98:A:PHE:HE2	3	1.14	0.67	1.34
(1,1465)	2:174:B:LEU:HD11	2:180:B:GLN:HE22	3	0.9	1.1	0.14
(1,1465)	2:174:B:LEU:HD12	2:180:B:GLN:HE22	3	0.9	1.1	0.14
(1,1465)	2:174:B:LEU:HD13	2:180:B:GLN:HE22	3	0.9	1.1	0.14
(1,2471)	1:72:A:VAL:HG21	1:71:A:GLN:HB3	3	0.85	0.51	1.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2471)	1:72:A:VAL:HG22	1:71:A:GLN:HB3	3	0.85	0.51	1.17
(1,2471)	1:72:A:VAL:HG23	1:71:A:GLN:HB3	3	0.85	0.51	1.17
(1,4323)	2:279:B:LEU:HD21	1:91:A:HIS:HB3	3	0.81	0.18	0.8
(1,4323)	2:279:B:LEU:HD22	1:91:A:HIS:HB3	3	0.81	0.18	0.8
(1,4323)	2:279:B:LEU:HD23	1:91:A:HIS:HB3	3	0.81	0.18	0.8
(1,4373)	2:169:B:VAL:HA	1:107:A:LEU:HD22	3	0.77	0.48	0.72
(1,4373)	2:169:B:VAL:HA	1:107:A:LEU:HD23	3	0.77	0.48	0.72
(1,4373)	2:172:B:TRP:HB2	1:107:A:LEU:HD22	3	0.77	0.48	0.72
(1,387)	2:196:B:ASP:HA	2:195:B:GLU:HG3	3	0.65	0.03	0.63
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD11	3	0.64	0.33	0.73
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD12	3	0.64	0.33	0.73
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD13	3	0.64	0.33	0.73
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD11	3	0.64	0.33	0.73
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD12	3	0.64	0.33	0.73
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD13	3	0.64	0.33	0.73
(1,4268)	1:81:A:LEU:HD22	1:78:A:TRP:HB2	3	0.62	0.3	0.62
(1,4268)	1:76:A:VAL:HG23	1:78:A:TRP:HB2	3	0.62	0.3	0.62
(1,4268)	1:76:A:VAL:HG21	1:78:A:TRP:HB2	3	0.62	0.3	0.62
(1,1338)	2:162:B:GLU:HG3	2:162:B:GLU:H	3	0.6	0.04	0.6
(1,4417)	1:109:A:GLU:HG2	1:112:A:ILE:HG23	3	0.58	0.18	0.48
(1,4417)	1:109:A:GLU:HG2	1:112:A:ILE:HG21	3	0.58	0.18	0.48
(1,4417)	1:109:A:GLU:HG2	1:112:A:ILE:HG22	3	0.58	0.18	0.48
(1,1303)	2:155:B:GLU:HG3	2:155:B:GLU:H	3	0.58	0.04	0.6
(1,1303)	2:155:B:GLU:HG2	2:155:B:GLU:H	3	0.58	0.04	0.6
(1,4600)	2:200:B:TYR:HE2	2:201:B:LYS:HG2	3	0.58	0.23	0.72
(1,4600)	2:200:B:TYR:HE1	2:201:B:LYS:HG2	3	0.58	0.23	0.72
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG11	3	0.53	0.28	0.65
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG12	3	0.53	0.28	0.65
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG13	3	0.53	0.28	0.65
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG11	3	0.53	0.28	0.65
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG12	3	0.53	0.28	0.65
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG13	3	0.53	0.28	0.65
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG11	3	0.53	0.28	0.65
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG12	3	0.53	0.28	0.65
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG13	3	0.53	0.28	0.65
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD21	3	0.53	0.27	0.42
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD22	3	0.53	0.27	0.42
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD23	3	0.53	0.27	0.42
(1,4440)	2:223:B:GLU:HG3	1:77:A:ILE:HG21	3	0.52	0.32	0.45
(1,4440)	2:218:B:VAL:HB	1:77:A:ILE:HG23	3	0.52	0.32	0.45
(1,4440)	2:223:B:GLU:HG3	1:77:A:ILE:HG22	3	0.52	0.32	0.45
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD21	3	0.5	0.21	0.63

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD22	3	0.5	0.21	0.63
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD23	3	0.5	0.21	0.63
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD21	3	0.44	0.04	0.43
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD22	3	0.44	0.04	0.43
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD23	3	0.44	0.04	0.43
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD11	3	0.44	0.28	0.28
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD12	3	0.44	0.28	0.28
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD13	3	0.44	0.28	0.28
(1,4396)	2:165:B:LYS:HE2	1:111:A:ILE:HD12	3	0.44	0.22	0.45
(1,4396)	2:165:B:LYS:HE2	1:111:A:ILE:HD11	3	0.44	0.22	0.45
(1,307)	2:193:B:ILE:HG12	2:188:B:LYS:HE3	3	0.43	0.17	0.52
(1,900)	2:269:B:ARG:HA	2:269:B:ARG:HD3	3	0.43	0.16	0.32
(1,900)	2:269:B:ARG:HA	2:269:B:ARG:HD2	3	0.43	0.16	0.32
(1,2945)	1:107:A:LEU:HD21	1:112:A:ILE:HG13	3	0.43	0.12	0.43
(1,2945)	1:107:A:LEU:HD22	1:112:A:ILE:HG13	3	0.43	0.12	0.43
(1,2945)	1:107:A:LEU:HD23	1:112:A:ILE:HG13	3	0.43	0.12	0.43
(1,3408)	1:119:A:LYS:HB2	1:119:A:LYS:H	3	0.43	0.08	0.44
(1,3928)	1:111:A:ILE:HD12	2:268:B:VAL:HG13	3	0.43	0.24	0.3
(1,3928)	1:111:A:ILE:HD13	2:268:B:VAL:HG13	3	0.43	0.24	0.3
(1,313)	2:192:B:SER:HB3	2:188:B:LYS:HG3	3	0.43	0.11	0.45
(1,313)	2:192:B:SER:HB2	2:188:B:LYS:HG3	3	0.43	0.11	0.45
(1,4631)	2:167:B:TRP:HZ3	2:308:B:ALA:HB3	3	0.42	0.09	0.47
(1,4631)	2:237:B:PHE:HE2	2:179:B:LYS:HB2	3	0.42	0.09	0.47
(1,4631)	2:167:B:TRP:HZ3	2:308:B:ALA:HB2	3	0.42	0.09	0.47
(1,3940)	2:274:B:LEU:HG	2:270:B:ILE:HD11	3	0.41	0.13	0.38
(1,3940)	2:274:B:LEU:HG	2:270:B:ILE:HD13	3	0.41	0.13	0.38
(1,3730)	2:267:B:PHE:HB3	2:158:B:VAL:HG11	3	0.41	0.38	0.16
(1,3730)	2:267:B:PHE:HB3	2:158:B:VAL:HG13	3	0.41	0.38	0.16
(1,3730)	2:225:B:PHE:HB3	2:263:B:LEU:HD22	3	0.41	0.38	0.16
(1,420)	2:199:B:ASN:HA	2:202:B:LYS:HE3	3	0.39	0.09	0.38
(1,420)	2:199:B:ASN:HA	2:202:B:LYS:HE2	3	0.39	0.09	0.38
(1,2341)	2:307:B:SER:HB3	2:309:B:SER:H	3	0.39	0.12	0.42
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD21	3	0.38	0.2	0.45
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD22	3	0.38	0.2	0.45
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD23	3	0.38	0.2	0.45
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD21	3	0.38	0.2	0.45
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD22	3	0.38	0.2	0.45
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD23	3	0.38	0.2	0.45
(1,299)	2:193:B:ILE:HD11	2:188:B:LYS:HD3	3	0.36	0.03	0.37
(1,299)	2:193:B:ILE:HD12	2:188:B:LYS:HD3	3	0.36	0.03	0.37
(1,299)	2:193:B:ILE:HD13	2:188:B:LYS:HD3	3	0.36	0.03	0.37
(1,1067)	2:298:B:LEU:HD11	2:295:B:LEU:HA	3	0.32	0.15	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1067)	2:298:B:LEU:HD12	2:295:B:LEU:HA	3	0.32	0.15	0.4
(1,1067)	2:298:B:LEU:HD13	2:295:B:LEU:HA	3	0.32	0.15	0.4
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD21	3	0.32	0.13	0.34
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD22	3	0.32	0.13	0.34
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD23	3	0.32	0.13	0.34
(1,1626)	2:195:B:GLU:HG2	2:199:B:ASN:HD22	3	0.3	0.14	0.35
(1,4491)	1:118:A:GLY:HA2	1:117:A:GLU:H	3	0.3	0.07	0.34
(1,4491)	1:118:A:GLY:HA3	1:117:A:GLU:H	3	0.3	0.07	0.34
(1,4424)	1:116:A:ARG:HG2	1:115:A:VAL:HG11	3	0.29	0.19	0.21
(1,4424)	1:116:A:ARG:HG2	1:115:A:VAL:HG12	3	0.29	0.19	0.21
(1,4424)	1:116:A:ARG:HG2	1:115:A:VAL:HG13	3	0.29	0.19	0.21
(2,307)	2:279:B:LEU:HD12	1:94:A:GLU:HA	3	0.28	0.06	0.31
(2,307)	2:279:B:LEU:HD11	1:87:A:MET:HA	3	0.28	0.06	0.31
(1,2593)	2:212:B:TYR:HD1	1:84:A:MET:HB2	3	0.28	0.11	0.24
(1,2593)	2:212:B:TYR:HD2	1:84:A:MET:HB2	3	0.28	0.11	0.24
(1,2593)	2:212:B:TYR:HD1	1:84:A:MET:HB3	3	0.28	0.11	0.24
(1,2593)	2:212:B:TYR:HD2	1:84:A:MET:HB3	3	0.28	0.11	0.24
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE1	3	0.26	0.07	0.31
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE2	3	0.26	0.07	0.31
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE3	3	0.26	0.07	0.31
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE1	3	0.24	0.12	0.16
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE2	3	0.24	0.12	0.16
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE3	3	0.24	0.12	0.16
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG21	3	0.22	0.08	0.26
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG22	3	0.22	0.08	0.26
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG23	3	0.22	0.08	0.26
(1,2996)	1:116:A:ARG:HD2	1:115:A:VAL:HG21	3	0.22	0.08	0.26
(1,2996)	1:116:A:ARG:HD2	1:115:A:VAL:HG22	3	0.22	0.08	0.26
(1,2996)	1:116:A:ARG:HD2	1:115:A:VAL:HG23	3	0.22	0.08	0.26
(1,1503)	2:184:B:LEU:HD11	2:184:B:LEU:H	3	0.21	0.01	0.22
(1,1503)	2:184:B:LEU:HD12	2:184:B:LEU:H	3	0.21	0.01	0.22
(1,1503)	2:184:B:LEU:HD13	2:184:B:LEU:H	3	0.21	0.01	0.22
(1,3910)	2:257:B:VAL:HG21	2:256:B:GLN:HG2	3	0.21	0.05	0.22
(1,3910)	2:257:B:VAL:HG23	2:256:B:GLN:HG3	3	0.21	0.05	0.22
(1,3910)	2:257:B:VAL:HG23	2:256:B:GLN:HG2	3	0.21	0.05	0.22
(1,4476)	1:92:A:GLU:HG2	1:90:A:LEU:H	3	0.21	0.06	0.24
(1,4476)	1:92:A:GLU:HG3	1:90:A:LEU:H	3	0.21	0.06	0.24
(1,3746)	2:306:B:PHE:HE1	2:298:B:LEU:HD21	3	0.2	0.05	0.19
(1,3746)	2:306:B:PHE:HE1	2:298:B:LEU:HD23	3	0.2	0.05	0.19
(1,3993)	2:296:B:LYS:HA	2:299:B:ALA:HB2	3	0.19	0.01	0.19
(1,2171)	2:282:B:LYS:HG2	2:283:B:SER:H	3	0.19	0.01	0.18
(1,4376)	1:112:A:ILE:HG13	1:108:A:PRO:HA	3	0.16	0.05	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4457)	1:82:A:SER:HA	1:85:A:TYR:H	3	0.16	0.03	0.14
(1,4457)	1:84:A:MET:HA	1:85:A:TYR:H	3	0.16	0.03	0.14
(1,978)	2:282:B:LYS:HD3	2:282:B:LYS:HB3	3	0.15	0.05	0.12
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD21	3	0.14	0.03	0.15
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD22	3	0.14	0.03	0.15
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD23	3	0.14	0.03	0.15
(1,1494)	2:183:B:TYR:HB2	2:183:B:TYR:H	3	0.13	0.03	0.13
(1,4565)	2:262:B:HIS:HD2	2:234:B:LEU:HG	3	0.13	0.0	0.13
(1,4565)	2:183:B:TYR:HE1	2:184:B:LEU:HG	3	0.13	0.0	0.13
(1,1130)	2:305:B:LEU:HD11	2:305:B:LEU:HA	3	0.12	0.03	0.1
(1,1130)	2:305:B:LEU:HD12	2:305:B:LEU:HA	3	0.12	0.03	0.1
(1,1130)	2:305:B:LEU:HD13	2:305:B:LEU:HA	3	0.12	0.03	0.1
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB1	3	0.11	0.01	0.11
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB2	3	0.11	0.01	0.11
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB3	3	0.11	0.01	0.11
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB1	3	0.11	0.01	0.11
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB2	3	0.11	0.01	0.11
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB3	3	0.11	0.01	0.11
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB1	3	0.11	0.01	0.11
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB2	3	0.11	0.01	0.11
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB3	3	0.11	0.01	0.11
(1,3220)	1:95:A:ILE:H	1:94:A:GLU:H	3	0.11	0.0	0.11
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG11	2	1.94	0.05	1.94
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG12	2	1.94	0.05	1.94
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG13	2	1.94	0.05	1.94
(1,4004)	2:305:B:LEU:HA	2:305:B:LEU:HD13	2	1.25	0.01	1.25
(1,4004)	2:274:B:LEU:HA	2:274:B:LEU:HD13	2	1.25	0.01	1.25
(1,4276)	1:98:A:PHE:HE2	1:96:A:LEU:HD21	2	0.89	0.22	0.89
(1,4276)	1:98:A:PHE:HE1	1:96:A:LEU:HD23	2	0.89	0.22	0.89
(1,3948)	2:276:B:TYR:HE2	2:273:B:MET:HE2	2	0.86	0.17	0.86
(1,2051)	2:190:B:VAL:HG21	2:263:B:LEU:H	2	0.83	0.52	0.83
(1,2051)	2:190:B:VAL:HG22	2:263:B:LEU:H	2	0.83	0.52	0.83
(1,2051)	2:190:B:VAL:HG23	2:263:B:LEU:H	2	0.83	0.52	0.83
(1,4449)	2:290:B:TYR:HE1	1:81:A:LEU:HD13	2	0.82	0.29	0.82
(1,4449)	2:290:B:TYR:HE2	1:81:A:LEU:HD12	2	0.82	0.29	0.82
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD21	2	0.82	0.07	0.82
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD22	2	0.82	0.07	0.82
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD23	2	0.82	0.07	0.82
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD21	2	0.82	0.07	0.82
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD22	2	0.82	0.07	0.82
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD23	2	0.82	0.07	0.82
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD21	2	0.82	0.07	0.82

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD22	2	0.82	0.07	0.82
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD23	2	0.82	0.07	0.82
(1,3930)	2:168:B:LEU:HD13	2:268:B:VAL:HG13	2	0.69	0.56	0.69
(1,3930)	2:168:B:LEU:HD11	2:268:B:VAL:HG12	2	0.69	0.56	0.69
(1,4601)	2:267:B:PHE:HE2	2:263:B:LEU:HD21	2	0.67	0.1	0.67
(1,4601)	2:267:B:PHE:HE2	2:263:B:LEU:HD22	2	0.67	0.1	0.67
(1,3721)	2:154:B:ALA:HB1	2:156:B:VAL:HA	2	0.66	0.21	0.66
(1,3721)	2:164:B:LEU:HG	2:165:B:LYS:HA	2	0.66	0.21	0.66
(1,4512)	2:235:B:TYR:HD1	2:175:B:ILE:HD13	2	0.62	0.12	0.62
(1,4512)	2:235:B:TYR:HD1	2:175:B:ILE:HD12	2	0.62	0.12	0.62
(1,3898)	2:254:B:MET:HE1	2:252:B:ALA:HB1	2	0.59	0.31	0.59
(1,3898)	2:254:B:MET:HE1	2:252:B:ALA:HB2	2	0.59	0.31	0.59
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG21	2	0.57	0.4	0.57
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG22	2	0.57	0.4	0.57
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG23	2	0.57	0.4	0.57
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG21	2	0.57	0.4	0.57
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG22	2	0.57	0.4	0.57
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG23	2	0.57	0.4	0.57
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG21	2	0.57	0.4	0.57
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG22	2	0.57	0.4	0.57
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG23	2	0.57	0.4	0.57
(1,2023)	2:257:B:VAL:HG11	2:256:B:GLN:H	2	0.55	0.13	0.55
(1,2023)	2:257:B:VAL:HG12	2:256:B:GLN:H	2	0.55	0.13	0.55
(1,2023)	2:257:B:VAL:HG13	2:256:B:GLN:H	2	0.55	0.13	0.55
(1,4587)	2:306:B:PHE:HE1	2:260:B:ALA:HB1	2	0.54	0.2	0.54
(1,4587)	2:306:B:PHE:HE2	2:305:B:LEU:HB3	2	0.54	0.2	0.54
(1,3613)	2:276:B:TYR:HE2	2:273:B:MET:HE2	2	0.53	0.16	0.53
(1,3613)	2:276:B:TYR:HE2	2:273:B:MET:HB3	2	0.53	0.16	0.53
(1,596)	2:234:B:LEU:HD21	2:230:B:GLY:HA3	2	0.52	0.12	0.52
(1,596)	2:234:B:LEU:HD22	2:230:B:GLY:HA3	2	0.52	0.12	0.52
(1,596)	2:234:B:LEU:HD23	2:230:B:GLY:HA3	2	0.52	0.12	0.52
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD21	2	0.49	0.05	0.49
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD22	2	0.49	0.05	0.49
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD23	2	0.49	0.05	0.49
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD21	2	0.49	0.05	0.49
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD22	2	0.49	0.05	0.49
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD23	2	0.49	0.05	0.49
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD21	2	0.49	0.05	0.49
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD22	2	0.49	0.05	0.49
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD23	2	0.49	0.05	0.49
(1,3999)	2:200:B:TYR:HE2	2:296:B:LYS:HE3	2	0.49	0.1	0.49
(1,3454)	2:292:B:HIS:HE1	2:159:B:LYS:HG3	2	0.48	0.22	0.48

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4532)	2:183:B:TYR:HD2	2:184:B:LEU:HA	2	0.48	0.25	0.48
(1,3912)	2:185:B:PRO:HB3	2:257:B:VAL:HG23	2	0.48	0.32	0.48
(1,3912)	2:185:B:PRO:HB3	2:257:B:VAL:HG21	2	0.48	0.32	0.48
(1,4035)	2:162:B:GLU:HG3	2:163:B:GLU:H	2	0.47	0.01	0.47
(1,4387)	1:112:A:ILE:HG23	1:109:A:GLU:HG2	2	0.46	0.02	0.46
(1,4387)	1:112:A:ILE:HG21	1:109:A:GLU:HG2	2	0.46	0.02	0.46
(1,4545)	2:200:B:TYR:HD2	2:201:B:LYS:HD2	2	0.45	0.05	0.45
(1,4545)	2:200:B:TYR:HD1	2:201:B:LYS:HD2	2	0.45	0.05	0.45
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD11	2	0.45	0.05	0.45
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD12	2	0.45	0.05	0.45
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD13	2	0.45	0.05	0.45
(1,4329)	1:89:A:ALA:HB2	1:92:A:GLU:HG3	2	0.44	0.06	0.44
(1,4329)	1:89:A:ALA:HB2	1:92:A:GLU:HG2	2	0.44	0.06	0.44
(1,1899)	2:239:B:ARG:HG2	2:239:B:ARG:H	2	0.43	0.12	0.43
(1,2458)	1:70:A:ARG:HG3	1:70:A:ARG:HA	2	0.42	0.0	0.42
(1,1832)	2:233:B:LEU:HD11	2:230:B:GLY:H	2	0.42	0.11	0.42
(1,1832)	2:233:B:LEU:HD12	2:230:B:GLY:H	2	0.42	0.11	0.42
(1,1832)	2:233:B:LEU:HD13	2:230:B:GLY:H	2	0.42	0.11	0.42
(1,4002)	2:188:B:LYS:HE2	2:305:B:LEU:HD13	2	0.41	0.13	0.41
(1,4002)	2:188:B:LYS:HE2	2:305:B:LEU:HD12	2	0.41	0.13	0.41
(1,4344)	1:92:A:GLU:HB3	1:95:A:ILE:HD12	2	0.41	0.28	0.41
(1,4344)	1:92:A:GLU:HB3	1:95:A:ILE:HD11	2	0.41	0.28	0.41
(1,4302)	1:91:A:HIS:HB2	1:92:A:GLU:HA	2	0.4	0.06	0.4
(1,4302)	1:91:A:HIS:HB2	1:88:A:GLN:HA	2	0.4	0.06	0.4
(1,4347)	1:97:A:PRO:HG3	1:95:A:ILE:HG22	2	0.4	0.12	0.4
(1,4347)	1:97:A:PRO:HG3	1:95:A:ILE:HG21	2	0.4	0.12	0.4
(1,681)	2:234:B:LEU:HD21	2:239:B:ARG:HG2	2	0.39	0.17	0.39
(1,681)	2:234:B:LEU:HD22	2:239:B:ARG:HG2	2	0.39	0.17	0.39
(1,681)	2:234:B:LEU:HD23	2:239:B:ARG:HG2	2	0.39	0.17	0.39
(1,4546)	2:224:B:TYR:HD1	2:270:B:ILE:HB	2	0.39	0.12	0.39
(1,4546)	2:200:B:TYR:HE2	2:201:B:LYS:HB2	2	0.39	0.12	0.39
(1,1888)	2:238:B:GLU:HG2	2:238:B:GLU:H	2	0.38	0.02	0.38
(1,1888)	2:238:B:GLU:HG3	2:238:B:GLU:H	2	0.38	0.02	0.38
(1,456)	2:245:B:ILE:HG21	2:244:B:GLU:HG2	2	0.38	0.01	0.38
(1,456)	2:245:B:ILE:HG22	2:244:B:GLU:HG2	2	0.38	0.01	0.38
(1,456)	2:245:B:ILE:HG23	2:244:B:GLU:HG2	2	0.38	0.01	0.38
(1,2040)	2:190:B:VAL:HG21	2:260:B:ALA:H	2	0.38	0.11	0.38
(1,2040)	2:190:B:VAL:HG22	2:260:B:ALA:H	2	0.38	0.11	0.38
(1,2040)	2:190:B:VAL:HG23	2:260:B:ALA:H	2	0.38	0.11	0.38
(1,2604)	1:87:A:MET:HB2	1:85:A:TYR:HA	2	0.36	0.14	0.36
(1,4222)	2:317:B:GLU:HB2	2:318:B:TYR:H	2	0.35	0.18	0.35
(1,2911)	1:114:A:GLU:HB3	1:111:A:ILE:HA	2	0.35	0.08	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4506)	2:235:B:TYR:HD1	2:175:B:ILE:HB	2	0.35	0.08	0.35
(1,4506)	2:172:B:TRP:HD1	2:175:B:ILE:HB	2	0.35	0.08	0.35
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD21	2	0.34	0.12	0.34
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD22	2	0.34	0.12	0.34
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD23	2	0.34	0.12	0.34
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD21	2	0.34	0.12	0.34
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD22	2	0.34	0.12	0.34
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD23	2	0.34	0.12	0.34
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD21	2	0.34	0.12	0.34
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD22	2	0.34	0.12	0.34
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD23	2	0.34	0.12	0.34
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG11	2	0.34	0.2	0.34
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG12	2	0.34	0.2	0.34
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG13	2	0.34	0.2	0.34
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD11	2	0.34	0.06	0.34
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD12	2	0.34	0.06	0.34
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD13	2	0.34	0.06	0.34
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD11	2	0.34	0.06	0.34
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD12	2	0.34	0.06	0.34
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD13	2	0.34	0.06	0.34
(1,4308)	1:90:A:LEU:HD11	1:90:A:LEU:HB2	2	0.34	0.01	0.34
(1,4308)	1:96:A:LEU:HD12	1:96:A:LEU:HB3	2	0.34	0.01	0.34
(1,2736)	1:96:A:LEU:HB3	1:97:A:PRO:HA	2	0.33	0.01	0.33
(1,3060)	1:79:A:ASP:HB2	1:76:A:VAL:HG11	2	0.32	0.16	0.32
(1,3060)	1:79:A:ASP:HB2	1:76:A:VAL:HG12	2	0.32	0.16	0.32
(1,3060)	1:79:A:ASP:HB2	1:76:A:VAL:HG13	2	0.32	0.16	0.32
(1,3060)	1:79:A:ASP:HB3	1:76:A:VAL:HG11	2	0.32	0.16	0.32
(1,3060)	1:79:A:ASP:HB3	1:76:A:VAL:HG12	2	0.32	0.16	0.32
(1,3060)	1:79:A:ASP:HB3	1:76:A:VAL:HG13	2	0.32	0.16	0.32
(1,385)	2:192:B:SER:HA	2:195:B:GLU:HG2	2	0.31	0.01	0.31
(1,797)	2:257:B:VAL:HG11	2:254:B:MET:HA	2	0.3	0.02	0.3
(1,797)	2:257:B:VAL:HG12	2:254:B:MET:HA	2	0.3	0.02	0.3
(1,797)	2:257:B:VAL:HG13	2:254:B:MET:HA	2	0.3	0.02	0.3
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB1	2	0.3	0.01	0.3
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB2	2	0.3	0.01	0.3
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB3	2	0.3	0.01	0.3
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB1	2	0.3	0.01	0.3
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB2	2	0.3	0.01	0.3
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB3	2	0.3	0.01	0.3
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB1	2	0.3	0.01	0.3
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB2	2	0.3	0.01	0.3
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB3	2	0.3	0.01	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG21	2	0.3	0.18	0.3
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG22	2	0.3	0.18	0.3
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG23	2	0.3	0.18	0.3
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG21	2	0.3	0.18	0.3
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG22	2	0.3	0.18	0.3
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG23	2	0.3	0.18	0.3
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG21	2	0.3	0.18	0.3
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG22	2	0.3	0.18	0.3
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG23	2	0.3	0.18	0.3
(1,4567)	2:306:B:PHE:HD2	2:305:B:LEU:HB2	2	0.3	0.18	0.3
(1,4567)	2:242:B:TYR:HE1	2:234:B:LEU:HD22	2	0.3	0.18	0.3
(1,3733)	2:165:B:LYS:HB3	2:160:B:ILE:HG21	2	0.3	0.12	0.3
(1,3733)	2:165:B:LYS:HB3	2:160:B:ILE:HG22	2	0.3	0.12	0.3
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD21	2	0.29	0.1	0.29
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD22	2	0.29	0.1	0.29
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD23	2	0.29	0.1	0.29
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD21	2	0.29	0.1	0.29
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD22	2	0.29	0.1	0.29
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD23	2	0.29	0.1	0.29
(1,4556)	2:290:B:TYR:HE1	2:217:B:VAL:HG21	2	0.29	0.1	0.29
(1,4556)	2:197:B:TYR:HE2	2:217:B:VAL:HG22	2	0.29	0.1	0.29
(1,344)	2:188:B:LYS:HE3	2:193:B:ILE:HA	2	0.28	0.05	0.28
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD21	2	0.28	0.04	0.28
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD22	2	0.28	0.04	0.28
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD23	2	0.28	0.04	0.28
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD21	2	0.28	0.04	0.28
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD22	2	0.28	0.04	0.28
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD23	2	0.28	0.04	0.28
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD21	2	0.28	0.06	0.28
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD22	2	0.28	0.06	0.28
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD23	2	0.28	0.06	0.28
(1,3359)	1:114:A:GLU:HB3	1:114:A:GLU:H	2	0.27	0.01	0.27
(1,3359)	1:114:A:GLU:HG2	1:114:A:GLU:H	2	0.27	0.01	0.27
(1,4133)	2:254:B:MET:HE3	2:246:B:LEU:H	2	0.27	0.0	0.27
(1,4133)	2:254:B:MET:HE1	2:246:B:LEU:H	2	0.27	0.0	0.27
(1,1739)	2:217:B:VAL:HB	2:218:B:VAL:H	2	0.26	0.02	0.26
(1,3810)	2:222:B:LYS:HB3	2:194:B:LEU:HD11	2	0.26	0.12	0.26
(1,3810)	2:222:B:LYS:HB3	2:194:B:LEU:HD12	2	0.26	0.12	0.26
(1,2145)	2:280:B:ASP:HB2	2:280:B:ASP:H	2	0.25	0.02	0.25
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD21	2	0.24	0.14	0.24
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD22	2	0.24	0.14	0.24
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD23	2	0.24	0.14	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD21	2	0.24	0.14	0.24
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD22	2	0.24	0.14	0.24
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD23	2	0.24	0.14	0.24
(1,3916)	2:263:B:LEU:HD23	2:263:B:LEU:HA	2	0.23	0.0	0.23
(1,3916)	2:263:B:LEU:HD21	2:263:B:LEU:HA	2	0.23	0.0	0.23
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD21	2	0.22	0.02	0.22
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD22	2	0.22	0.02	0.22
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD23	2	0.22	0.02	0.22
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD21	2	0.22	0.02	0.22
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD22	2	0.22	0.02	0.22
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD23	2	0.22	0.02	0.22
(1,2466)	1:72:A:VAL:HG11	1:71:A:GLN:HA	2	0.22	0.08	0.22
(1,2466)	1:72:A:VAL:HG12	1:71:A:GLN:HA	2	0.22	0.08	0.22
(1,2466)	1:72:A:VAL:HG13	1:71:A:GLN:HA	2	0.22	0.08	0.22
(1,3402)	1:117:A:GLU:HB3	1:119:A:LYS:H	2	0.21	0.1	0.21
(1,2135)	2:278:B:PRO:HA	2:279:B:LEU:H	2	0.2	0.02	0.2
(1,2320)	2:305:B:LEU:HB3	2:306:B:PHE:H	2	0.2	0.0	0.2
(1,4438)	2:166:B:PRO:HA	1:111:A:ILE:HG23	2	0.2	0.08	0.2
(1,1003)	2:288:B:LEU:HD11	2:285:B:ALA:HA	2	0.2	0.06	0.2
(1,1003)	2:288:B:LEU:HD12	2:285:B:ALA:HA	2	0.2	0.06	0.2
(1,1003)	2:288:B:LEU:HD13	2:285:B:ALA:HA	2	0.2	0.06	0.2
(1,2029)	2:257:B:VAL:HG11	2:257:B:VAL:H	2	0.2	0.02	0.2
(1,2029)	2:257:B:VAL:HG12	2:257:B:VAL:H	2	0.2	0.02	0.2
(1,2029)	2:257:B:VAL:HG13	2:257:B:VAL:H	2	0.2	0.02	0.2
(1,3965)	2:290:B:TYR:HE2	2:286:B:LEU:HG	2	0.2	0.05	0.2
(1,4554)	2:290:B:TYR:HD2	2:217:B:VAL:HG13	2	0.19	0.05	0.19
(1,4554)	2:290:B:TYR:HD1	2:217:B:VAL:HG13	2	0.19	0.05	0.19
(1,4573)	2:249:B:HIS:HD2	2:245:B:ILE:HG22	2	0.19	0.04	0.19
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG21	2	0.18	0.08	0.18
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG22	2	0.18	0.08	0.18
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG23	2	0.18	0.08	0.18
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG21	2	0.18	0.08	0.18
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG22	2	0.18	0.08	0.18
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG23	2	0.18	0.08	0.18
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG21	2	0.18	0.08	0.18
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG22	2	0.18	0.08	0.18
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG23	2	0.18	0.08	0.18
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD11	2	0.18	0.02	0.18
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD12	2	0.18	0.02	0.18
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD13	2	0.18	0.02	0.18
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD11	2	0.18	0.02	0.18
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD12	2	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD13	2	0.18	0.02	0.18
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD11	2	0.18	0.02	0.18
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD12	2	0.18	0.02	0.18
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD13	2	0.18	0.02	0.18
(1,4571)	2:318:B:TYR:HE2	2:241:B:GLN:HA	2	0.18	0.04	0.18
(1,4571)	2:318:B:TYR:HE1	2:241:B:GLN:HA	2	0.18	0.04	0.18
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD21	2	0.18	0.02	0.18
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD22	2	0.18	0.02	0.18
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD23	2	0.18	0.02	0.18
(1,1844)	2:232:B:GLN:HG3	2:232:B:GLN:H	2	0.17	0.05	0.17
(1,1844)	2:232:B:GLN:HG2	2:232:B:GLN:H	2	0.17	0.05	0.17
(1,301)	2:192:B:SER:HB2	2:188:B:LYS:HD2	2	0.16	0.06	0.16
(1,301)	2:192:B:SER:HB3	2:188:B:LYS:HD2	2	0.16	0.06	0.16
(1,1561)	2:190:B:VAL:HB	2:191:B:ASP:H	2	0.16	0.05	0.16
(1,3752)	2:160:B:ILE:HG21	2:165:B:LYS:HG3	2	0.16	0.04	0.16
(1,3752)	2:160:B:ILE:HG22	2:165:B:LYS:HG3	2	0.16	0.04	0.16
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG21	2	0.16	0.04	0.16
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG22	2	0.16	0.04	0.16
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG23	2	0.16	0.04	0.16
(1,1316)	2:157:B:LYS:HB3	2:157:B:LYS:H	2	0.16	0.02	0.16
(1,37)	2:159:B:LYS:HA	2:159:B:LYS:HG3	2	0.15	0.02	0.15
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE1	2	0.15	0.03	0.15
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE2	2	0.15	0.03	0.15
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE3	2	0.15	0.03	0.15
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE1	2	0.15	0.03	0.15
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE2	2	0.15	0.03	0.15
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE3	2	0.15	0.03	0.15
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE1	2	0.15	0.03	0.15
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE2	2	0.15	0.03	0.15
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE3	2	0.15	0.03	0.15
(1,1299)	2:154:B:ALA:HA	2:155:B:GLU:H	2	0.14	0.0	0.14
(1,2640)	1:87:A:MET:HB3	1:87:A:MET:HG2	2	0.14	0.04	0.14
(1,2640)	1:87:A:MET:HB2	1:87:A:MET:HG2	2	0.14	0.04	0.14
(1,2963)	1:110:A:GLU:HA	1:113:A:GLN:HG3	2	0.14	0.01	0.14
(1,4208)	2:305:B:LEU:HG	2:305:B:LEU:H	2	0.14	0.02	0.14
(1,4493)	1:90:A:LEU:HD13	1:90:A:LEU:H	2	0.14	0.02	0.14
(1,4493)	1:90:A:LEU:HD12	1:90:A:LEU:H	2	0.14	0.02	0.14
(1,2721)	1:97:A:PRO:HD2	1:96:A:LEU:HA	2	0.13	0.02	0.13
(1,4173)	2:281:B:GLU:HA	2:285:B:ALA:H	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD11	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD12	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD13	2	0.13	0.02	0.13

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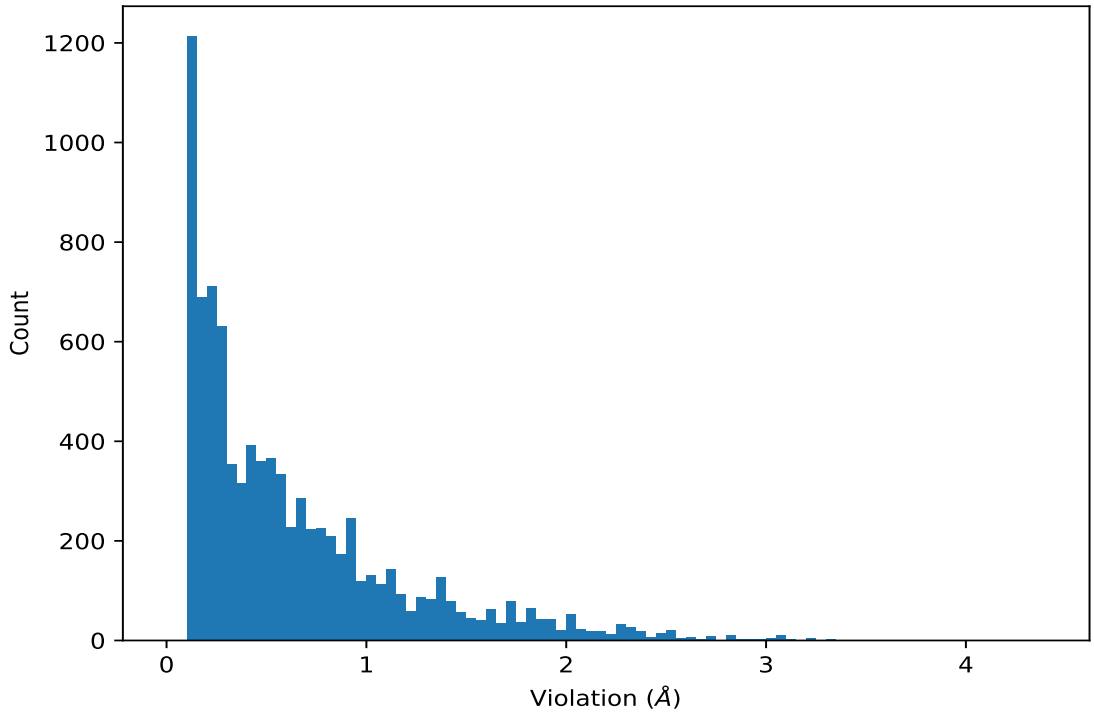
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD21	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD22	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD23	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD11	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD12	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD13	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD21	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD22	2	0.13	0.02	0.13
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD23	2	0.13	0.02	0.13
(1,4150)	2:263:B:LEU:HD22	2:263:B:LEU:H	2	0.12	0.02	0.12
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE1	2	0.12	0.01	0.12
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE2	2	0.12	0.01	0.12
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE3	2	0.12	0.01	0.12
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG21	2	0.12	0.01	0.12
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG22	2	0.12	0.01	0.12
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG23	2	0.12	0.01	0.12
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG21	2	0.12	0.01	0.12
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG22	2	0.12	0.01	0.12
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG23	2	0.12	0.01	0.12
(1,478)	2:218:B:VAL:HB	2:215:B:ASN:HA	2	0.12	0.02	0.12
(1,1337)	2:162:B:GLU:HB2	2:162:B:GLU:H	2	0.12	0.02	0.12
(1,2943)	1:107:A:LEU:HG	1:112:A:ILE:HG13	2	0.12	0.02	0.12
(1,2169)	2:282:B:LYS:HB2	2:283:B:SER:H	2	0.12	0.0	0.12
(1,664)	2:239:B:ARG:HA	2:239:B:ARG:HD3	2	0.11	0.01	0.11
(1,1978)	2:250:B:PRO:HA	2:251:B:ASP:H	2	0.11	0.0	0.11
(1,2155)	2:280:B:ASP:HB3	2:282:B:LYS:H	2	0.11	0.0	0.11
(1,2746)	1:98:A:PHE:HD1	1:97:A:PRO:HB3	2	0.11	0.0	0.11
(1,2746)	1:98:A:PHE:HD2	1:97:A:PRO:HB3	2	0.11	0.0	0.11
(1,4175)	2:284:B:LEU:HB3	2:285:B:ALA:H	2	0.11	0.0	0.11
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG21	2	0.11	0.01	0.11
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG22	2	0.11	0.01	0.11
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG23	2	0.11	0.01	0.11
(1,1232)	2:320:B:ARG:HB2	2:320:B:ARG:HD2	2	0.11	0.0	0.11
(1,2965)	1:113:A:GLN:HA	1:113:A:GLN:HG2	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3980)	2:164:B:LEU:HD23	2:295:B:LEU:HD23	16	4.39
(1,3842)	2:214:B:VAL:HG23	2:218:B:VAL:HG11	17	4.31
(1,3980)	2:164:B:LEU:HD22	2:295:B:LEU:HD22	12	4.29
(1,3842)	2:214:B:VAL:HG22	2:218:B:VAL:HG13	7	4.18
(1,3989)	2:190:B:VAL:HG22	2:298:B:LEU:HD13	12	4.07
(1,3842)	2:214:B:VAL:HG22	2:218:B:VAL:HG11	10	4.01
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD21	12	3.87
(1,4313)	1:87:A:MET:HE2	1:90:A:LEU:HD11	6	3.73
(1,3989)	2:190:B:VAL:HG21	2:298:B:LEU:HD12	9	3.57
(1,3989)	2:190:B:VAL:HG22	2:298:B:LEU:HD12	16	3.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	5	3.45
(1,3942)	2:233:B:LEU:HD22	2:270:B:ILE:HG21	10	3.37
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG22	3	3.31
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD22	16	3.31
(1,4442)	1:74:A:SER:HB3	1:76:A:VAL:HG21	6	3.3
(1,3842)	2:214:B:VAL:HG22	2:207:B:THR:HG21	8	3.24
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD21	9	3.24
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD12	11	3.23
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	20	3.2
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	2	3.19
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD12	9	3.15
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	4	3.13
(1,4296)	1:90:A:LEU:HD22	1:87:A:MET:HE2	17	3.11
(1,3980)	2:298:B:LEU:HD12	2:295:B:LEU:HD21	13	3.08
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	3	3.06
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	3	3.06
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	3	3.06
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	3	3.06
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	3	3.06
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	3	3.06
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	3	3.06
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	3	3.06
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	3	3.06
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	16	3.04
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	7	3.03
(1,4328)	1:95:A:ILE:HD13	1:92:A:GLU:HB2	18	3.02
(1,3945)	2:274:B:LEU:HD22	2:271:B:GLY:HA3	10	3.01
(1,3936)	2:265:B:ARG:HB2	2:269:B:ARG:HD2	19	2.99
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD11	20	2.97
(1,3842)	2:214:B:VAL:HG22	2:207:B:THR:HG21	15	2.96
(1,4296)	1:90:A:LEU:HD21	1:87:A:MET:HE3	2	2.93
(1,3945)	2:274:B:LEU:HD21	2:271:B:GLY:HA3	17	2.91
(1,3942)	2:274:B:LEU:HD21	2:270:B:ILE:HG21	2	2.9
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG21	17	2.88
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD11	13	2.87
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG23	4	2.83
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	8	2.82
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	8	2.82
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	8	2.82
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	8	2.82
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	8	2.82
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	8	2.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	8	2.82
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	8	2.82
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	8	2.82
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD22	13	2.77
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD21	11	2.74
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD22	11	2.74
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD23	11	2.74
(1,4442)	1:74:A:SER:HB3	1:76:A:VAL:HG23	8	2.73
(1,4269)	1:81:A:LEU:HD11	1:79:A:ASP:HA	15	2.73
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD12	10	2.72
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD11	2	2.72
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD23	3	2.7
(1,3989)	2:295:B:LEU:HD21	2:298:B:LEU:HD12	13	2.68
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD12	10	2.66
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD11	5	2.65
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	5	2.65
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	5	2.65
(1,4640)	2:267:B:PHE:HD1	2:168:B:LEU:HD23	1	2.6
(1,4269)	1:81:A:LEU:HD13	1:79:A:ASP:HA	10	2.6
(1,3989)	2:295:B:LEU:HD21	2:298:B:LEU:HD12	17	2.6
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD11	6	2.59
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD11	10	2.58
(1,3980)	2:298:B:LEU:HD11	2:295:B:LEU:HD22	3	2.58
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD12	14	2.56
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD12	14	2.54
(1,3988)	2:263:B:LEU:HD12	2:298:B:LEU:HD11	12	2.53
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD11	8	2.5
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	1	2.5
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	1	2.5
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	1	2.5
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	1	2.5
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	1	2.5
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	1	2.5
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	17	2.5
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	17	2.5
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	17	2.5
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	11	2.5
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	11	2.5
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	11	2.5
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	11	2.5
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	11	2.5
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	11	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	11	2.5
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	11	2.5
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	11	2.5
(1,3936)	2:268:B:VAL:HG22	2:269:B:ARG:HD2	20	2.49
(1,3945)	2:274:B:LEU:HD22	2:271:B:GLY:HA3	6	2.46
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	14	2.46
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	14	2.46
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	14	2.46
(1,1465)	2:174:B:LEU:HD11	2:180:B:GLN:HE22	13	2.46
(1,1465)	2:174:B:LEU:HD12	2:180:B:GLN:HE22	13	2.46
(1,1465)	2:174:B:LEU:HD13	2:180:B:GLN:HE22	13	2.46
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	3	2.46
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	3	2.46
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	3	2.46
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG21	18	2.45
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD11	20	2.45
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	20	2.45
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	20	2.45
(1,4054)	2:313:B:VAL:HG13	2:180:B:GLN:HE22	2	2.44
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD22	8	2.43
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	5	2.42
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	2	2.42
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	2	2.42
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	2	2.42
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD11	9	2.4
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	13	2.4
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	13	2.4
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	13	2.4
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	17	2.39
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	17	2.39
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	17	2.39
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	11	2.38
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	11	2.38
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	11	2.38
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	11	2.38
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	11	2.38
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	11	2.38
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	8	2.38
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	8	2.38
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	8	2.38
(1,4027)	2:321:B:LYS:HA	2:323:B:VAL:HG22	6	2.37
(1,3911)	2:252:B:ALA:HB3	2:257:B:VAL:HG13	20	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3950)	2:270:B:ILE:HG21	2:274:B:LEU:HD23	13	2.34
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	9	2.34
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	9	2.34
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	9	2.34
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	9	2.34
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	9	2.34
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	9	2.34
(1,336)	2:263:B:LEU:HB2	2:190:B:VAL:HG21	11	2.34
(1,336)	2:263:B:LEU:HB2	2:190:B:VAL:HG22	11	2.34
(1,336)	2:263:B:LEU:HB2	2:190:B:VAL:HG23	11	2.34
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	9	2.33
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	9	2.33
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	9	2.33
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	9	2.33
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	9	2.33
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	9	2.33
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	2	2.33
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	2	2.33
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	2	2.33
(1,2287)	2:305:B:LEU:HD21	2:301:B:ASN:H	12	2.32
(1,2287)	2:305:B:LEU:HD22	2:301:B:ASN:H	12	2.32
(1,2287)	2:305:B:LEU:HD23	2:301:B:ASN:H	12	2.32
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	20	2.31
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	20	2.31
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	20	2.31
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	20	2.31
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	20	2.31
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	20	2.31
(1,4269)	1:76:A:VAL:HG21	1:79:A:ASP:HA	7	2.3
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG23	18	2.3
(1,4028)	2:279:B:LEU:HD22	2:277:B:THR:HB	11	2.29
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	17	2.29
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	17	2.29
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	17	2.29
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	17	2.29
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	17	2.29
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	17	2.29
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	6	2.29
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	6	2.29
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	6	2.29
(1,3950)	2:279:B:LEU:HD22	2:274:B:LEU:HD22	17	2.28
(1,3935)	2:268:B:VAL:HG22	2:269:B:ARG:HD3	15	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	12	2.28
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD21	5	2.28
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD22	5	2.28
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD23	5	2.28
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	4	2.27
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	4	2.27
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	4	2.27
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	4	2.27
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	4	2.27
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	4	2.27
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG21	20	2.27
(1,4269)	1:76:A:VAL:HG23	1:79:A:ASP:HA	20	2.27
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	5	2.27
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	5	2.27
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	5	2.27
(1,4312)	1:73:A:PRO:HB3	1:96:A:LEU:HD11	10	2.26
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	20	2.25
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	20	2.25
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	20	2.25
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	13	2.23
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	16	2.23
(1,3443)	2:227:B:VAL:HG21	1:100:A:ASN:HD22	12	2.22
(1,3443)	2:227:B:VAL:HG22	1:100:A:ASN:HD22	12	2.22
(1,3443)	2:227:B:VAL:HG23	1:100:A:ASN:HD22	12	2.22
(1,4333)	1:90:A:LEU:HD21	1:93:A:SER:HA	3	2.21
(1,3918)	2:298:B:LEU:HD13	2:263:B:LEU:HD13	16	2.21
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	3	2.21
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	3	2.21
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	3	2.21
(1,4534)	2:183:B:TYR:HD1	2:238:B:GLU:HB2	14	2.2
(1,4269)	1:76:A:VAL:HG22	1:79:A:ASP:HA	16	2.2
(1,3935)	2:268:B:VAL:HG23	2:269:B:ARG:HD3	4	2.2
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	14	2.19
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	14	2.19
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	14	2.19
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	14	2.19
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	14	2.19
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	14	2.19
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG11	7	2.18
(1,3989)	2:295:B:LEU:HD22	2:298:B:LEU:HD11	3	2.18
(1,4333)	1:95:A:ILE:HG21	1:93:A:SER:HA	8	2.17
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	6	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	6	2.17
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	6	2.17
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	6	2.17
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	6	2.17
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	6	2.17
(1,4269)	1:76:A:VAL:HG23	1:79:A:ASP:HA	18	2.16
(1,4054)	2:313:B:VAL:HG11	2:180:B:GLN:HE22	11	2.16
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD22	5	2.15
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD12	15	2.14
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	20	2.13
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	20	2.13
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	20	2.13
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	20	2.13
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	20	2.13
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	20	2.13
(1,3950)	2:270:B:ILE:HG22	2:274:B:LEU:HD21	4	2.13
(2,59)	1:78:A:TRP:HH2	1:76:A:VAL:HG13	6	2.12
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	15	2.11
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG13	15	2.11
(1,4372)	1:112:A:ILE:HG13	1:107:A:LEU:HD21	15	2.11
(1,3989)	2:295:B:LEU:HD23	2:298:B:LEU:HD12	20	2.11
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD22	8	2.1
(1,4333)	1:90:A:LEU:HD21	1:93:A:SER:HA	5	2.1
(1,4269)	1:76:A:VAL:HG22	1:79:A:ASP:HA	12	2.1
(1,3950)	2:270:B:ILE:HG22	2:274:B:LEU:HD23	16	2.1
(1,3945)	2:274:B:LEU:HD21	2:271:B:GLY:HA3	4	2.1
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	2	2.09
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD11	4	2.09
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD22	6	2.09
(1,3795)	2:194:B:LEU:HD23	2:190:B:VAL:HG11	11	2.09
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG13	9	2.08
(1,4027)	2:321:B:LYS:HA	2:323:B:VAL:HG21	8	2.08
(1,3989)	2:295:B:LEU:HD21	2:298:B:LEU:HD12	8	2.08
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	9	2.08
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	9	2.08
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	9	2.08
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	14	2.07
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	14	2.07
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	14	2.07
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	14	2.07
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	14	2.07
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	14	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	14	2.07
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	14	2.07
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	14	2.07
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	12	2.06
(1,3842)	2:214:B:VAL:HG21	2:207:B:THR:HG23	11	2.06
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	4	2.06
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	4	2.06
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	4	2.06
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	12	2.05
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	12	2.05
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	12	2.05
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	12	2.05
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	12	2.05
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	12	2.05
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	6	2.05
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	6	2.05
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	6	2.05
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	6	2.05
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	6	2.05
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	6	2.05
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	6	2.05
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	6	2.05
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	6	2.05
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG11	8	2.04
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	9	2.04
(1,4497)	2:292:B:HIS:HE1	2:158:B:VAL:HG23	9	2.04
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG13	17	2.04
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG21	13	2.04
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	19	2.04
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	19	2.04
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	19	2.04
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	19	2.04
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	19	2.04
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	19	2.04
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	19	2.04
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	19	2.04
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	19	2.04
(1,4534)	2:183:B:TYR:HD2	2:238:B:GLU:HB2	17	2.03
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	18	2.03
(1,3935)	2:268:B:VAL:HG21	2:269:B:ARG:HD3	19	2.03
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	2	2.03
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	2	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	2	2.03
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	11	2.03
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	11	2.03
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	11	2.03
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG11	10	2.01
(1,3988)	2:263:B:LEU:HD13	2:298:B:LEU:HD13	16	2.01
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	20	2.01
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	20	2.01
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	20	2.01
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD21	10	2.0
(1,4296)	1:90:A:LEU:HD11	1:87:A:MET:HE3	1	2.0
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD11	3	2.0
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD12	3	2.0
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD13	3	2.0
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	5	2.0
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	5	2.0
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	5	2.0
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	5	2.0
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	5	2.0
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	5	2.0
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG21	8	1.99
(1,4333)	1:95:A:ILE:HG21	1:93:A:SER:HA	10	1.99
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG11	11	1.99
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG12	11	1.99
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG13	11	1.99
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG11	18	1.98
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG13	13	1.98
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD12	2	1.98
(1,4269)	1:81:A:LEU:HD11	1:79:A:ASP:HA	4	1.98
(1,4333)	2:279:B:LEU:HD21	1:93:A:SER:HA	20	1.97
(1,3936)	2:268:B:VAL:HG23	2:269:B:ARG:HD2	12	1.97
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	20	1.97
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	20	1.97
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	20	1.97
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	20	1.97
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	20	1.97
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	20	1.97
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	20	1.97
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	20	1.97
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	20	1.97
(1,4333)	1:90:A:LEU:HD21	1:93:A:SER:HA	12	1.96
(1,4333)	1:95:A:ILE:HG23	1:93:A:SER:HA	16	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	11	1.95
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD23	5	1.95
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	11	1.95
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	11	1.95
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	11	1.95
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	12	1.95
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	12	1.95
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	12	1.95
(1,2287)	2:305:B:LEU:HD21	2:301:B:ASN:H	8	1.95
(1,2287)	2:305:B:LEU:HD22	2:301:B:ASN:H	8	1.95
(1,2287)	2:305:B:LEU:HD23	2:301:B:ASN:H	8	1.95
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	2	1.95
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	2	1.95
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	2	1.95
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG13	4	1.94
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG11	10	1.94
(1,4282)	1:87:A:MET:HE3	1:83:A:THR:HG23	11	1.94
(1,2811)	1:106:A:VAL:HG11	1:104:A:ASN:HB3	14	1.94
(1,2811)	1:106:A:VAL:HG12	1:104:A:ASN:HB3	14	1.94
(1,2811)	1:106:A:VAL:HG13	1:104:A:ASN:HB3	14	1.94
(1,2293)	2:305:B:LEU:HD21	2:302:B:SER:H	12	1.94
(1,2293)	2:305:B:LEU:HD22	2:302:B:SER:H	12	1.94
(1,2293)	2:305:B:LEU:HD23	2:302:B:SER:H	12	1.94
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	3	1.94
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG13	16	1.93
(1,4282)	1:87:A:MET:HE1	1:83:A:THR:HG23	10	1.93
(1,3980)	2:164:B:LEU:HD22	2:295:B:LEU:HD21	6	1.93
(1,3842)	2:214:B:VAL:HG23	2:207:B:THR:HG21	9	1.93
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	4	1.93
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	4	1.93
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	4	1.93
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD11	10	1.93
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	10	1.93
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	10	1.93
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG13	3	1.92
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG11	7	1.92
(1,3421)	2:236:B:LYS:HE2	1:104:A:ASN:HD22	17	1.92
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG12	11	1.91
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG11	20	1.91
(1,4333)	1:95:A:ILE:HG23	1:93:A:SER:HA	11	1.91
(1,4054)	2:313:B:VAL:HG11	2:180:B:GLN:HE22	5	1.91
(1,239)	2:238:B:GLU:HA	2:181:B:LEU:HD11	6	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	2:238:B:GLU:HA	2:181:B:LEU:HD12	6	1.91
(1,239)	2:238:B:GLU:HA	2:181:B:LEU:HD13	6	1.91
(1,4333)	1:90:A:LEU:HD21	1:93:A:SER:HA	18	1.9
(1,4054)	2:313:B:VAL:HG12	2:180:B:GLN:HE22	10	1.9
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG11	4	1.9
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG12	4	1.9
(1,485)	1:78:A:TRP:HZ2	2:217:B:VAL:HG13	4	1.9
(1,4328)	2:279:B:LEU:HD21	1:94:A:GLU:HB2	1	1.89
(1,4269)	1:76:A:VAL:HG23	1:79:A:ASP:HA	13	1.89
(1,3935)	2:268:B:VAL:HG23	2:269:B:ARG:HD3	16	1.89
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	5	1.89
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	5	1.89
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	5	1.89
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD21	15	1.89
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD22	15	1.89
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD23	15	1.89
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG11	1	1.88
(1,3989)	2:295:B:LEU:HD21	2:298:B:LEU:HD12	5	1.88
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	5	1.88
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	5	1.88
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	5	1.88
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	5	1.88
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	5	1.88
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	5	1.88
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	6	1.87
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	6	1.87
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	6	1.87
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	11	1.86
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG13	2	1.86
(1,4282)	1:87:A:MET:HE1	1:83:A:THR:HG23	15	1.86
(1,3918)	2:193:B:ILE:HD13	2:263:B:LEU:HD13	12	1.86
(1,3419)	2:236:B:LYS:HD3	1:104:A:ASN:HD22	14	1.86
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	7	1.86
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	7	1.86
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	7	1.86
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	7	1.85
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	7	1.85
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	7	1.85
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	7	1.85
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	7	1.85
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	7	1.85
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB3	1	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD13	14	1.85
(1,4333)	1:90:A:LEU:HD13	1:93:A:SER:HA	9	1.85
(1,3936)	2:268:B:VAL:HG21	2:269:B:ARG:HD2	5	1.85
(2,261)	2:227:B:VAL:HG11	1:98:A:PHE:HE2	7	1.84
(2,259)	2:227:B:VAL:HG11	1:98:A:PHE:HE2	7	1.84
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG22	12	1.84
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG13	15	1.84
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	10	1.84
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	10	1.84
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	10	1.84
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	10	1.84
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	10	1.84
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	10	1.84
(1,4282)	1:87:A:MET:HE1	1:83:A:THR:HG23	20	1.84
(1,3935)	2:265:B:ARG:HB2	2:269:B:ARG:HD3	9	1.84
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	12	1.84
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	12	1.84
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	12	1.84
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	9	1.84
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	9	1.84
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	9	1.84
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	9	1.84
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	9	1.84
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	9	1.84
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	9	1.84
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	9	1.84
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	9	1.84
(1,4333)	2:279:B:LEU:HD22	1:93:A:SER:HA	4	1.83
(1,3950)	2:279:B:LEU:HD22	2:274:B:LEU:HD22	10	1.83
(1,3942)	2:274:B:LEU:HD21	2:270:B:ILE:HG22	4	1.83
(1,3935)	2:268:B:VAL:HG21	2:269:B:ARG:HD3	5	1.83
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	13	1.83
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	13	1.83
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	13	1.83
(1,4505)	2:311:B:TYR:HD2	2:181:B:LEU:HD21	20	1.82
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG22	11	1.82
(1,4333)	1:95:A:ILE:HG23	1:93:A:SER:HA	1	1.82
(1,4282)	1:87:A:MET:HE2	1:83:A:THR:HG23	19	1.82
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	10	1.82
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	10	1.82
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	10	1.82
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	14	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	14	1.81
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	14	1.81
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	9	1.81
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	9	1.81
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	9	1.81
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	16	1.81
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	16	1.81
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	16	1.81
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	4	1.81
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	4	1.81
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	4	1.81
(1,4589)	2:182:B:PHE:HD2	2:259:B:GLY:HA2	6	1.8
(1,4343)	1:93:A:SER:HB3	1:95:A:ILE:HD12	5	1.8
(1,4316)	1:87:A:MET:HE3	1:90:A:LEU:HD23	18	1.8
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG22	16	1.8
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	10	1.8
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	10	1.8
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	10	1.8
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG21	14	1.8
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG22	14	1.8
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG23	14	1.8
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG21	14	1.8
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG22	14	1.8
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG23	14	1.8
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG21	14	1.8
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG22	14	1.8
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG23	14	1.8
(1,4534)	2:183:B:TYR:HD2	2:238:B:GLU:HB2	12	1.79
(1,3942)	2:274:B:LEU:HD22	2:270:B:ILE:HG23	6	1.79
(1,3935)	2:265:B:ARG:HB2	2:269:B:ARG:HD3	2	1.79
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG21	6	1.79
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	12	1.79
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	12	1.79
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	12	1.79
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	4	1.79
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	4	1.79
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	4	1.79
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG21	5	1.78
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD23	3	1.78
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	19	1.78
(1,4363)	2:235:B:TYR:HD1	1:106:A:VAL:HG22	18	1.78
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	3	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3724)	2:271:B:GLY:HA3	2:156:B:VAL:HG12	15	1.78
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	14	1.78
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	14	1.78
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	14	1.78
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	14	1.78
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	14	1.78
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	14	1.78
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD11	12	1.78
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD12	12	1.78
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD13	12	1.78
(1,4282)	1:87:A:MET:HE3	1:83:A:THR:HG22	3	1.77
(1,4269)	1:76:A:VAL:HG21	1:79:A:ASP:HA	19	1.77
(1,3967)	2:224:B:TYR:HA	2:266:B:LEU:HD12	10	1.77
(1,3935)	2:268:B:VAL:HG23	2:269:B:ARG:HD3	12	1.77
(1,4282)	1:87:A:MET:HE3	1:83:A:THR:HG21	2	1.76
(1,4282)	1:87:A:MET:HE3	1:83:A:THR:HG22	7	1.76
(1,4054)	2:313:B:VAL:HG11	2:180:B:GLN:HE22	8	1.76
(1,4054)	2:313:B:VAL:HG13	2:180:B:GLN:HE22	20	1.76
(1,2808)	1:106:A:VAL:HG11	1:104:A:ASN:HA	20	1.76
(1,2808)	1:106:A:VAL:HG12	1:104:A:ASN:HA	20	1.76
(1,2808)	1:106:A:VAL:HG13	1:104:A:ASN:HA	20	1.76
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD12	9	1.75
(1,4269)	1:76:A:VAL:HG23	1:79:A:ASP:HA	8	1.75
(1,4333)	2:279:B:LEU:HD21	1:93:A:SER:HA	15	1.74
(1,4282)	1:87:A:MET:HE1	1:83:A:THR:HG21	12	1.74
(1,4054)	2:313:B:VAL:HG11	2:180:B:GLN:HE22	16	1.74
(1,3980)	2:298:B:LEU:HD12	2:295:B:LEU:HD21	1	1.74
(1,3936)	2:268:B:VAL:HG23	2:269:B:ARG:HD2	11	1.74
(1,3901)	2:257:B:VAL:HG21	2:252:B:ALA:HB1	18	1.74
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	16	1.74
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	16	1.74
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	16	1.74
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	16	1.74
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	16	1.74
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	16	1.74
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	16	1.74
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	16	1.74
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	16	1.74
(1,2811)	1:106:A:VAL:HG11	1:104:A:ASN:HB3	13	1.74
(1,2811)	1:106:A:VAL:HG12	1:104:A:ASN:HB3	13	1.74
(1,2811)	1:106:A:VAL:HG13	1:104:A:ASN:HB3	13	1.74
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	5	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	5	1.74
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	5	1.74
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	5	1.74
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	5	1.74
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	5	1.74
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	5	1.74
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	5	1.74
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	5	1.74
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG22	9	1.73
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	16	1.73
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	16	1.73
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	16	1.73
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	16	1.73
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	16	1.73
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	16	1.73
(1,4343)	1:74:A:SER:HB2	1:95:A:ILE:HD12	12	1.73
(1,4282)	1:87:A:MET:HE1	1:83:A:THR:HG22	1	1.73
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	7	1.73
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	7	1.73
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	7	1.73
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	7	1.73
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	7	1.73
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	7	1.73
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	7	1.73
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	7	1.73
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	7	1.73
(1,2287)	2:305:B:LEU:HD21	2:301:B:ASN:H	11	1.73
(1,2287)	2:305:B:LEU:HD22	2:301:B:ASN:H	11	1.73
(1,2287)	2:305:B:LEU:HD23	2:301:B:ASN:H	11	1.73
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	6	1.73
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	6	1.73
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	6	1.73
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	13	1.72
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	13	1.72
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	13	1.72
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	13	1.72
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	13	1.72
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	13	1.72
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG13	20	1.72
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG21	5	1.72
(1,3875)	2:242:B:TYR:HB3	2:234:B:LEU:HD23	11	1.72
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	8	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	8	1.72
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	8	1.72
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD21	16	1.72
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG22	2	1.71
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG22	17	1.71
(1,4555)	2:294:B:PHE:HD2	2:217:B:VAL:HG13	19	1.71
(1,4363)	2:172:B:TRP:HD1	1:106:A:VAL:HG21	19	1.71
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	15	1.71
(1,4269)	1:76:A:VAL:HG22	1:79:A:ASP:HA	9	1.71
(1,3774)	2:245:B:ILE:HG12	2:184:B:LEU:HD22	1	1.71
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	16	1.71
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	16	1.71
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	16	1.71
(1,2287)	2:305:B:LEU:HD21	2:301:B:ASN:H	16	1.71
(1,2287)	2:305:B:LEU:HD22	2:301:B:ASN:H	16	1.71
(1,2287)	2:305:B:LEU:HD23	2:301:B:ASN:H	16	1.71
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	11	1.71
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	11	1.71
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	11	1.71
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG23	14	1.7
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	12	1.69
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	12	1.69
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	12	1.69
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	12	1.69
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	12	1.69
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	12	1.69
(1,4269)	1:76:A:VAL:HG21	1:79:A:ASP:HA	11	1.69
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD11	13	1.69
(1,3988)	2:263:B:LEU:HD12	2:298:B:LEU:HD11	14	1.69
(1,3795)	2:221:B:ILE:HG22	2:190:B:VAL:HG13	14	1.69
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	11	1.69
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	11	1.69
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	11	1.69
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	2	1.69
(1,2812)	1:106:A:VAL:HG11	1:104:A:ASN:HB2	12	1.68
(1,2812)	1:106:A:VAL:HG12	1:104:A:ASN:HB2	12	1.68
(1,2812)	1:106:A:VAL:HG13	1:104:A:ASN:HB2	12	1.68
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	17	1.68
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	17	1.68
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	17	1.68
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG23	13	1.67
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	15	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	17	1.67
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	17	1.67
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	17	1.67
(2,59)	1:78:A:TRP:HZ3	1:76:A:VAL:HG21	19	1.66
(1,4505)	2:311:B:TYR:HD1	2:181:B:LEU:HD22	7	1.66
(1,4421)	1:111:A:ILE:HD12	1:110:A:GLU:HB2	20	1.66
(1,4343)	1:93:A:SER:HB2	1:95:A:ILE:HD11	13	1.66
(1,4269)	1:76:A:VAL:HG23	1:79:A:ASP:HA	17	1.66
(1,4243)	1:72:A:VAL:HG21	1:71:A:GLN:HB2	4	1.66
(1,677)	2:234:B:LEU:HD21	2:239:B:ARG:HG3	11	1.66
(1,677)	2:234:B:LEU:HD22	2:239:B:ARG:HG3	11	1.66
(1,677)	2:234:B:LEU:HD23	2:239:B:ARG:HG3	11	1.66
(1,4444)	2:273:B:MET:HB3	1:96:A:LEU:HD13	4	1.65
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD23	14	1.65
(1,4282)	1:87:A:MET:HE2	1:83:A:THR:HG23	8	1.65
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG23	5	1.65
(1,3875)	2:242:B:TYR:HB3	2:234:B:LEU:HD22	20	1.65
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	2	1.65
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	2	1.65
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	2	1.65
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	1	1.65
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	1	1.65
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	1	1.65
(1,4604)	2:225:B:PHE:HE2	2:229:B:LEU:HG	10	1.64
(1,4314)	2:283:B:SER:HB2	1:90:A:LEU:HD22	17	1.64
(1,4312)	1:73:A:PRO:HB3	1:96:A:LEU:HD13	12	1.64
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD23	10	1.64
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	7	1.64
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	7	1.64
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	7	1.64
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	6	1.64
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	6	1.64
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	6	1.64
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	9	1.64
(1,4575)	2:242:B:TYR:HE2	2:246:B:LEU:HD13	17	1.63
(1,4243)	1:115:A:VAL:HG22	1:114:A:GLU:HB2	8	1.63
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	1	1.63
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	1	1.63
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	1	1.63
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	1	1.63
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	1	1.63
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	1	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4555)	2:294:B:PHE:HD2	2:264:B:LEU:HD11	10	1.62
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD13	11	1.62
(1,4269)	1:76:A:VAL:HG23	1:79:A:ASP:HA	3	1.62
(1,3989)	2:295:B:LEU:HD23	2:298:B:LEU:HD12	6	1.62
(1,2293)	2:305:B:LEU:HD21	2:302:B:SER:H	8	1.62
(1,2293)	2:305:B:LEU:HD22	2:302:B:SER:H	8	1.62
(1,2293)	2:305:B:LEU:HD23	2:302:B:SER:H	8	1.62
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	15	1.61
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	15	1.61
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	15	1.61
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	15	1.61
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	15	1.61
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	15	1.61
(1,4421)	1:111:A:ILE:HD12	1:110:A:GLU:HB2	11	1.61
(1,4316)	1:87:A:MET:HE1	1:90:A:LEU:HD22	6	1.61
(1,4269)	1:81:A:LEU:HD12	1:79:A:ASP:HA	5	1.61
(1,3936)	2:268:B:VAL:HG21	2:269:B:ARG:HD2	6	1.61
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG23	9	1.61
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB2	15	1.6
(1,4333)	1:90:A:LEU:HD12	1:93:A:SER:HA	7	1.6
(1,4269)	1:76:A:VAL:HG21	1:79:A:ASP:HA	6	1.6
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG23	12	1.6
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD22	6	1.6
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	6	1.6
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	6	1.6
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	6	1.6
(1,2293)	2:305:B:LEU:HD21	2:302:B:SER:H	11	1.6
(1,2293)	2:305:B:LEU:HD22	2:302:B:SER:H	11	1.6
(1,2293)	2:305:B:LEU:HD23	2:302:B:SER:H	11	1.6
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	20	1.6
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	20	1.6
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	20	1.6
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD21	10	1.6
(1,3918)	2:193:B:ILE:HD13	2:263:B:LEU:HD13	14	1.59
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	14	1.59
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	14	1.59
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	14	1.59
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	14	1.59
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	14	1.59
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	14	1.59
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	10	1.59
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	10	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	10	1.59
(1,158)	2:311:B:TYR:HD1	2:174:B:LEU:HD22	20	1.59
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	3	1.58
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	3	1.58
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	3	1.58
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	3	1.58
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	3	1.58
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	3	1.58
(1,4421)	1:111:A:ILE:HD11	1:110:A:GLU:HB2	13	1.58
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG22	11	1.58
(1,4343)	1:93:A:SER:HB2	1:95:A:ILE:HD12	6	1.58
(1,4312)	1:73:A:PRO:HB3	1:96:A:LEU:HD12	1	1.58
(1,4282)	1:88:A:GLN:HB2	1:83:A:THR:HG23	4	1.58
(1,3911)	2:252:B:ALA:HB3	2:257:B:VAL:HG11	11	1.58
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG11	19	1.57
(1,4421)	1:111:A:ILE:HD12	1:110:A:GLU:HB2	14	1.57
(1,3936)	2:268:B:VAL:HG21	2:269:B:ARG:HD2	2	1.57
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD21	16	1.57
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD22	16	1.57
(1,3654)	2:297:B:TYR:HE1	2:298:B:LEU:HD23	16	1.57
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD21	16	1.57
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD22	16	1.57
(1,3654)	2:297:B:TYR:HE2	2:298:B:LEU:HD23	16	1.57
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG12	12	1.56
(1,4054)	2:313:B:VAL:HG12	2:180:B:GLN:HE22	18	1.56
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	20	1.56
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	20	1.56
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	20	1.56
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD11	6	1.55
(1,4328)	2:279:B:LEU:HD22	1:94:A:GLU:HB2	12	1.55
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	5	1.55
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	5	1.55
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	5	1.55
(1,4421)	1:111:A:ILE:HD11	1:110:A:GLU:HB2	2	1.54
(1,4243)	1:115:A:VAL:HG23	1:114:A:GLU:HB2	3	1.54
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD11	15	1.54
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD23	9	1.54
(1,3491)	2:237:B:PHE:HD1	2:181:B:LEU:HD11	6	1.54
(1,3491)	2:237:B:PHE:HD1	2:181:B:LEU:HD12	6	1.54
(1,3491)	2:237:B:PHE:HD1	2:181:B:LEU:HD13	6	1.54
(1,3491)	2:237:B:PHE:HD2	2:181:B:LEU:HD11	6	1.54
(1,3491)	2:237:B:PHE:HD2	2:181:B:LEU:HD12	6	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3491)	2:237:B:PHE:HD2	2:181:B:LEU:HD13	6	1.54
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	5	1.54
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	5	1.54
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	5	1.54
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD12	16	1.53
(1,4333)	1:90:A:LEU:HD12	1:93:A:SER:HA	13	1.53
(1,4243)	1:115:A:VAL:HG21	1:114:A:GLU:HB2	18	1.53
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG23	2	1.53
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD21	13	1.53
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD22	13	1.53
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD23	13	1.53
(1,158)	2:311:B:TYR:HD1	2:174:B:LEU:HD21	7	1.53
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	7	1.52
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG12	11	1.52
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG22	15	1.52
(1,2775)	1:96:A:LEU:HD11	1:100:A:ASN:HB3	3	1.52
(1,2775)	1:96:A:LEU:HD12	1:100:A:ASN:HB3	3	1.52
(1,2775)	1:96:A:LEU:HD13	1:100:A:ASN:HB3	3	1.52
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD21	11	1.52
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD22	11	1.52
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD23	11	1.52
(1,4555)	2:294:B:PHE:HD1	2:214:B:VAL:HG13	16	1.51
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD13	16	1.51
(1,4421)	1:111:A:ILE:HD11	1:110:A:GLU:HB2	10	1.51
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD11	10	1.51
(1,4027)	2:320:B:ARG:HA	2:323:B:VAL:HG23	15	1.51
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG21	10	1.51
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	2	1.51
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	2	1.51
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	2	1.51
(1,4520)	2:237:B:PHE:HE1	2:179:B:LYS:HE3	13	1.5
(1,4505)	2:311:B:TYR:HD1	2:181:B:LEU:HD21	3	1.5
(1,4333)	1:90:A:LEU:HD13	1:93:A:SER:HA	14	1.5
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	14	1.5
(1,4312)	1:94:A:GLU:HG3	1:90:A:LEU:HD12	8	1.5
(1,4282)	1:87:A:MET:HE2	1:83:A:THR:HG22	13	1.5
(1,3837)	2:198:B:ALA:HB3	2:214:B:VAL:HG21	5	1.5
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG22	6	1.49
(1,4243)	1:115:A:VAL:HG23	1:114:A:GLU:HB2	2	1.49
(1,3724)	2:271:B:GLY:HA3	2:156:B:VAL:HG11	5	1.49
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	6	1.49
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	6	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	6	1.49
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HB3	7	1.48
(1,4054)	2:313:B:VAL:HG11	2:180:B:GLN:HE22	19	1.48
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD22	12	1.48
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	7	1.48
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	7	1.48
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	7	1.48
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD21	7	1.47
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HB3	6	1.47
(1,4279)	1:88:A:GLN:HG2	1:90:A:LEU:HD22	20	1.47
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	9	1.47
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	9	1.47
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	9	1.47
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	9	1.47
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	9	1.47
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	9	1.47
(1,2287)	2:305:B:LEU:HD21	2:301:B:ASN:H	13	1.47
(1,2287)	2:305:B:LEU:HD22	2:301:B:ASN:H	13	1.47
(1,2287)	2:305:B:LEU:HD23	2:301:B:ASN:H	13	1.47
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	9	1.47
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	9	1.47
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	9	1.47
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG21	16	1.47
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG22	16	1.47
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG23	16	1.47
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG21	16	1.47
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG22	16	1.47
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG23	16	1.47
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG21	16	1.47
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG22	16	1.47
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG23	16	1.47
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	17	1.47
(1,4269)	1:76:A:VAL:HG23	1:79:A:ASP:HA	1	1.46
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	5	1.46
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	5	1.46
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	5	1.46
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	5	1.46
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	5	1.46
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	5	1.46
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	5	1.46
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	5	1.46
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	5	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	9	1.46
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	9	1.46
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	9	1.46
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG2	20	1.46
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG2	20	1.46
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG2	20	1.46
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	19	1.46
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	19	1.46
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	19	1.46
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	11	1.46
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD12	13	1.45
(1,4363)	2:172:B:TRP:HD1	1:106:A:VAL:HG21	11	1.45
(1,4296)	2:279:B:LEU:HD13	1:87:A:MET:HE2	15	1.45
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD23	3	1.45
(1,4269)	1:76:A:VAL:HG21	1:79:A:ASP:HA	14	1.45
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	20	1.45
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	20	1.45
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	20	1.45
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	20	1.45
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	20	1.45
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	20	1.45
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG22	1	1.44
(1,4421)	1:111:A:ILE:HD11	1:110:A:GLU:HB2	12	1.44
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG22	1	1.44
(1,4337)	1:73:A:PRO:HB3	1:74:A:SER:HB2	5	1.44
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD22	14	1.44
(1,4243)	1:115:A:VAL:HG22	1:114:A:GLU:HB2	5	1.44
(1,4054)	2:313:B:VAL:HG12	2:180:B:GLN:HE22	15	1.44
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	12	1.44
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	12	1.44
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	12	1.44
(1,4385)	1:112:A:ILE:HG23	1:109:A:GLU:HB3	19	1.43
(1,4282)	1:87:A:MET:HE2	1:83:A:THR:HG23	5	1.43
(1,3936)	2:265:B:ARG:HB2	2:269:B:ARG:HD2	15	1.43
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD11	15	1.43
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	15	1.43
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	15	1.43
(1,4333)	1:90:A:LEU:HD13	1:93:A:SER:HA	6	1.42
(1,3936)	2:268:B:VAL:HG21	2:269:B:ARG:HD2	10	1.42
(1,3935)	2:265:B:ARG:HB2	2:269:B:ARG:HD3	6	1.42
(1,333)	2:259:B:GLY:HA3	2:190:B:VAL:HG21	14	1.42
(1,333)	2:259:B:GLY:HA3	2:190:B:VAL:HG22	14	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	2:259:B:GLY:HA3	2:190:B:VAL:HG23	14	1.42
(2,5)	2:262:B:HIS:HD2	2:229:B:LEU:HD11	20	1.41
(2,5)	2:262:B:HIS:HD2	2:229:B:LEU:HD12	20	1.41
(2,5)	2:262:B:HIS:HD2	2:229:B:LEU:HD13	20	1.41
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB2	7	1.41
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD11	17	1.41
(1,4346)	1:94:A:GLU:HB3	1:95:A:ILE:HG21	13	1.41
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD21	8	1.41
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD23	16	1.41
(1,4028)	1:96:A:LEU:HD11	2:277:B:THR:HB	17	1.41
(1,3936)	2:265:B:ARG:HB2	2:269:B:ARG:HD2	9	1.41
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	2	1.41
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	2	1.41
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	2	1.41
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	7	1.41
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	7	1.41
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	7	1.41
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	6	1.41
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	6	1.41
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	6	1.41
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	14	1.41
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	14	1.41
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	14	1.41
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	3	1.41
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	3	1.41
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	3	1.41
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	6	1.41
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	6	1.41
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	6	1.41
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG21	3	1.41
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG22	3	1.41
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG23	3	1.41
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG21	3	1.41
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG22	3	1.41
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG23	3	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG21	3	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG22	3	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG23	3	1.41
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG21	8	1.41
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG22	8	1.41
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG23	8	1.41
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG21	8	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG22	8	1.41
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG23	8	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG21	8	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG22	8	1.41
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG23	8	1.41
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	20	1.4
(1,4421)	1:111:A:ILE:HD11	1:110:A:GLU:HB2	4	1.4
(1,4296)	1:90:A:LEU:HD11	1:87:A:MET:HE1	10	1.4
(1,3962)	2:156:B:VAL:HA	2:284:B:LEU:HD11	14	1.4
(1,3842)	2:214:B:VAL:HG23	2:207:B:THR:HG21	6	1.4
(1,3837)	2:198:B:ALA:HB3	2:214:B:VAL:HG23	14	1.4
(1,3745)	2:165:B:LYS:HA	2:164:B:LEU:HD22	20	1.4
(1,2812)	1:106:A:VAL:HG11	1:104:A:ASN:HB2	8	1.4
(1,2812)	1:106:A:VAL:HG12	1:104:A:ASN:HB2	8	1.4
(1,2812)	1:106:A:VAL:HG13	1:104:A:ASN:HB2	8	1.4
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	18	1.4
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	18	1.4
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	18	1.4
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	5	1.4
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	5	1.4
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	5	1.4
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	12	1.4
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	12	1.4
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	12	1.4
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	15	1.4
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	15	1.4
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	15	1.4
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD11	11	1.4
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD12	11	1.4
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD13	11	1.4
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD11	11	1.4
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD12	11	1.4
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD13	11	1.4
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD11	11	1.4
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD12	11	1.4
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD13	11	1.4
(1,4555)	2:294:B:PHE:HD2	2:217:B:VAL:HG11	13	1.39
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB2	6	1.39
(1,4243)	1:115:A:VAL:HG23	1:114:A:GLU:HB2	7	1.39
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	6	1.39
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	6	1.39
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	6	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	5	1.39
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	5	1.39
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	5	1.39
(1,2007)	2:226:B:ASN:HD21	2:255:B:SER:H	1	1.39
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	2	1.39
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	2	1.39
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	2	1.39
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	4	1.39
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	4	1.39
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	4	1.39
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	10	1.39
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	10	1.39
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	10	1.39
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	11	1.39
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	11	1.39
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	11	1.39
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	16	1.39
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	16	1.39
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	16	1.39
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG12	1	1.38
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB2	3	1.38
(1,4373)	2:169:B:VAL:HA	1:107:A:LEU:HD22	8	1.38
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD12	5	1.38
(1,4296)	2:279:B:LEU:HD13	1:87:A:MET:HE1	9	1.38
(1,3949)	2:302:B:SER:HB2	2:305:B:LEU:HD11	1	1.38
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	4	1.38
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	4	1.38
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	4	1.38
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	10	1.38
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	10	1.38
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	10	1.38
(1,1161)	2:180:B:GLN:HG2	2:313:B:VAL:HA	13	1.38
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	3	1.38
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	3	1.38
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	3	1.38
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	17	1.38
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	17	1.38
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	17	1.38
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	20	1.38
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	20	1.38
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	20	1.38
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	6	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	6	1.38
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	6	1.38
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	19	1.38
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB2	9	1.37
(1,4346)	1:72:A:VAL:HB	1:95:A:ILE:HG21	18	1.37
(1,4314)	1:74:A:SER:HB3	1:96:A:LEU:HD21	12	1.37
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	13	1.37
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD11	16	1.37
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD12	16	1.37
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD13	16	1.37
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	20	1.37
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	20	1.37
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	20	1.37
(1,3184)	1:90:A:LEU:HD21	1:89:A:ALA:H	1	1.37
(1,3184)	1:90:A:LEU:HD22	1:89:A:ALA:H	1	1.37
(1,3184)	1:90:A:LEU:HD23	1:89:A:ALA:H	1	1.37
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	15	1.37
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	15	1.37
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	15	1.37
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	7	1.37
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	7	1.37
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	7	1.37
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG11	1	1.36
(1,4269)	1:81:A:LEU:HD13	1:79:A:ASP:HA	2	1.36
(1,4243)	1:115:A:VAL:HG21	1:114:A:GLU:HB2	20	1.36
(1,3875)	2:242:B:TYR:HB3	2:234:B:LEU:HD23	15	1.36
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	13	1.36
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	13	1.36
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	13	1.36
(1,158)	2:311:B:TYR:HD1	2:174:B:LEU:HD23	1	1.36
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG11	8	1.35
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	8	1.35
(1,3852)	2:218:B:VAL:HG21	2:202:B:LYS:HE3	14	1.35
(1,3774)	2:245:B:ILE:HG12	2:184:B:LEU:HD22	11	1.35
(1,2051)	2:190:B:VAL:HG21	2:263:B:LEU:H	11	1.35
(1,2051)	2:190:B:VAL:HG22	2:263:B:LEU:H	11	1.35
(1,2051)	2:190:B:VAL:HG23	2:263:B:LEU:H	11	1.35
(1,1156)	2:313:B:VAL:HG11	2:312:B:GLU:HA	8	1.35
(1,1156)	2:313:B:VAL:HG12	2:312:B:GLU:HA	8	1.35
(1,1156)	2:313:B:VAL:HG13	2:312:B:GLU:HA	8	1.35
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	16	1.35
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	16	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	16	1.35
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	16	1.35
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	16	1.35
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	16	1.35
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	16	1.35
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	16	1.35
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	16	1.35
(2,261)	2:227:B:VAL:HG22	1:98:A:PHE:HD1	10	1.34
(2,259)	2:227:B:VAL:HG22	1:98:A:PHE:HD1	10	1.34
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	6	1.34
(1,4382)	1:111:A:ILE:HG12	1:108:A:PRO:HD3	11	1.34
(1,4243)	1:115:A:VAL:HG21	1:114:A:GLU:HB2	16	1.34
(1,3989)	2:295:B:LEU:HD21	2:298:B:LEU:HD12	1	1.34
(1,3936)	2:268:B:VAL:HG23	2:269:B:ARG:HD2	4	1.34
(1,3918)	2:298:B:LEU:HD13	2:263:B:LEU:HD12	8	1.34
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	6	1.34
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	6	1.34
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	6	1.34
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	6	1.34
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	6	1.34
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	6	1.34
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	3	1.34
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	3	1.34
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	3	1.34
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	3	1.34
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	3	1.34
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	3	1.34
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD11	11	1.34
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	11	1.34
(1,631)	2:262:B:HIS:HD2	2:234:B:LEU:HD13	11	1.34
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	7	1.33
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	7	1.33
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	7	1.33
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	7	1.33
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	7	1.33
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	7	1.33
(1,4520)	2:212:B:TYR:HD1	2:215:B:ASN:HB2	9	1.33
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE3	10	1.33
(1,4054)	2:313:B:VAL:HG12	2:180:B:GLN:HE22	17	1.33
(1,3842)	2:214:B:VAL:HG22	2:207:B:THR:HG21	1	1.33
(1,3803)	2:194:B:LEU:HD21	2:193:B:ILE:HG23	9	1.33
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	9	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	9	1.33
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	9	1.33
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	8	1.33
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	8	1.33
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	8	1.33
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	8	1.33
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	8	1.33
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	8	1.33
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	18	1.32
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG13	5	1.32
(1,4312)	1:94:A:GLU:HG2	1:90:A:LEU:HD11	3	1.32
(1,4237)	2:218:B:VAL:HG13	2:198:B:ALA:H	9	1.32
(1,4237)	2:218:B:VAL:HG11	2:198:B:ALA:H	17	1.32
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG23	16	1.32
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	5	1.32
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	5	1.32
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	5	1.32
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG13	4	1.31
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD12	8	1.31
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	7	1.31
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	7	1.31
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	7	1.31
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	7	1.31
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	7	1.31
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	7	1.31
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	7	1.31
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	7	1.31
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	7	1.31
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE2	2	1.3
(1,4520)	2:212:B:TYR:HD2	2:215:B:ASN:HB2	12	1.3
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD12	18	1.3
(1,4333)	1:95:A:ILE:HG22	1:93:A:SER:HA	19	1.3
(1,4313)	1:87:A:MET:HE3	1:90:A:LEU:HD11	1	1.3
(1,3967)	2:285:B:ALA:HA	2:288:B:LEU:HD11	5	1.3
(1,3857)	2:224:B:TYR:HD1	2:227:B:VAL:HG13	8	1.3
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD22	18	1.3
(1,3419)	2:236:B:LYS:HD3	1:104:A:ASN:HD22	13	1.3
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	16	1.3
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	16	1.3
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	16	1.3
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	1	1.3
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	1	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	1	1.3
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	13	1.3
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	13	1.3
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	13	1.3
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD21	4	1.3
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD22	4	1.3
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD23	4	1.3
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD12	16	1.29
(1,3852)	2:218:B:VAL:HG22	2:202:B:LYS:HE2	2	1.29
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	16	1.29
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	16	1.29
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	16	1.29
(1,4421)	1:111:A:ILE:HD12	1:110:A:GLU:HB2	18	1.28
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE3	1	1.28
(1,4282)	1:88:A:GLN:HB2	1:83:A:THR:HG21	18	1.28
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	17	1.28
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	17	1.28
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	17	1.28
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	17	1.28
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	17	1.28
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	17	1.28
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	13	1.28
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	13	1.28
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	13	1.28
(1,2007)	2:226:B:ASN:HD21	2:255:B:SER:H	3	1.28
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	14	1.28
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	14	1.28
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	14	1.28
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	14	1.28
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	14	1.28
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	14	1.28
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	14	1.28
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	14	1.28
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	14	1.28
(1,4140)	2:254:B:MET:HE1	2:252:B:ALA:H	13	1.27
(1,2775)	1:96:A:LEU:HD11	1:100:A:ASN:HB3	12	1.27
(1,2775)	1:96:A:LEU:HD12	1:100:A:ASN:HB3	12	1.27
(1,2775)	1:96:A:LEU:HD13	1:100:A:ASN:HB3	12	1.27
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	18	1.27
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	18	1.27
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	18	1.27
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	18	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	18	1.27
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	18	1.27
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	18	1.27
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	18	1.27
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	18	1.27
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	18	1.27
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	18	1.27
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	18	1.27
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD21	14	1.27
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD22	14	1.27
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD23	14	1.27
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD22	19	1.26
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG11	10	1.26
(1,4421)	1:111:A:ILE:HD12	1:110:A:GLU:HB2	5	1.26
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB2	19	1.26
(1,4282)	1:88:A:GLN:HB2	1:83:A:THR:HG23	6	1.26
(1,4004)	2:305:B:LEU:HA	2:305:B:LEU:HD13	17	1.26
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD21	2	1.26
(1,2471)	1:72:A:VAL:HG21	1:71:A:GLN:HB3	3	1.26
(1,2471)	1:72:A:VAL:HG22	1:71:A:GLN:HB3	3	1.26
(1,2471)	1:72:A:VAL:HG23	1:71:A:GLN:HB3	3	1.26
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB1	14	1.26
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB2	14	1.26
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB3	14	1.26
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB1	14	1.26
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB2	14	1.26
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB3	14	1.26
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB1	14	1.26
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB2	14	1.26
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB3	14	1.26
(1,454)	2:202:B:LYS:HD3	2:211:B:GLU:HG3	2	1.26
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	10	1.25
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	9	1.25
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD23	3	1.25
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD11	20	1.25
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG23	11	1.25
(1,3930)	2:168:B:LEU:HD11	2:268:B:VAL:HG12	15	1.25
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	15	1.25
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	15	1.25
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	15	1.25
(1,2293)	2:305:B:LEU:HD21	2:302:B:SER:H	16	1.25
(1,2293)	2:305:B:LEU:HD22	2:302:B:SER:H	16	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2293)	2:305:B:LEU:HD23	2:302:B:SER:H	16	1.25
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG21	12	1.25
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG22	12	1.25
(1,364)	2:263:B:LEU:HD11	2:193:B:ILE:HG23	12	1.25
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG21	12	1.25
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG22	12	1.25
(1,364)	2:263:B:LEU:HD12	2:193:B:ILE:HG23	12	1.25
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG21	12	1.25
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG22	12	1.25
(1,364)	2:263:B:LEU:HD13	2:193:B:ILE:HG23	12	1.25
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG12	11	1.24
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE2	6	1.24
(1,4346)	1:94:A:GLU:HB3	1:95:A:ILE:HG21	4	1.24
(1,4337)	1:73:A:PRO:HB3	1:74:A:SER:HB2	12	1.24
(1,4327)	1:95:A:ILE:HD13	1:92:A:GLU:HB3	18	1.24
(1,4004)	2:274:B:LEU:HA	2:274:B:LEU:HD13	12	1.24
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD12	19	1.24
(1,3935)	2:268:B:VAL:HG22	2:269:B:ARG:HD3	20	1.24
(1,3837)	2:198:B:ALA:HB1	2:214:B:VAL:HG21	11	1.24
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	1	1.24
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	1	1.24
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	1	1.24
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	12	1.24
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	12	1.24
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	12	1.24
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	4	1.24
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	4	1.24
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	4	1.24
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD21	19	1.23
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	20	1.23
(1,4328)	1:95:A:ILE:HD12	1:92:A:GLU:HB2	10	1.23
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD23	11	1.23
(1,3989)	2:295:B:LEU:HD23	2:298:B:LEU:HD11	14	1.23
(1,3980)	2:164:B:LEU:HD23	2:295:B:LEU:HD22	9	1.23
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	12	1.23
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	12	1.23
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	12	1.23
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	12	1.23
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	12	1.23
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	12	1.23
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	13	1.23
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	13	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	13	1.23
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	13	1.23
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	13	1.23
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	13	1.23
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	13	1.23
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	13	1.23
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	13	1.23
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	13	1.23
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	13	1.23
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	13	1.23
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HB3	5	1.22
(1,4444)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	1	1.22
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG12	6	1.22
(1,4296)	1:90:A:LEU:HD22	1:87:A:MET:HE2	20	1.22
(1,4054)	2:313:B:VAL:HG13	2:180:B:GLN:HE22	6	1.22
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE2	10	1.22
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	16	1.22
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	16	1.22
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	16	1.22
(1,2293)	2:305:B:LEU:HD21	2:302:B:SER:H	13	1.22
(1,2293)	2:305:B:LEU:HD22	2:302:B:SER:H	13	1.22
(1,2293)	2:305:B:LEU:HD23	2:302:B:SER:H	13	1.22
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HB3	12	1.21
(1,4407)	2:162:B:GLU:HG2	1:111:A:ILE:HG21	20	1.21
(1,4343)	1:74:A:SER:HB3	1:95:A:ILE:HD12	4	1.21
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD21	3	1.21
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE1	14	1.21
(1,298)	2:192:B:SER:HB2	2:188:B:LYS:HD3	13	1.21
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD22	14	1.2
(1,4421)	1:111:A:ILE:HD11	1:110:A:GLU:HB2	16	1.2
(1,4346)	1:92:A:GLU:HB3	1:95:A:ILE:HG23	5	1.2
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	17	1.2
(1,4237)	2:218:B:VAL:HG13	2:198:B:ALA:H	4	1.2
(1,3979)	2:160:B:ILE:HG23	2:295:B:LEU:HD21	20	1.2
(1,3842)	2:214:B:VAL:HG21	2:218:B:VAL:HG12	12	1.2
(1,3803)	2:194:B:LEU:HD22	2:193:B:ILE:HG23	1	1.2
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD11	8	1.2
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD12	8	1.2
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD13	8	1.2
(1,1476)	2:180:B:GLN:HG3	2:180:B:GLN:H	13	1.2
(1,4604)	2:225:B:PHE:HE1	2:266:B:LEU:HD12	16	1.19
(1,4421)	1:111:A:ILE:HD13	1:110:A:GLU:HB2	17	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4385)	1:112:A:ILE:HG21	1:109:A:GLU:HB3	6	1.19
(1,4312)	1:94:A:GLU:HG2	1:90:A:LEU:HD12	4	1.19
(1,4054)	2:313:B:VAL:HG13	2:180:B:GLN:HE22	14	1.19
(1,3745)	2:165:B:LYS:HA	2:164:B:LEU:HD23	11	1.19
(1,4497)	2:292:B:HIS:HE1	2:295:B:LEU:HD12	6	1.18
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD21	8	1.18
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD21	11	1.18
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG21	18	1.18
(1,4324)	1:81:A:LEU:HD13	1:80:A:HIS:HB2	4	1.18
(1,4282)	1:88:A:GLN:HB2	1:83:A:THR:HG23	16	1.18
(1,4271)	2:212:B:TYR:HD2	1:81:A:LEU:HA	9	1.18
(1,3949)	2:302:B:SER:HB2	2:305:B:LEU:HD11	9	1.18
(1,3896)	2:246:B:LEU:HA	2:246:B:LEU:HD23	10	1.18
(1,3842)	2:214:B:VAL:HG23	2:218:B:VAL:HG13	5	1.18
(1,3745)	2:294:B:PHE:HA	2:298:B:LEU:HD23	2	1.18
(1,3421)	2:236:B:LYS:HE2	1:104:A:ASN:HD22	7	1.18
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	7	1.18
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	7	1.18
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	7	1.18
(1,671)	2:234:B:LEU:HD21	2:239:B:ARG:HD2	15	1.18
(1,671)	2:234:B:LEU:HD22	2:239:B:ARG:HD2	15	1.18
(1,671)	2:234:B:LEU:HD23	2:239:B:ARG:HD2	15	1.18
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD21	14	1.18
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD22	14	1.18
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD23	14	1.18
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD21	14	1.18
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD22	14	1.18
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD23	14	1.18
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD21	14	1.18
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD22	14	1.18
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD23	14	1.18
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG22	7	1.17
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG22	3	1.17
(1,4361)	1:105:A:PHE:HD2	1:106:A:VAL:HG12	2	1.17
(1,4327)	2:279:B:LEU:HD22	1:94:A:GLU:HB3	3	1.17
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD22	9	1.17
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG23	1	1.17
(1,3920)	2:194:B:LEU:HD21	2:263:B:LEU:HD13	5	1.17
(1,3896)	2:246:B:LEU:HA	2:246:B:LEU:HD22	5	1.17
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG21	5	1.17
(1,3843)	2:194:B:LEU:HD12	2:218:B:VAL:HG21	6	1.17
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	14	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	14	1.17
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	14	1.17
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	14	1.17
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	14	1.17
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	14	1.17
(1,2866)	1:112:A:ILE:HG12	1:107:A:LEU:HD21	15	1.17
(1,2866)	1:112:A:ILE:HG12	1:107:A:LEU:HD22	15	1.17
(1,2866)	1:112:A:ILE:HG12	1:107:A:LEU:HD23	15	1.17
(1,2471)	1:72:A:VAL:HG21	1:71:A:GLN:HB3	18	1.17
(1,2471)	1:72:A:VAL:HG22	1:71:A:GLN:HB3	18	1.17
(1,2471)	1:72:A:VAL:HG23	1:71:A:GLN:HB3	18	1.17
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	9	1.17
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	9	1.17
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	9	1.17
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	9	1.17
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	9	1.17
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	9	1.17
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	9	1.17
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	9	1.17
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	9	1.17
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	13	1.16
(1,4328)	2:279:B:LEU:HD22	1:94:A:GLU:HB2	11	1.16
(1,4296)	2:279:B:LEU:HD13	1:87:A:MET:HE2	7	1.16
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD11	18	1.16
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE3	2	1.16
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	2	1.16
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	2	1.16
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	2	1.16
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	11	1.16
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	11	1.16
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	11	1.16
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	13	1.16
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	13	1.16
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	13	1.16
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	7	1.16
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	7	1.16
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	7	1.16
(1,4505)	2:311:B:TYR:HD1	2:181:B:LEU:HD23	16	1.15
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD23	14	1.15
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD21	12	1.15
(1,3979)	2:160:B:ILE:HG22	2:295:B:LEU:HD21	14	1.15
(1,3962)	2:156:B:VAL:HA	2:284:B:LEU:HD13	8	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD11	18	1.15
(1,3724)	2:271:B:GLY:HA3	2:156:B:VAL:HG12	1	1.15
(1,2659)	1:92:A:GLU:HB2	1:89:A:ALA:HB1	4	1.15
(1,2659)	1:92:A:GLU:HB2	1:89:A:ALA:HB2	4	1.15
(1,2659)	1:92:A:GLU:HB2	1:89:A:ALA:HB3	4	1.15
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD11	1	1.15
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD12	1	1.15
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD13	1	1.15
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD11	1	1.15
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD12	1	1.15
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD13	1	1.15
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	16	1.15
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	16	1.15
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	16	1.15
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	14	1.15
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	14	1.15
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	14	1.15
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD21	12	1.15
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD22	12	1.15
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD23	12	1.15
(1,4622)	2:267:B:PHE:HZ	2:298:B:LEU:HD11	12	1.14
(1,4327)	1:95:A:ILE:HD12	1:92:A:GLU:HB3	11	1.14
(1,4316)	1:87:A:MET:HE3	1:90:A:LEU:HD21	1	1.14
(1,4243)	1:115:A:VAL:HG22	1:114:A:GLU:HB2	10	1.14
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG22	12	1.14
(1,3857)	2:224:B:TYR:HD1	2:227:B:VAL:HG12	7	1.14
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	5	1.14
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	5	1.14
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	5	1.14
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	5	1.14
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	5	1.14
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	5	1.14
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	1	1.14
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	1	1.14
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	1	1.14
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	1	1.14
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	1	1.14
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	1	1.14
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	1	1.14
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	1	1.14
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	1	1.14
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	14	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	14	1.14
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	14	1.14
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD11	20	1.14
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD12	20	1.14
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD13	20	1.14
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD11	20	1.14
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD12	20	1.14
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD13	20	1.14
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD11	20	1.14
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD12	20	1.14
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD13	20	1.14
(1,589)	2:242:B:TYR:HD1	2:229:B:LEU:HD21	14	1.14
(1,589)	2:242:B:TYR:HD1	2:229:B:LEU:HD22	14	1.14
(1,589)	2:242:B:TYR:HD1	2:229:B:LEU:HD23	14	1.14
(1,589)	2:242:B:TYR:HD2	2:229:B:LEU:HD21	14	1.14
(1,589)	2:242:B:TYR:HD2	2:229:B:LEU:HD22	14	1.14
(1,589)	2:242:B:TYR:HD2	2:229:B:LEU:HD23	14	1.14
(1,4560)	2:225:B:PHE:HD1	2:221:B:ILE:HG22	7	1.13
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG12	13	1.13
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD12	3	1.13
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD21	19	1.13
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE1	20	1.13
(1,4243)	1:72:A:VAL:HG22	1:71:A:GLN:HB2	13	1.13
(1,4243)	1:115:A:VAL:HG22	1:114:A:GLU:HB2	14	1.13
(1,4237)	2:218:B:VAL:HG11	2:198:B:ALA:H	11	1.13
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD12	5	1.13
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD22	2	1.13
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	5	1.13
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	5	1.13
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	5	1.13
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	4	1.13
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	4	1.13
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	4	1.13
(1,158)	2:311:B:TYR:HD1	2:174:B:LEU:HD23	12	1.13
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	17	1.12
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD23	10	1.12
(1,4296)	2:279:B:LEU:HD13	1:87:A:MET:HE1	5	1.12
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD13	4	1.12
(1,3949)	2:302:B:SER:HB2	2:305:B:LEU:HD12	15	1.12
(1,3768)	2:235:B:TYR:HE1	2:176:B:THR:HG21	18	1.12
(1,3745)	2:165:B:LYS:HA	2:164:B:LEU:HD21	17	1.12
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	15	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	15	1.12
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	15	1.12
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	2	1.12
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	2	1.12
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	2	1.12
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	16	1.12
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	16	1.12
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	16	1.12
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD11	16	1.12
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD12	16	1.12
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD13	16	1.12
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD11	16	1.12
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD12	16	1.12
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD13	16	1.12
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD11	16	1.12
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD12	16	1.12
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD13	16	1.12
(1,4640)	2:267:B:PHE:HD2	2:168:B:LEU:HD21	8	1.11
(1,4505)	2:311:B:TYR:HD2	2:181:B:LEU:HD21	15	1.11
(1,4449)	2:290:B:TYR:HE2	1:81:A:LEU:HD12	1	1.11
(1,4276)	1:98:A:PHE:HE1	1:96:A:LEU:HD23	2	1.11
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD11	3	1.11
(1,3947)	2:272:B:ALA:HB2	2:273:B:MET:HE2	5	1.11
(1,3935)	2:268:B:VAL:HG21	2:269:B:ARG:HD3	10	1.11
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD22	3	1.11
(1,3837)	2:198:B:ALA:HB2	2:214:B:VAL:HG22	7	1.11
(1,855)	2:270:B:ILE:HD11	2:291:B:LEU:HD11	9	1.11
(1,855)	2:270:B:ILE:HD11	2:291:B:LEU:HD12	9	1.11
(1,855)	2:270:B:ILE:HD11	2:291:B:LEU:HD13	9	1.11
(1,855)	2:270:B:ILE:HD12	2:291:B:LEU:HD11	9	1.11
(1,855)	2:270:B:ILE:HD12	2:291:B:LEU:HD12	9	1.11
(1,855)	2:270:B:ILE:HD12	2:291:B:LEU:HD13	9	1.11
(1,855)	2:270:B:ILE:HD13	2:291:B:LEU:HD11	9	1.11
(1,855)	2:270:B:ILE:HD13	2:291:B:LEU:HD12	9	1.11
(1,855)	2:270:B:ILE:HD13	2:291:B:LEU:HD13	9	1.11
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	2	1.11
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	2	1.11
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	2	1.11
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	2	1.11
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	2	1.11
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	2	1.11
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	2	1.11
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	2	1.11
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	2	1.11
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	2	1.11
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	2	1.11
(1,4492)	1:85:A:TYR:HE2	1:86:A:ASP:H	18	1.1
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	3	1.1
(1,4280)	2:290:B:TYR:HE2	1:81:A:LEU:HD23	7	1.1
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG22	20	1.1
(1,3803)	2:298:B:LEU:HD22	2:193:B:ILE:HG22	17	1.1
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	20	1.1
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	20	1.1
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	20	1.1
(1,4513)	2:235:B:TYR:HE2	2:175:B:ILE:HD11	8	1.09
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD13	4	1.09
(1,4385)	1:112:A:ILE:HG22	1:109:A:GLU:HB3	2	1.09
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD22	17	1.09
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD12	15	1.09
(1,3742)	2:164:B:LEU:HA	2:164:B:LEU:HD23	20	1.09
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	4	1.09
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	4	1.09
(1,298)	2:192:B:SER:HB2	2:188:B:LYS:HD3	10	1.09
(1,4492)	1:85:A:TYR:HE2	1:86:A:ASP:H	12	1.08
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	10	1.08
(1,3967)	2:224:B:TYR:HA	2:266:B:LEU:HD13	3	1.08
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD21	4	1.08
(1,3859)	2:266:B:LEU:HD12	2:228:B:MET:HE2	7	1.08
(1,3852)	2:218:B:VAL:HG22	2:202:B:LYS:HE3	18	1.08
(1,3742)	2:164:B:LEU:HA	2:164:B:LEU:HD21	11	1.08
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD11	9	1.08
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD12	9	1.08
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD13	9	1.08
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD21	8	1.08
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD22	8	1.08
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD23	8	1.08
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	11	1.08
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	11	1.08
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	11	1.08
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	18	1.08
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	18	1.08
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	18	1.08
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	10	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	10	1.08
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	10	1.08
(1,4555)	2:294:B:PHE:HD1	2:214:B:VAL:HG13	1	1.07
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	14	1.07
(1,4343)	1:74:A:SER:HB3	1:95:A:ILE:HD12	19	1.07
(1,4153)	2:298:B:LEU:HD11	2:264:B:LEU:H	1	1.07
(1,3949)	2:302:B:SER:HB2	2:305:B:LEU:HD11	14	1.07
(1,3857)	1:98:A:PHE:HE2	2:227:B:VAL:HG11	2	1.07
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE2	13	1.07
(1,3742)	2:234:B:LEU:HA	2:234:B:LEU:HD13	5	1.07
(1,3420)	2:236:B:LYS:HG2	1:104:A:ASN:HD22	12	1.07
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	12	1.07
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	12	1.07
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	12	1.07
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	12	1.07
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	12	1.07
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	12	1.07
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	12	1.07
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	12	1.07
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	12	1.07
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	12	1.07
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	12	1.07
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	12	1.07
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	18	1.07
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	18	1.07
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	18	1.07
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	13	1.07
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	13	1.07
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	13	1.07
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	3	1.07
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	3	1.07
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	3	1.07
(1,4604)	2:225:B:PHE:HE1	2:266:B:LEU:HD13	19	1.06
(1,4560)	2:225:B:PHE:HD1	2:221:B:ILE:HG21	11	1.06
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	10	1.06
(1,4237)	2:218:B:VAL:HG13	2:198:B:ALA:H	15	1.06
(1,3945)	2:274:B:LEU:HD21	2:271:B:GLY:HA3	7	1.06
(1,3812)	2:193:B:ILE:HG23	2:194:B:LEU:HD22	5	1.06
(1,3812)	2:193:B:ILE:HG23	2:194:B:LEU:HD22	14	1.06
(1,3803)	2:194:B:LEU:HD22	2:193:B:ILE:HG23	5	1.06
(1,3803)	2:194:B:LEU:HD22	2:193:B:ILE:HG23	14	1.06
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	1	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	1	1.06
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	1	1.06
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	9	1.06
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	9	1.06
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	9	1.06
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	20	1.05
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	20	1.05
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	20	1.05
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	20	1.05
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	20	1.05
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	20	1.05
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	2	1.05
(1,4609)	2:224:B:TYR:HD2	2:223:B:GLU:HB3	10	1.05
(1,4497)	2:292:B:HIS:HE1	2:158:B:VAL:HG22	13	1.05
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD13	5	1.05
(1,4328)	2:279:B:LEU:HD23	1:94:A:GLU:HB2	17	1.05
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD21	5	1.05
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD13	17	1.05
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD22	10	1.05
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD22	6	1.05
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD23	15	1.05
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE1	16	1.05
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	14	1.05
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	14	1.05
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	14	1.05
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	5	1.05
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	5	1.05
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	5	1.05
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	17	1.05
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	17	1.05
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	17	1.05
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	17	1.05
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	17	1.05
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	17	1.05
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	17	1.05
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	17	1.05
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	17	1.05
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD21	9	1.05
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD22	9	1.05
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD23	9	1.05
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD21	10	1.05
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD22	10	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD23	10	1.05
(1,4560)	2:225:B:PHE:HD1	2:221:B:ILE:HG21	8	1.04
(1,4333)	1:90:A:LEU:HD12	1:93:A:SER:HA	17	1.04
(1,4314)	2:283:B:SER:HB2	1:90:A:LEU:HD21	10	1.04
(1,4140)	2:254:B:MET:HE1	2:252:B:ALA:H	18	1.04
(1,4011)	2:314:B:ALA:HB3	2:313:B:VAL:HG21	2	1.04
(1,4011)	2:314:B:ALA:HB3	2:313:B:VAL:HG21	4	1.04
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG21	8	1.04
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD22	7	1.04
(1,3852)	2:218:B:VAL:HG21	2:202:B:LYS:HE2	12	1.04
(1,3742)	2:164:B:LEU:HA	2:164:B:LEU:HD22	15	1.04
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	19	1.04
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	19	1.04
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	19	1.04
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD11	15	1.04
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD12	15	1.04
(1,962)	2:233:B:LEU:HD21	2:266:B:LEU:HD13	15	1.04
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD11	15	1.04
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD12	15	1.04
(1,962)	2:233:B:LEU:HD22	2:266:B:LEU:HD13	15	1.04
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD11	15	1.04
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD12	15	1.04
(1,962)	2:233:B:LEU:HD23	2:266:B:LEU:HD13	15	1.04
(1,671)	2:234:B:LEU:HD21	2:239:B:ARG:HD2	11	1.04
(1,671)	2:234:B:LEU:HD22	2:239:B:ARG:HD2	11	1.04
(1,671)	2:234:B:LEU:HD23	2:239:B:ARG:HD2	11	1.04
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	8	1.04
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	14	1.03
(1,4609)	2:224:B:TYR:HD2	2:223:B:GLU:HB3	1	1.03
(1,4505)	2:311:B:TYR:HD2	2:181:B:LEU:HD22	14	1.03
(1,4444)	1:97:A:PRO:HG3	1:96:A:LEU:HD11	8	1.03
(1,4433)	2:169:B:VAL:HG21	1:116:A:ARG:HG3	11	1.03
(1,4323)	2:279:B:LEU:HD23	1:91:A:HIS:HB3	4	1.03
(1,4296)	1:90:A:LEU:HD13	1:87:A:MET:HE3	18	1.03
(1,4167)	2:279:B:LEU:HD11	2:280:B:ASP:H	1	1.03
(1,3967)	2:224:B:TYR:HA	2:266:B:LEU:HD12	20	1.03
(1,3948)	2:276:B:TYR:HE2	2:273:B:MET:HE2	3	1.03
(1,3936)	2:265:B:ARG:HB2	2:269:B:ARG:HD2	7	1.03
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG23	4	1.03
(1,3921)	2:194:B:LEU:HD22	2:263:B:LEU:HD22	3	1.03
(1,3915)	2:305:B:LEU:HD21	2:260:B:ALA:HB1	14	1.03
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD22	11	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3745)	2:165:B:LYS:HA	2:164:B:LEU:HD23	5	1.03
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	8	1.03
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	8	1.03
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	8	1.03
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	8	1.03
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	8	1.03
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	8	1.03
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	8	1.03
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	8	1.03
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	8	1.03
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HE1	17	1.02
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	2	1.02
(1,4505)	2:311:B:TYR:HD2	2:181:B:LEU:HD21	17	1.02
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	8	1.02
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE1	6	1.02
(1,4030)	2:192:B:SER:HB2	2:188:B:LYS:HG2	1	1.02
(1,4027)	2:320:B:ARG:HA	2:323:B:VAL:HG22	7	1.02
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD13	5	1.02
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD11	6	1.02
(1,3896)	2:288:B:LEU:HA	2:288:B:LEU:HD22	13	1.02
(1,3184)	1:90:A:LEU:HD21	1:89:A:ALA:H	15	1.02
(1,3184)	1:90:A:LEU:HD22	1:89:A:ALA:H	15	1.02
(1,3184)	1:90:A:LEU:HD23	1:89:A:ALA:H	15	1.02
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	20	1.02
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	20	1.02
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	20	1.02
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	3	1.01
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	3	1.01
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	3	1.01
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	3	1.01
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	3	1.01
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	3	1.01
(1,4492)	2:212:B:TYR:HE1	1:81:A:LEU:H	8	1.01
(1,4324)	1:95:A:ILE:HG23	1:91:A:HIS:HB2	18	1.01
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD11	2	1.01
(1,4054)	2:313:B:VAL:HG12	2:180:B:GLN:HE22	7	1.01
(1,4030)	2:192:B:SER:HB2	2:188:B:LYS:HG2	13	1.01
(1,3789)	2:193:B:ILE:HD11	2:188:B:LYS:HE2	12	1.01
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	16	1.01
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	16	1.01
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	16	1.01
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	15	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	15	1.01
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	15	1.01
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	16	1.01
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	16	1.01
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	16	1.01
(1,815)	2:253:B:PRO:HB2	2:256:B:GLN:HG3	11	1.01
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	5	1.0
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	4	1.0
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE3	19	1.0
(1,3842)	2:214:B:VAL:HG23	2:218:B:VAL:HG11	16	1.0
(1,3443)	2:227:B:VAL:HG21	1:100:A:ASN:HD22	15	1.0
(1,3443)	2:227:B:VAL:HG22	1:100:A:ASN:HD22	15	1.0
(1,3443)	2:227:B:VAL:HG23	1:100:A:ASN:HD22	15	1.0
(1,3028)	1:107:A:LEU:HD21	1:112:A:ILE:HD11	15	1.0
(1,3028)	1:107:A:LEU:HD21	1:112:A:ILE:HD12	15	1.0
(1,3028)	1:107:A:LEU:HD21	1:112:A:ILE:HD13	15	1.0
(1,3028)	1:107:A:LEU:HD22	1:112:A:ILE:HD11	15	1.0
(1,3028)	1:107:A:LEU:HD22	1:112:A:ILE:HD12	15	1.0
(1,3028)	1:107:A:LEU:HD22	1:112:A:ILE:HD13	15	1.0
(1,3028)	1:107:A:LEU:HD23	1:112:A:ILE:HD11	15	1.0
(1,3028)	1:107:A:LEU:HD23	1:112:A:ILE:HD12	15	1.0
(1,3028)	1:107:A:LEU:HD23	1:112:A:ILE:HD13	15	1.0
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	5	1.0
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	5	1.0
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	5	1.0
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD21	2	1.0
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD22	2	1.0
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD23	2	1.0
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD11	3	1.0
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD12	3	1.0
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD13	3	1.0
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD11	3	1.0
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD12	3	1.0
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD13	3	1.0
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	1	1.0
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	1	1.0
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	1	1.0
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	15	1.0
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	15	1.0
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	15	1.0
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	15	1.0
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	15	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	15	1.0
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	15	1.0
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	15	1.0
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	15	1.0
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD11	2	1.0
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD12	2	1.0
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD13	2	1.0
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD13	6	0.99
(1,4445)	1:74:A:SER:HA	1:72:A:VAL:HG11	6	0.99
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG21	10	0.99
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	15	0.99
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD11	9	0.99
(1,4346)	1:72:A:VAL:HB	1:95:A:ILE:HG23	19	0.99
(1,4268)	1:81:A:LEU:HD22	1:78:A:TRP:HB2	8	0.99
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD13	2	0.99
(1,3837)	2:198:B:ALA:HB1	2:214:B:VAL:HG23	4	0.99
(1,3745)	2:294:B:PHE:HA	2:298:B:LEU:HD21	15	0.99
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	8	0.99
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	8	0.99
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	8	0.99
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	9	0.99
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	9	0.99
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	9	0.99
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	9	0.99
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	9	0.99
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	9	0.99
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	9	0.99
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	9	0.99
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	9	0.99
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	1	0.99
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	1	0.99
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	1	0.99
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	1	0.99
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	1	0.99
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	1	0.99
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	1	0.99
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	1	0.99
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	1	0.99
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD21	7	0.98
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD13	5	0.98
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	18	0.98
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG21	10	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4324)	1:81:A:LEU:HD12	1:80:A:HIS:HB2	8	0.98
(1,4008)	2:170:B:ASP:HB3	2:169:B:VAL:HG11	19	0.98
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG21	7	0.98
(1,3852)	2:218:B:VAL:HG21	2:202:B:LYS:HE3	1	0.98
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD11	13	0.98
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD12	13	0.98
(1,3638)	2:292:B:HIS:HD2	2:295:B:LEU:HD13	13	0.98
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD11	5	0.98
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD12	5	0.98
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD13	5	0.98
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD11	5	0.98
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD12	5	0.98
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD13	5	0.98
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	20	0.98
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	20	0.98
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	20	0.98
(1,1521)	2:187:B:LYS:HG3	2:187:B:LYS:H	1	0.98
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	12	0.98
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	12	0.98
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	12	0.98
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	4	0.98
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	4	0.98
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	4	0.98
(1,454)	2:202:B:LYS:HD3	2:211:B:GLU:HG3	4	0.98
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD12	4	0.97
(1,4589)	2:182:B:PHE:HD2	2:259:B:GLY:HA2	4	0.97
(1,4589)	2:182:B:PHE:HD2	2:259:B:GLY:HA2	19	0.97
(1,4520)	2:237:B:PHE:HE1	2:179:B:LYS:HE3	19	0.97
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	4	0.97
(1,4492)	1:85:A:TYR:HE2	1:86:A:ASP:H	5	0.97
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG12	8	0.97
(1,4328)	2:279:B:LEU:HD22	1:94:A:GLU:HB2	3	0.97
(1,4296)	1:90:A:LEU:HD12	1:87:A:MET:HE1	3	0.97
(1,4153)	2:298:B:LEU:HD13	2:264:B:LEU:H	12	0.97
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG23	3	0.97
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG22	11	0.97
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG23	17	0.97
(1,3843)	1:96:A:LEU:HD21	2:227:B:VAL:HG11	16	0.97
(1,3745)	2:302:B:SER:HA	2:298:B:LEU:HD21	8	0.97
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG21	11	0.97
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG22	11	0.97
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG23	11	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG21	11	0.97
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG22	11	0.97
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG23	11	0.97
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG21	11	0.97
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG22	11	0.97
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG23	11	0.97
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	15	0.97
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	15	0.97
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	15	0.97
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	15	0.97
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	15	0.97
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	15	0.97
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	15	0.97
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	15	0.97
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	15	0.97
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD21	2	0.97
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD22	2	0.97
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD23	2	0.97
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	15	0.96
(1,4525)	2:306:B:PHE:HD1	2:260:B:ALA:HB2	17	0.96
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG12	11	0.96
(1,4421)	1:111:A:ILE:HD11	1:110:A:GLU:HB2	8	0.96
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD11	15	0.96
(1,3859)	2:266:B:LEU:HD12	2:228:B:MET:HE1	20	0.96
(1,3441)	2:227:B:VAL:HG21	1:100:A:ASN:HD21	16	0.96
(1,3441)	2:227:B:VAL:HG22	1:100:A:ASN:HD21	16	0.96
(1,3441)	2:227:B:VAL:HG23	1:100:A:ASN:HD21	16	0.96
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	4	0.96
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	4	0.96
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	4	0.96
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	13	0.96
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	13	0.96
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	13	0.96
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	13	0.96
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	13	0.96
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	13	0.96
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	13	0.96
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	13	0.96
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	13	0.96
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	3	0.96
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	3	0.96
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	3	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	10	0.95
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	10	0.95
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	10	0.95
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	10	0.95
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	10	0.95
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	10	0.95
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	11	0.95
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	11	0.95
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	11	0.95
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	11	0.95
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	11	0.95
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	11	0.95
(1,4622)	2:267:B:PHE:HZ	2:298:B:LEU:HD13	16	0.95
(1,4555)	2:294:B:PHE:HD2	2:217:B:VAL:HG11	3	0.95
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE3	16	0.95
(1,4505)	2:311:B:TYR:HD2	2:181:B:LEU:HD22	12	0.95
(1,4492)	2:212:B:TYR:HE2	1:81:A:LEU:H	16	0.95
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG11	14	0.95
(1,4346)	1:72:A:VAL:HB	1:95:A:ILE:HG22	9	0.95
(1,4011)	2:314:B:ALA:HB3	2:313:B:VAL:HG23	20	0.95
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD13	10	0.95
(1,3837)	2:198:B:ALA:HB2	2:214:B:VAL:HG21	15	0.95
(1,3730)	2:225:B:PHE:HB3	2:263:B:LEU:HD22	6	0.95
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD21	16	0.95
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD22	16	0.95
(1,3653)	2:297:B:TYR:HD1	2:298:B:LEU:HD23	16	0.95
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD21	16	0.95
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD22	16	0.95
(1,3653)	2:297:B:TYR:HD2	2:298:B:LEU:HD23	16	0.95
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE3	2	0.95
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE3	2	0.95
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	11	0.95
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	11	0.95
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	11	0.95
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	11	0.95
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	11	0.95
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	11	0.95
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	11	0.95
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	11	0.95
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	11	0.95
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	20	0.95
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	20	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	20	0.95
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	1	0.95
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	1	0.95
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	1	0.95
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	1	0.95
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	1	0.95
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	1	0.95
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	1	0.95
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	1	0.95
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	1	0.95
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	19	0.95
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	19	0.95
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	19	0.95
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	5	0.95
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	5	0.95
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	5	0.95
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD21	11	0.95
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD22	11	0.95
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD23	11	0.95
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD21	20	0.95
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD22	20	0.95
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD23	20	0.95
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	1	0.95
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	1	0.95
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	1	0.95
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	1	0.95
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	1	0.95
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	1	0.95
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	1	0.95
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	1	0.95
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	1	0.95
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	13	0.94
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	13	0.94
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	13	0.94
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	13	0.94
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	13	0.94
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	13	0.94
(1,4591)	2:182:B:PHE:HD2	2:261:B:PRO:HD2	15	0.94
(1,4440)	2:218:B:VAL:HB	1:77:A:ILE:HG23	6	0.94
(1,4011)	2:314:B:ALA:HB1	2:313:B:VAL:HG22	10	0.94
(1,4011)	2:314:B:ALA:HB1	2:313:B:VAL:HG21	13	0.94
(1,3990)	2:263:B:LEU:HD12	2:194:B:LEU:HD21	14	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD23	17	0.94
(1,3184)	1:90:A:LEU:HD21	1:89:A:ALA:H	9	0.94
(1,3184)	1:90:A:LEU:HD22	1:89:A:ALA:H	9	0.94
(1,3184)	1:90:A:LEU:HD23	1:89:A:ALA:H	9	0.94
(1,3184)	1:90:A:LEU:HD21	1:89:A:ALA:H	20	0.94
(1,3184)	1:90:A:LEU:HD22	1:89:A:ALA:H	20	0.94
(1,3184)	1:90:A:LEU:HD23	1:89:A:ALA:H	20	0.94
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	6	0.94
(1,4644)	2:182:B:PHE:HD1	2:184:B:LEU:HB2	7	0.93
(1,4634)	2:237:B:PHE:HE2	2:314:B:ALA:HB3	4	0.93
(1,4555)	2:294:B:PHE:HD2	2:264:B:LEU:HD13	18	0.93
(1,4547)	2:200:B:TYR:HD1	2:204:B:ARG:HD2	19	0.93
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD13	18	0.93
(1,4385)	1:112:A:ILE:HG22	1:109:A:GLU:HB3	9	0.93
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG23	14	0.93
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD13	1	0.93
(1,3901)	2:246:B:LEU:HD12	2:252:B:ALA:HB3	7	0.93
(1,3611)	2:224:B:TYR:HE1	2:273:B:MET:HE3	3	0.93
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	7	0.93
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	7	0.93
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	7	0.93
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	14	0.93
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	14	0.93
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	14	0.93
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	8	0.93
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	8	0.93
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	8	0.93
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG2	11	0.93
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG2	11	0.93
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG2	11	0.93
(1,815)	2:253:B:PRO:HG2	2:256:B:GLN:HG3	17	0.93
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	19	0.93
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	19	0.93
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	19	0.93
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	2	0.93
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	2	0.93
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	2	0.93
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	19	0.93
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	19	0.93
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	19	0.93
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	19	0.93
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	19	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	19	0.93
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	19	0.93
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	19	0.93
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	19	0.93
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD11	4	0.92
(1,4644)	2:182:B:PHE:HD1	2:184:B:LEU:HB2	14	0.92
(1,4621)	2:267:B:PHE:HE2	2:298:B:LEU:HD11	12	0.92
(1,4611)	2:290:B:TYR:HD1	2:210:B:LYS:HD2	1	0.92
(1,4520)	2:237:B:PHE:HE1	2:179:B:LYS:HE2	11	0.92
(1,4511)	2:182:B:PHE:HD1	2:184:B:LEU:HB3	20	0.92
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG12	7	0.92
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	9	0.92
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD13	2	0.92
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG23	2	0.92
(1,3934)	2:173:B:ASP:HA	2:169:B:VAL:HG13	6	0.92
(1,3921)	2:194:B:LEU:HD21	2:263:B:LEU:HD21	16	0.92
(1,3896)	2:246:B:LEU:HA	2:246:B:LEU:HD23	20	0.92
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE3	4	0.92
(1,3745)	2:302:B:SER:HA	2:298:B:LEU:HD23	18	0.92
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	16	0.92
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	16	0.92
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	16	0.92
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	16	0.92
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	16	0.92
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	16	0.92
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	16	0.92
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	16	0.92
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	16	0.92
(1,677)	2:234:B:LEU:HD21	2:239:B:ARG:HG3	10	0.92
(1,677)	2:234:B:LEU:HD22	2:239:B:ARG:HG3	10	0.92
(1,677)	2:234:B:LEU:HD23	2:239:B:ARG:HG3	10	0.92
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	18	0.92
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	8	0.91
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	8	0.91
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	8	0.91
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	8	0.91
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	8	0.91
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	8	0.91
(1,4505)	2:311:B:TYR:HD2	2:181:B:LEU:HD22	1	0.91
(1,4357)	2:273:B:MET:HE2	1:100:A:ASN:HA	16	0.91
(1,4337)	1:73:A:PRO:HB3	1:74:A:SER:HB2	18	0.91
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE1	13	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD13	18	0.91
(1,3893)	2:246:B:LEU:HB2	2:245:B:ILE:HG22	1	0.91
(1,3859)	2:266:B:LEU:HD13	2:228:B:MET:HE3	15	0.91
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE3	11	0.91
(1,3768)	2:235:B:TYR:HE1	2:176:B:THR:HG23	9	0.91
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	3	0.91
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	3	0.91
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	16	0.91
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	16	0.91
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	16	0.91
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	2	0.91
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	2	0.91
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	2	0.91
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	18	0.91
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	18	0.91
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	18	0.91
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	8	0.91
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	8	0.91
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	8	0.91
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD21	20	0.91
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD22	20	0.91
(1,591)	2:254:B:MET:HG3	2:229:B:LEU:HD23	20	0.91
(1,324)	2:194:B:LEU:HD11	2:190:B:VAL:HG11	11	0.91
(1,324)	2:194:B:LEU:HD11	2:190:B:VAL:HG12	11	0.91
(1,324)	2:194:B:LEU:HD11	2:190:B:VAL:HG13	11	0.91
(1,324)	2:194:B:LEU:HD12	2:190:B:VAL:HG11	11	0.91
(1,324)	2:194:B:LEU:HD12	2:190:B:VAL:HG12	11	0.91
(1,324)	2:194:B:LEU:HD12	2:190:B:VAL:HG13	11	0.91
(1,324)	2:194:B:LEU:HD13	2:190:B:VAL:HG11	11	0.91
(1,324)	2:194:B:LEU:HD13	2:190:B:VAL:HG12	11	0.91
(1,324)	2:194:B:LEU:HD13	2:190:B:VAL:HG13	11	0.91
(1,158)	2:311:B:TYR:HD1	2:174:B:LEU:HD21	15	0.91
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	12	0.9
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	12	0.9
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	12	0.9
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	12	0.9
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	12	0.9
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	12	0.9
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	1	0.9
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	15	0.9
(1,4497)	2:292:B:HIS:HE1	2:295:B:LEU:HD12	2	0.9
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	19	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4327)	1:95:A:ILE:HD12	1:92:A:GLU:HB3	1	0.9
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD22	2	0.9
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	19	0.9
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD21	1	0.9
(1,3921)	2:274:B:LEU:HD21	2:156:B:VAL:HG23	14	0.9
(1,3898)	2:254:B:MET:HE1	2:252:B:ALA:HB2	13	0.9
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE3	3	0.9
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	16	0.9
(1,3749)	2:160:B:ILE:HG22	2:165:B:LYS:HE3	19	0.9
(1,3722)	2:257:B:VAL:HA	2:257:B:VAL:HG13	16	0.9
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD21	8	0.9
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD22	8	0.9
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD23	8	0.9
(1,2812)	1:106:A:VAL:HG11	1:104:A:ASN:HB2	13	0.9
(1,2812)	1:106:A:VAL:HG12	1:104:A:ASN:HB2	13	0.9
(1,2812)	1:106:A:VAL:HG13	1:104:A:ASN:HB2	13	0.9
(1,2812)	1:106:A:VAL:HG11	1:104:A:ASN:HB2	14	0.9
(1,2812)	1:106:A:VAL:HG12	1:104:A:ASN:HB2	14	0.9
(1,2812)	1:106:A:VAL:HG13	1:104:A:ASN:HB2	14	0.9
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	9	0.9
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	9	0.9
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	9	0.9
(1,677)	2:234:B:LEU:HD21	2:239:B:ARG:HG3	20	0.9
(1,677)	2:234:B:LEU:HD22	2:239:B:ARG:HG3	20	0.9
(1,677)	2:234:B:LEU:HD23	2:239:B:ARG:HG3	20	0.9
(1,292)	2:188:B:LYS:HD3	2:188:B:LYS:HA	4	0.9
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	12	0.9
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	12	0.9
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	12	0.9
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	12	0.9
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	12	0.9
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	12	0.9
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	12	0.9
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	12	0.9
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	12	0.9
(1,4492)	1:85:A:TYR:HE2	1:86:A:ASP:H	4	0.89
(1,4447)	2:232:B:GLN:HG2	1:103:A:ARG:HG2	19	0.89
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG12	5	0.89
(1,4357)	2:273:B:MET:HE3	1:100:A:ASN:HA	17	0.89
(1,4317)	1:87:A:MET:HB2	1:90:A:LEU:HD23	5	0.89
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE3	12	0.89
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	12	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4237)	2:218:B:VAL:HG13	2:198:B:ALA:H	20	0.89
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG22	15	0.89
(1,3824)	2:214:B:VAL:HG23	2:202:B:LYS:HE3	10	0.89
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	3	0.89
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	3	0.89
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	3	0.89
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	7	0.89
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	7	0.89
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	7	0.89
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	11	0.89
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	11	0.89
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	11	0.89
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	5	0.89
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	5	0.89
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	5	0.89
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	5	0.89
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	5	0.89
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	5	0.89
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	5	0.89
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	5	0.89
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	5	0.89
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	8	0.89
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	8	0.89
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	8	0.89
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD21	14	0.89
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD22	14	0.89
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD23	14	0.89
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD21	14	0.89
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD22	14	0.89
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD23	14	0.89
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD21	14	0.89
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD22	14	0.89
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD23	14	0.89
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	3	0.89
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	3	0.89
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	3	0.89
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	3	0.89
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	3	0.89
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	3	0.89
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	3	0.89
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	3	0.89
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	3	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	10	0.88
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD22	11	0.88
(1,4011)	2:314:B:ALA:HB2	2:313:B:VAL:HG22	5	0.88
(1,3979)	2:160:B:ILE:HG22	2:295:B:LEU:HD22	5	0.88
(1,3453)	2:292:B:HIS:HE1	2:158:B:VAL:HG11	10	0.88
(1,3453)	2:292:B:HIS:HE1	2:158:B:VAL:HG12	10	0.88
(1,3453)	2:292:B:HIS:HE1	2:158:B:VAL:HG13	10	0.88
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	12	0.88
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	12	0.88
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	12	0.88
(1,4612)	2:290:B:TYR:HE1	2:210:B:LYS:HD2	7	0.87
(1,4609)	2:224:B:TYR:HD2	2:223:B:GLU:HB3	9	0.87
(1,4533)	2:183:B:TYR:HE2	2:321:B:LYS:HE3	20	0.87
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG22	15	0.87
(1,4282)	1:88:A:GLN:HB2	1:83:A:THR:HG22	14	0.87
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD11	7	0.87
(1,3803)	2:194:B:LEU:HD21	2:193:B:ILE:HG23	20	0.87
(1,3721)	2:164:B:LEU:HG	2:165:B:LYS:HA	4	0.87
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	7	0.87
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	7	0.87
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	10	0.87
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	10	0.87
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	14	0.87
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	14	0.87
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	4	0.87
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	4	0.87
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	4	0.87
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	9	0.87
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	9	0.87
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	9	0.87
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	2	0.87
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	2	0.87
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	2	0.87
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	13	0.87
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	13	0.87
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	13	0.87
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	12	0.87
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	12	0.87
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	12	0.87
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	12	0.87
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	12	0.87
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	12	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	12	0.87
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	12	0.87
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	12	0.87
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	10	0.87
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	10	0.87
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	10	0.87
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	10	0.87
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	10	0.87
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	10	0.87
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	10	0.87
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	10	0.87
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	10	0.87
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	14	0.87
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	14	0.87
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	14	0.87
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	14	0.87
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	14	0.87
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	14	0.87
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	14	0.87
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	14	0.87
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	14	0.87
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	9	0.87
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	9	0.87
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	9	0.87
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	9	0.87
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	9	0.87
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	9	0.87
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	9	0.87
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	9	0.87
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	9	0.87
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	3	0.87
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	3	0.87
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	3	0.87
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	3	0.87
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	3	0.87
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	3	0.87
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	3	0.87
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	3	0.87
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	3	0.87
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	15	0.87
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	15	0.87
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	15	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	15	0.87
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	15	0.87
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	15	0.87
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	15	0.87
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	15	0.87
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	15	0.87
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD11	9	0.87
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD12	9	0.87
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD13	9	0.87
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	18	0.86
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	18	0.86
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	18	0.86
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	18	0.86
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	18	0.86
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	18	0.86
(1,4611)	2:290:B:TYR:HD1	2:210:B:LYS:HD2	9	0.86
(1,4325)	2:277:B:THR:HG21	1:94:A:GLU:HB3	3	0.86
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	16	0.86
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD13	4	0.86
(1,3441)	2:227:B:VAL:HG21	1:100:A:ASN:HD21	12	0.86
(1,3441)	2:227:B:VAL:HG22	1:100:A:ASN:HD21	12	0.86
(1,3441)	2:227:B:VAL:HG23	1:100:A:ASN:HD21	12	0.86
(1,3419)	2:236:B:LYS:HD3	1:104:A:ASN:HD22	17	0.86
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	13	0.86
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	13	0.86
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	13	0.86
(1,2160)	2:282:B:LYS:HB3	2:282:B:LYS:H	7	0.86
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	19	0.86
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	19	0.86
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	19	0.86
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	19	0.86
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	19	0.86
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	19	0.86
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	19	0.86
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	19	0.86
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	19	0.86
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	7	0.86
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	7	0.86
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	7	0.86
(1,298)	2:192:B:SER:HB2	2:188:B:LYS:HD3	18	0.86
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	13	0.85
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD11	1	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4030)	2:192:B:SER:HB2	2:188:B:LYS:HG2	17	0.85
(1,4011)	2:314:B:ALA:HB1	2:313:B:VAL:HG21	16	0.85
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG21	14	0.85
(1,3837)	2:210:B:LYS:HG3	2:214:B:VAL:HG22	16	0.85
(1,2160)	2:282:B:LYS:HB3	2:282:B:LYS:H	18	0.85
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	11	0.85
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	11	0.85
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	11	0.85
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	11	0.85
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	11	0.85
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	11	0.85
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	11	0.85
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	11	0.85
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	11	0.85
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	6	0.85
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	6	0.85
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	6	0.85
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	6	0.85
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	6	0.85
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	6	0.85
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	6	0.85
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	6	0.85
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	6	0.85
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	9	0.85
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	9	0.85
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	9	0.85
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	14	0.85
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	14	0.85
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	14	0.85
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	10	0.85
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	10	0.85
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	10	0.85
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	12	0.85
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	12	0.85
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	12	0.85
(1,4555)	2:294:B:PHE:HD2	2:264:B:LEU:HD13	17	0.84
(1,4497)	2:292:B:HIS:HE1	2:295:B:LEU:HD11	20	0.84
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD12	12	0.84
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD21	11	0.84
(1,4237)	2:218:B:VAL:HG13	2:198:B:ALA:H	7	0.84
(1,3857)	2:224:B:TYR:HD1	2:227:B:VAL:HG12	11	0.84
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB2	9	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	5	0.84
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	10	0.84
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	10	0.84
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	10	0.84
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	10	0.84
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	10	0.84
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	10	0.84
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD11	12	0.84
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD12	12	0.84
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD13	12	0.84
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	14	0.84
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	14	0.84
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	14	0.84
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	6	0.84
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	6	0.84
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	6	0.84
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	15	0.84
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	15	0.84
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	15	0.84
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	6	0.84
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	6	0.84
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	6	0.84
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	5	0.84
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	5	0.84
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	5	0.84
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	5	0.84
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	5	0.84
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	5	0.84
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	5	0.84
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	5	0.84
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	5	0.84
(1,4621)	2:267:B:PHE:HE2	2:298:B:LEU:HD12	17	0.83
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE3	8	0.83
(1,4417)	1:109:A:GLU:HG2	1:112:A:ILE:HG22	12	0.83
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD22	7	0.83
(1,4296)	1:90:A:LEU:HD13	1:87:A:MET:HE1	11	0.83
(1,4153)	2:298:B:LEU:HD11	2:264:B:LEU:H	17	0.83
(1,4030)	2:192:B:SER:HB2	2:188:B:LYS:HG2	11	0.83
(1,3824)	2:214:B:VAL:HG23	2:202:B:LYS:HE3	9	0.83
(1,3750)	1:111:A:ILE:HD11	2:165:B:LYS:HE2	17	0.83
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	11	0.83
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	11	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	11	0.83
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD11	3	0.83
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD12	3	0.83
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD13	3	0.83
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD11	3	0.83
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD12	3	0.83
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD13	3	0.83
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD11	3	0.83
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD12	3	0.83
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD13	3	0.83
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG12	2	0.82
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE3	20	0.82
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	12	0.82
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	10	0.82
(1,4363)	2:172:B:TRP:HD1	1:106:A:VAL:HG22	17	0.82
(1,4316)	1:87:A:MET:HE1	1:90:A:LEU:HD21	4	0.82
(1,4316)	1:87:A:MET:HE1	1:90:A:LEU:HD23	15	0.82
(1,4030)	2:192:B:SER:HB2	2:188:B:LYS:HG2	18	0.82
(1,4001)	2:273:B:MET:HB3	2:274:B:LEU:HD13	12	0.82
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG21	15	0.82
(1,3875)	2:242:B:TYR:HB3	2:234:B:LEU:HD21	10	0.82
(1,3776)	2:257:B:VAL:HG22	2:185:B:PRO:HB3	6	0.82
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	8	0.82
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	8	0.82
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	8	0.82
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	15	0.82
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	15	0.82
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	15	0.82
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	6	0.82
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	6	0.82
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	6	0.82
(1,815)	2:253:B:PRO:HG2	2:256:B:GLN:HG3	5	0.82
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG11	6	0.81
(1,4513)	2:235:B:TYR:HE2	2:175:B:ILE:HD11	20	0.81
(1,4511)	2:182:B:PHE:HD1	2:184:B:LEU:HB3	4	0.81
(1,4496)	2:267:B:PHE:HD1	2:158:B:VAL:HG13	14	0.81
(1,4317)	1:87:A:MET:HB2	1:90:A:LEU:HD23	12	0.81
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	4	0.81
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD11	14	0.81
(1,4237)	2:218:B:VAL:HG11	2:198:B:ALA:H	8	0.81
(1,3920)	2:194:B:LEU:HD23	2:263:B:LEU:HD12	9	0.81
(1,3824)	2:214:B:VAL:HG23	2:202:B:LYS:HE3	6	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3812)	2:193:B:ILE:HG23	2:194:B:LEU:HD22	16	0.81
(1,3803)	2:194:B:LEU:HD22	2:193:B:ILE:HG23	16	0.81
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	13	0.81
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	13	0.81
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	13	0.81
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	13	0.81
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	13	0.81
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	13	0.81
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	4	0.81
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	4	0.81
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	4	0.81
(1,2160)	2:282:B:LYS:HB3	2:282:B:LYS:H	17	0.81
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	15	0.81
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	15	0.81
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	15	0.81
(1,532)	2:218:B:VAL:HG21	2:221:B:ILE:HD11	16	0.81
(1,532)	2:218:B:VAL:HG21	2:221:B:ILE:HD12	16	0.81
(1,532)	2:218:B:VAL:HG21	2:221:B:ILE:HD13	16	0.81
(1,532)	2:218:B:VAL:HG22	2:221:B:ILE:HD11	16	0.81
(1,532)	2:218:B:VAL:HG22	2:221:B:ILE:HD12	16	0.81
(1,532)	2:218:B:VAL:HG22	2:221:B:ILE:HD13	16	0.81
(1,532)	2:218:B:VAL:HG23	2:221:B:ILE:HD11	16	0.81
(1,532)	2:218:B:VAL:HG23	2:221:B:ILE:HD12	16	0.81
(1,532)	2:218:B:VAL:HG23	2:221:B:ILE:HD13	16	0.81
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD11	16	0.81
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD12	16	0.81
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD13	16	0.81
(1,4634)	2:237:B:PHE:HE2	2:181:B:LEU:HG	7	0.8
(1,4472)	1:93:A:SER:HB3	1:90:A:LEU:H	5	0.8
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG21	12	0.8
(1,4324)	1:81:A:LEU:HD13	1:80:A:HIS:HB2	14	0.8
(1,4323)	2:279:B:LEU:HD21	1:91:A:HIS:HB3	9	0.8
(1,3912)	2:185:B:PRO:HB3	2:257:B:VAL:HG21	7	0.8
(1,3901)	2:246:B:LEU:HD12	2:252:B:ALA:HB2	4	0.8
(1,3796)	2:255:B:SER:HB3	2:190:B:VAL:HG12	4	0.8
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD23	14	0.8
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	10	0.8
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	10	0.8
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	10	0.8
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG11	20	0.8
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG12	20	0.8
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG13	20	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG11	20	0.8
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG12	20	0.8
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG13	20	0.8
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG11	20	0.8
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG12	20	0.8
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG13	20	0.8
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	3	0.8
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	3	0.8
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	3	0.8
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	3	0.8
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	3	0.8
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	3	0.8
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	3	0.8
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	3	0.8
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	3	0.8
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	5	0.8
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	5	0.8
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	5	0.8
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	5	0.8
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	5	0.8
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	5	0.8
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	5	0.8
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	5	0.8
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	5	0.8
(1,671)	2:234:B:LEU:HD21	2:239:B:ARG:HD2	5	0.8
(1,671)	2:234:B:LEU:HD22	2:239:B:ARG:HD2	5	0.8
(1,671)	2:234:B:LEU:HD23	2:239:B:ARG:HD2	5	0.8
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	20	0.8
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	20	0.8
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	20	0.8
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	20	0.8
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	20	0.8
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	20	0.8
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	20	0.8
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	20	0.8
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	20	0.8
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD21	14	0.8
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD22	14	0.8
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD23	14	0.8
(1,4575)	2:242:B:TYR:HE1	2:234:B:LEU:HD12	20	0.79
(1,4560)	2:225:B:PHE:HD1	2:221:B:ILE:HG21	4	0.79
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	19	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4511)	2:182:B:PHE:HD1	2:184:B:LEU:HB3	14	0.79
(1,4497)	2:292:B:HIS:HE1	2:295:B:LEU:HD13	17	0.79
(1,4496)	2:267:B:PHE:HD2	2:263:B:LEU:HD23	5	0.79
(1,4444)	1:97:A:PRO:HG3	1:96:A:LEU:HD12	12	0.79
(1,4382)	2:168:B:LEU:HD12	1:108:A:PRO:HD3	18	0.79
(1,4324)	1:81:A:LEU:HD11	1:80:A:HIS:HB2	3	0.79
(1,4014)	2:181:B:LEU:HD13	2:314:B:ALA:HB2	13	0.79
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD13	6	0.79
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE1	12	0.79
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG23	4	0.79
(1,3845)	2:202:B:LYS:HE2	2:218:B:VAL:HG22	2	0.79
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB1	8	0.79
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE3	17	0.79
(1,3744)	2:299:B:ALA:HA	2:164:B:LEU:HD21	5	0.79
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	4	0.79
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	4	0.79
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	4	0.79
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	4	0.79
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	4	0.79
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	4	0.79
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	4	0.79
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	4	0.79
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	4	0.79
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	7	0.79
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	7	0.79
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	7	0.79
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	2	0.79
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	2	0.79
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	2	0.79
(1,1120)	2:305:B:LEU:HD21	2:301:B:ASN:HB2	11	0.79
(1,1120)	2:305:B:LEU:HD22	2:301:B:ASN:HB2	11	0.79
(1,1120)	2:305:B:LEU:HD23	2:301:B:ASN:HB2	11	0.79
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	1	0.79
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	1	0.79
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	1	0.79
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	10	0.79
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	10	0.79
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	10	0.79
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	16	0.79
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	16	0.79
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD11	8	0.79
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD12	8	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD13	8	0.79
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	9	0.78
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	9	0.78
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	9	0.78
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	9	0.78
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	9	0.78
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	9	0.78
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG12	7	0.78
(1,4447)	2:232:B:GLN:HG2	1:103:A:ARG:HG2	11	0.78
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG12	13	0.78
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	17	0.78
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	6	0.78
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE3	1	0.78
(1,3824)	2:214:B:VAL:HG22	2:202:B:LYS:HE2	19	0.78
(1,3803)	2:194:B:LEU:HD23	2:193:B:ILE:HG21	6	0.78
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE3	1	0.78
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE3	1	0.78
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	9	0.78
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	9	0.78
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	9	0.78
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	18	0.78
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	18	0.78
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	18	0.78
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	1	0.78
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	1	0.78
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	1	0.78
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	12	0.78
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	12	0.78
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	12	0.78
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	13	0.78
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	13	0.78
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	13	0.78
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	8	0.78
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	8	0.78
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	8	0.78
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	8	0.78
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	8	0.78
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	8	0.78
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	8	0.78
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	8	0.78
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	8	0.78
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD11	20	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4609)	2:224:B:TYR:HD2	2:223:B:GLU:HB3	2	0.77
(1,4601)	2:267:B:PHE:HE2	2:263:B:LEU:HD22	12	0.77
(1,4600)	2:200:B:TYR:HE1	2:201:B:LYS:HG2	16	0.77
(1,4579)	2:306:B:PHE:HD2	2:261:B:PRO:HG3	20	0.77
(1,4511)	2:182:B:PHE:HD1	2:175:B:ILE:HD12	1	0.77
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	2	0.77
(1,4357)	2:273:B:MET:HE2	1:100:A:ASN:HA	4	0.77
(1,4324)	1:81:A:LEU:HD11	1:80:A:HIS:HB2	15	0.77
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE1	7	0.77
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	11	0.77
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD13	17	0.77
(1,3928)	1:111:A:ILE:HD12	2:268:B:VAL:HG13	19	0.77
(1,3921)	2:194:B:LEU:HD23	2:263:B:LEU:HD22	12	0.77
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	13	0.77
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	4	0.77
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	4	0.77
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	4	0.77
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	4	0.77
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	4	0.77
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	4	0.77
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB3	20	0.77
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB3	20	0.77
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB3	20	0.77
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	9	0.77
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	9	0.77
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	9	0.77
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	7	0.77
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	7	0.77
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	7	0.77
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	7	0.77
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	7	0.77
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	7	0.77
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	7	0.77
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	7	0.77
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	7	0.77
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	15	0.77
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	15	0.77
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD11	10	0.77
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD12	10	0.77
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD13	10	0.77
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	10	0.76
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HE2	16	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4558)	2:224:B:TYR:HD1	2:270:B:ILE:HD12	7	0.76
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	6	0.76
(1,4390)	1:115:A:VAL:HG22	1:111:A:ILE:HA	8	0.76
(1,4384)	2:169:B:VAL:HG23	1:109:A:GLU:HA	10	0.76
(1,4324)	1:95:A:ILE:HG22	1:91:A:HIS:HB2	19	0.76
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD22	15	0.76
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD13	13	0.76
(1,4054)	2:313:B:VAL:HG11	2:180:B:GLN:HE22	4	0.76
(1,3901)	2:257:B:VAL:HG23	2:252:B:ALA:HB2	5	0.76
(1,3824)	2:214:B:VAL:HG22	2:202:B:LYS:HE3	7	0.76
(1,3812)	2:218:B:VAL:HG23	2:194:B:LEU:HD22	17	0.76
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	8	0.76
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	9	0.76
(1,3420)	2:236:B:LYS:HG2	1:104:A:ASN:HD22	14	0.76
(1,3298)	1:106:A:VAL:HG21	1:109:A:GLU:H	14	0.76
(1,3298)	1:106:A:VAL:HG22	1:109:A:GLU:H	14	0.76
(1,3298)	1:106:A:VAL:HG23	1:109:A:GLU:H	14	0.76
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB2	17	0.76
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB2	17	0.76
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB2	17	0.76
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	6	0.76
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	4	0.76
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	4	0.76
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	4	0.76
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	4	0.76
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	4	0.76
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	4	0.76
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	4	0.76
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	4	0.76
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	4	0.76
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	8	0.76
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	8	0.76
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	8	0.76
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	8	0.76
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	8	0.76
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	8	0.76
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	8	0.76
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	8	0.76
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	8	0.76
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD21	15	0.76
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD22	15	0.76
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD23	15	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4547)	2:200:B:TYR:HD1	2:204:B:ARG:HD2	16	0.75
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	8	0.75
(1,4527)	2:306:B:PHE:HD1	2:305:B:LEU:HG	12	0.75
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG22	16	0.75
(1,4361)	2:235:B:TYR:HE1	1:106:A:VAL:HG11	3	0.75
(1,4296)	2:279:B:LEU:HD11	1:87:A:MET:HE1	4	0.75
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE3	3	0.75
(1,4153)	2:298:B:LEU:HD13	2:264:B:LEU:H	14	0.75
(1,4030)	2:192:B:SER:HB2	2:188:B:LYS:HG2	10	0.75
(1,3947)	2:272:B:ALA:HB2	2:273:B:MET:HE3	10	0.75
(1,3935)	2:265:B:ARG:HB2	2:269:B:ARG:HD3	11	0.75
(1,3921)	2:221:B:ILE:HG21	2:263:B:LEU:HD21	18	0.75
(1,3911)	2:252:B:ALA:HB3	2:257:B:VAL:HG13	18	0.75
(1,3880)	2:236:B:LYS:HA	2:239:B:ARG:HG2	15	0.75
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB3	19	0.75
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	11	0.75
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	17	0.75
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	6	0.75
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	6	0.75
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	6	0.75
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	6	0.75
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	6	0.75
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	6	0.75
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	6	0.75
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	6	0.75
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	6	0.75
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	6	0.75
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	6	0.75
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	6	0.75
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	11	0.75
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	11	0.75
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	11	0.75
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD11	5	0.75
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD12	5	0.75
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD13	5	0.75
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD11	5	0.75
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD12	5	0.75
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD13	5	0.75
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	10	0.75
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD11	10	0.75
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD12	10	0.75
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD13	10	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD11	10	0.75
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	10	0.75
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD13	10	0.75
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD21	11	0.75
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD22	11	0.75
(1,376)	2:190:B:VAL:HG11	2:194:B:LEU:HD23	11	0.75
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD21	11	0.75
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD22	11	0.75
(1,376)	2:190:B:VAL:HG12	2:194:B:LEU:HD23	11	0.75
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD21	11	0.75
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD22	11	0.75
(1,376)	2:190:B:VAL:HG13	2:194:B:LEU:HD23	11	0.75
(1,4587)	2:306:B:PHE:HE1	2:260:B:ALA:HB1	17	0.74
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	18	0.74
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	19	0.74
(1,4497)	2:292:B:HIS:HE1	2:158:B:VAL:HG23	16	0.74
(1,4433)	2:169:B:VAL:HG21	1:116:A:ARG:HG3	8	0.74
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD12	8	0.74
(1,4384)	2:169:B:VAL:HG23	1:109:A:GLU:HA	18	0.74
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	12	0.74
(1,4327)	1:95:A:ILE:HD11	1:92:A:GLU:HB3	7	0.74
(1,4312)	2:223:B:GLU:HG3	1:96:A:LEU:HD11	9	0.74
(1,4008)	2:170:B:ASP:HB3	2:169:B:VAL:HG11	18	0.74
(1,3945)	2:274:B:LEU:HD21	2:271:B:GLY:HA3	11	0.74
(1,3776)	2:257:B:VAL:HG22	2:185:B:PRO:HB3	17	0.74
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	20	0.74
(1,3250)	1:103:A:ARG:HD3	1:102:A:GLU:H	15	0.74
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	17	0.74
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	17	0.74
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	17	0.74
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD21	20	0.74
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD22	20	0.74
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD23	20	0.74
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD3	1	0.74
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	13	0.74
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	20	0.74
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	2	0.74
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	2	0.74
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	2	0.74
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	2	0.74
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	2	0.74
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	2	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	2	0.74
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	2	0.74
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	2	0.74
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	5	0.73
(1,4532)	2:183:B:TYR:HD2	2:184:B:LEU:HA	7	0.73
(1,4520)	2:212:B:TYR:HD2	2:215:B:ASN:HB2	18	0.73
(1,4512)	2:235:B:TYR:HD1	2:175:B:ILE:HD12	14	0.73
(1,4497)	2:292:B:HIS:HE1	2:158:B:VAL:HG21	3	0.73
(1,4492)	2:212:B:TYR:HE1	1:81:A:LEU:H	7	0.73
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	11	0.73
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	7	0.73
(1,4324)	1:81:A:LEU:HD13	1:80:A:HIS:HB2	11	0.73
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD22	4	0.73
(1,4008)	2:170:B:ASP:HB3	2:169:B:VAL:HG13	5	0.73
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	5	0.73
(1,3852)	2:218:B:VAL:HG22	2:222:B:LYS:HE2	5	0.73
(1,3749)	2:160:B:ILE:HG21	2:165:B:LYS:HE3	17	0.73
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	6	0.73
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	12	0.73
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	16	0.73
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	18	0.73
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD11	10	0.73
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD12	10	0.73
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD13	10	0.73
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD11	10	0.73
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD12	10	0.73
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD13	10	0.73
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	2	0.73
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	2	0.73
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	2	0.73
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD3	20	0.73
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD3	20	0.73
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD3	20	0.73
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	16	0.73
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	16	0.73
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	16	0.73
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD3	14	0.73
(1,1526)	2:187:B:LYS:HB2	2:188:B:LYS:H	1	0.73
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	16	0.73
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	16	0.73
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	16	0.73
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	16	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	16	0.73
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	16	0.73
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	16	0.73
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	16	0.73
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	16	0.73
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	18	0.73
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	18	0.73
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	18	0.73
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	18	0.73
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	18	0.73
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	18	0.73
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	18	0.73
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	18	0.73
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	18	0.73
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	13	0.73
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	13	0.73
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	13	0.73
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	8	0.73
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	8	0.73
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	8	0.73
(1,87)	2:302:B:SER:HB3	2:164:B:LEU:HD21	5	0.73
(1,87)	2:302:B:SER:HB3	2:164:B:LEU:HD22	5	0.73
(1,87)	2:302:B:SER:HB3	2:164:B:LEU:HD23	5	0.73
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD11	6	0.73
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD12	6	0.73
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD13	6	0.73
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	6	0.72
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	6	0.72
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	6	0.72
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	6	0.72
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	6	0.72
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	6	0.72
(1,4600)	2:200:B:TYR:HE2	2:201:B:LYS:HG2	14	0.72
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE3	15	0.72
(1,4492)	2:212:B:TYR:HE2	1:81:A:LEU:H	13	0.72
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD12	1	0.72
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	17	0.72
(1,4373)	2:169:B:VAL:HA	1:107:A:LEU:HD23	3	0.72
(1,4364)	1:111:A:ILE:HD12	1:107:A:LEU:HA	19	0.72
(1,4363)	2:172:B:TRP:HD1	1:106:A:VAL:HG22	7	0.72
(1,4361)	2:235:B:TYR:HE1	1:106:A:VAL:HG13	13	0.72
(1,4140)	2:254:B:MET:HE3	2:252:B:ALA:H	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4011)	2:314:B:ALA:HB1	2:313:B:VAL:HG23	6	0.72
(1,3843)	1:96:A:LEU:HD21	2:227:B:VAL:HG12	7	0.72
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB3	17	0.72
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD22	13	0.72
(1,3734)	2:161:B:PRO:HB2	2:160:B:ILE:HG23	16	0.72
(1,3689)	2:318:B:TYR:HE1	2:241:B:GLN:HG2	14	0.72
(1,3689)	2:318:B:TYR:HE2	2:241:B:GLN:HG2	14	0.72
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	3	0.72
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	4	0.72
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	13	0.72
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	10	0.72
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	10	0.72
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	10	0.72
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	15	0.72
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	15	0.72
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	15	0.72
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	3	0.72
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	3	0.72
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	3	0.72
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	8	0.72
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	8	0.72
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	8	0.72
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD21	4	0.72
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD22	4	0.72
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD23	4	0.72
(1,2136)	2:278:B:PRO:HB2	2:279:B:LEU:H	3	0.72
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	16	0.72
(1,815)	2:253:B:PRO:HB2	2:256:B:GLN:HG2	13	0.72
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	20	0.72
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	20	0.72
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	20	0.72
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	20	0.72
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	20	0.72
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	20	0.72
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	20	0.72
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	20	0.72
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	20	0.72
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	16	0.72
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	16	0.72
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	16	0.72
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	4	0.72
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	4	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	4	0.72
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	8	0.72
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	8	0.72
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	8	0.72
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	8	0.72
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	8	0.72
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	8	0.72
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	8	0.72
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	8	0.72
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	8	0.72
(1,4604)	2:225:B:PHE:HE1	2:266:B:LEU:HD12	6	0.71
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD21	5	0.71
(1,4390)	1:115:A:VAL:HG22	1:111:A:ILE:HA	14	0.71
(1,4385)	1:112:A:ILE:HG22	1:109:A:GLU:HB3	5	0.71
(1,4334)	1:96:A:LEU:HD13	1:74:A:SER:HB3	12	0.71
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	16	0.71
(1,4014)	2:181:B:LEU:HD12	2:314:B:ALA:HB3	4	0.71
(1,3921)	2:221:B:ILE:HG22	2:263:B:LEU:HD23	1	0.71
(1,3915)	2:305:B:LEU:HD21	2:260:B:ALA:HB3	3	0.71
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	2	0.71
(1,3250)	1:103:A:ARG:HD3	1:102:A:GLU:H	12	0.71
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	4	0.71
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	4	0.71
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	4	0.71
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	13	0.71
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	13	0.71
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	13	0.71
(1,1120)	2:305:B:LEU:HD21	2:301:B:ASN:HB2	12	0.71
(1,1120)	2:305:B:LEU:HD22	2:301:B:ASN:HB2	12	0.71
(1,1120)	2:305:B:LEU:HD23	2:301:B:ASN:HB2	12	0.71
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	2	0.71
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	16	0.71
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	16	0.71
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	16	0.71
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	16	0.71
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	16	0.71
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	16	0.71
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	16	0.71
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	16	0.71
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	16	0.71
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	7	0.71
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	7	0.71
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	11	0.71
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	11	0.71
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	11	0.71
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	18	0.71
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	18	0.71
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	18	0.71
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD11	12	0.71
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD12	12	0.71
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD13	12	0.71
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD11	12	0.71
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD12	12	0.71
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD13	12	0.71
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD11	12	0.71
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD12	12	0.71
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD13	12	0.71
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD11	11	0.71
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD12	11	0.71
(1,85)	2:295:B:LEU:HD21	2:164:B:LEU:HD13	11	0.71
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD11	11	0.71
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD12	11	0.71
(1,85)	2:295:B:LEU:HD22	2:164:B:LEU:HD13	11	0.71
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD11	11	0.71
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD12	11	0.71
(1,85)	2:295:B:LEU:HD23	2:164:B:LEU:HD13	11	0.71
(1,4597)	2:267:B:PHE:HE1	2:295:B:LEU:HB2	11	0.7
(1,4589)	2:182:B:PHE:HD2	2:259:B:GLY:HA2	9	0.7
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG13	15	0.7
(1,4511)	2:182:B:PHE:HD1	2:184:B:LEU:HB3	7	0.7
(1,4492)	2:212:B:TYR:HE2	1:81:A:LEU:H	10	0.7
(1,4472)	1:93:A:SER:HB2	1:95:A:ILE:H	12	0.7
(1,4396)	2:165:B:LYS:HE2	1:111:A:ILE:HD12	2	0.7
(1,4324)	1:81:A:LEU:HD11	1:80:A:HIS:HB2	16	0.7
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD11	10	0.7
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE3	14	0.7
(1,3832)	2:217:B:VAL:HG12	2:213:B:ALA:HB1	18	0.7
(1,3832)	2:214:B:VAL:HG12	2:213:B:ALA:HB1	20	0.7
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	18	0.7
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD21	19	0.7
(1,3766)	2:235:B:TYR:HD1	2:175:B:ILE:HD12	17	0.7
(1,3454)	2:292:B:HIS:HE1	2:159:B:LYS:HG3	6	0.7
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	4	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	4	0.7
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	4	0.7
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	20	0.7
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	20	0.7
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	20	0.7
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	12	0.7
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	12	0.7
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	12	0.7
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	13	0.7
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	13	0.7
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	13	0.7
(1,2007)	2:226:B:ASN:HD21	2:255:B:SER:H	2	0.7
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB1	16	0.7
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB2	16	0.7
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB3	16	0.7
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB1	16	0.7
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB2	16	0.7
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB3	16	0.7
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB1	16	0.7
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB2	16	0.7
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB3	16	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	8	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	8	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	8	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	12	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	12	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	12	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB1	20	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB2	20	0.7
(1,925)	2:273:B:MET:HB3	2:272:B:ALA:HB3	20	0.7
(1,676)	2:242:B:TYR:HD1	2:239:B:ARG:HD2	11	0.7
(1,676)	2:242:B:TYR:HD2	2:239:B:ARG:HD2	11	0.7
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	12	0.7
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	12	0.7
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	12	0.7
(1,4612)	2:262:B:HIS:HD2	2:265:B:ARG:HG3	11	0.69
(1,4575)	2:242:B:TYR:HE2	2:246:B:LEU:HD11	9	0.69
(1,4564)	2:197:B:TYR:HE2	2:198:B:ALA:HB1	17	0.69
(1,4511)	2:182:B:PHE:HD2	2:184:B:LEU:HB3	17	0.69
(1,4390)	1:115:A:VAL:HG22	1:111:A:ILE:HA	10	0.69
(1,4384)	2:169:B:VAL:HG23	1:109:A:GLU:HA	19	0.69
(1,4382)	2:168:B:LEU:HD13	1:108:A:PRO:HD3	8	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4344)	1:92:A:GLU:HB3	1:95:A:ILE:HD11	4	0.69
(1,4316)	1:88:A:GLN:HB2	1:90:A:LEU:HD22	13	0.69
(1,4031)	2:298:B:LEU:HB2	2:193:B:ILE:HD12	14	0.69
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD21	11	0.69
(1,3948)	2:276:B:TYR:HE2	2:273:B:MET:HE2	1	0.69
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	11	0.69
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD21	5	0.69
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	11	0.69
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	11	0.69
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	11	0.69
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	11	0.69
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	11	0.69
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	11	0.69
(1,3613)	2:276:B:TYR:HE2	2:273:B:MET:HE2	1	0.69
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	1	0.69
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	7	0.69
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	6	0.69
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	6	0.69
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG11	14	0.69
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG12	14	0.69
(1,2827)	1:105:A:PHE:HA	1:106:A:VAL:HG13	14	0.69
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD21	15	0.69
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD22	15	0.69
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD23	15	0.69
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	5	0.69
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	5	0.69
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	5	0.69
(1,2023)	2:257:B:VAL:HG11	2:256:B:GLN:H	11	0.69
(1,2023)	2:257:B:VAL:HG12	2:256:B:GLN:H	11	0.69
(1,2023)	2:257:B:VAL:HG13	2:256:B:GLN:H	11	0.69
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	6	0.69
(1,1054)	2:295:B:LEU:HD11	2:292:B:HIS:HA	9	0.69
(1,1054)	2:295:B:LEU:HD12	2:292:B:HIS:HA	9	0.69
(1,1054)	2:295:B:LEU:HD13	2:292:B:HIS:HA	9	0.69
(1,815)	2:253:B:PRO:HG2	2:256:B:GLN:HG3	8	0.69
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	3	0.69
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	3	0.69
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	3	0.69
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD21	1	0.69
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD22	1	0.69
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD23	1	0.69
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD21	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD22	1	0.69
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD23	1	0.69
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD21	1	0.69
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD22	1	0.69
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD23	1	0.69
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	8	0.69
(1,387)	2:196:B:ASP:HA	2:195:B:GLU:HG3	9	0.69
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD21	14	0.69
(1,4612)	2:290:B:TYR:HE2	2:286:B:LEU:HG	14	0.68
(1,4609)	2:224:B:TYR:HD2	2:223:B:GLU:HB3	11	0.68
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD13	7	0.68
(1,4243)	1:72:A:VAL:HG23	1:71:A:GLN:HB2	15	0.68
(1,3945)	2:274:B:LEU:HD21	2:271:B:GLY:HA3	19	0.68
(1,3920)	2:194:B:LEU:HD23	2:263:B:LEU:HD13	10	0.68
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB2	15	0.68
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB3	16	0.68
(1,3796)	2:255:B:SER:HB3	2:190:B:VAL:HG11	19	0.68
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD23	10	0.68
(1,2806)	2:232:B:GLN:HA	1:103:A:ARG:HG2	19	0.68
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD11	6	0.68
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD12	6	0.68
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD13	6	0.68
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD11	6	0.68
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	6	0.68
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD13	6	0.68
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD11	10	0.67
(1,4460)	1:87:A:MET:HG3	1:87:A:MET:H	2	0.67
(1,4444)	1:97:A:PRO:HG3	1:96:A:LEU:HD13	6	0.67
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD12	4	0.67
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	16	0.67
(1,4384)	2:169:B:VAL:HG22	1:109:A:GLU:HA	20	0.67
(1,4324)	1:81:A:LEU:HD13	1:80:A:HIS:HB2	10	0.67
(1,4280)	2:290:B:TYR:HE2	1:81:A:LEU:HD21	6	0.67
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD21	10	0.67
(1,4276)	1:98:A:PHE:HE2	1:96:A:LEU:HD21	8	0.67
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG12	7	0.67
(1,3950)	2:270:B:ILE:HG22	2:274:B:LEU:HD21	19	0.67
(1,3947)	2:272:B:ALA:HB2	2:273:B:MET:HE3	11	0.67
(1,3859)	2:266:B:LEU:HD11	2:228:B:MET:HE2	13	0.67
(1,3749)	2:160:B:ILE:HG21	2:165:B:LYS:HE3	1	0.67
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	20	0.67
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	20	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3441)	2:227:B:VAL:HG21	1:100:A:ASN:HD21	11	0.67
(1,3441)	2:227:B:VAL:HG22	1:100:A:ASN:HD21	11	0.67
(1,3441)	2:227:B:VAL:HG23	1:100:A:ASN:HD21	11	0.67
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD21	9	0.67
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD22	9	0.67
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD23	9	0.67
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	8	0.67
(1,1702)	2:211:B:GLU:HB3	2:212:B:TYR:H	4	0.67
(1,1576)	2:193:B:ILE:HG13	2:193:B:ILE:H	17	0.67
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	4	0.67
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	4	0.67
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	4	0.67
(1,954)	2:274:B:LEU:HD11	2:277:B:THR:HB	13	0.67
(1,954)	2:274:B:LEU:HD12	2:277:B:THR:HB	13	0.67
(1,954)	2:274:B:LEU:HD13	2:277:B:THR:HB	13	0.67
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	10	0.67
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	10	0.67
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	10	0.67
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	10	0.67
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	10	0.67
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	10	0.67
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	10	0.67
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	10	0.67
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	10	0.67
(1,4611)	2:290:B:TYR:HD2	2:286:B:LEU:HG	5	0.66
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HB3	8	0.66
(1,4560)	2:225:B:PHE:HD1	2:233:B:LEU:HD11	14	0.66
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	9	0.66
(1,4460)	1:87:A:MET:HG3	1:87:A:MET:H	17	0.66
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG11	4	0.66
(1,4390)	1:115:A:VAL:HG23	1:111:A:ILE:HA	17	0.66
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	2	0.66
(1,4296)	2:279:B:LEU:HD11	1:87:A:MET:HE1	13	0.66
(1,4198)	2:164:B:LEU:HD21	2:299:B:ALA:H	5	0.66
(1,4167)	2:279:B:LEU:HD13	2:280:B:ASP:H	20	0.66
(1,4140)	2:185:B:PRO:HB3	2:252:B:ALA:H	4	0.66
(1,4028)	1:96:A:LEU:HD12	2:277:B:THR:HB	2	0.66
(1,4014)	2:181:B:LEU:HD13	2:314:B:ALA:HB3	7	0.66
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG12	1	0.66
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD12	2	0.66
(1,4001)	2:273:B:MET:HB3	2:274:B:LEU:HD13	3	0.66
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD12	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG21	5	0.66
(1,3824)	2:214:B:VAL:HG23	2:202:B:LYS:HE2	14	0.66
(1,3039)	2:231:B:THR:HA	1:102:A:GLU:HG3	13	0.66
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	1	0.66
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	1	0.66
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	1	0.66
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD21	8	0.66
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD22	8	0.66
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD23	8	0.66
(1,2775)	1:96:A:LEU:HD11	1:100:A:ASN:HB3	6	0.66
(1,2775)	1:96:A:LEU:HD12	1:100:A:ASN:HB3	6	0.66
(1,2775)	1:96:A:LEU:HD13	1:100:A:ASN:HB3	6	0.66
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	10	0.66
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	10	0.66
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	10	0.66
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	20	0.66
(1,900)	2:269:B:ARG:HA	2:269:B:ARG:HD3	7	0.66
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	2	0.66
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	2	0.66
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	2	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	2	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	2	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	2	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	2	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	2	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	2	0.66
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	13	0.66
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	13	0.66
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	13	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	13	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	13	0.66
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	13	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	13	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	13	0.66
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	13	0.66
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD11	17	0.66
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD12	17	0.66
(1,173)	2:181:B:LEU:HD11	2:175:B:ILE:HD13	17	0.66
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD11	17	0.66
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD12	17	0.66
(1,173)	2:181:B:LEU:HD12	2:175:B:ILE:HD13	17	0.66
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD11	17	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD12	17	0.66
(1,173)	2:181:B:LEU:HD13	2:175:B:ILE:HD13	17	0.66
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD11	14	0.66
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD12	14	0.66
(1,3)	2:289:B:ASN:HB2	2:286:B:LEU:HD13	14	0.66
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD12	2	0.65
(1,4564)	2:197:B:TYR:HE2	2:198:B:ALA:HB3	4	0.65
(1,4547)	2:200:B:TYR:HD1	2:204:B:ARG:HD3	3	0.65
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	9	0.65
(1,4511)	2:182:B:PHE:HD2	2:181:B:LEU:HG	9	0.65
(1,4382)	2:168:B:LEU:HD13	1:108:A:PRO:HD3	12	0.65
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	15	0.65
(1,4271)	2:212:B:TYR:HD1	1:81:A:LEU:HA	4	0.65
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	20	0.65
(1,3911)	2:252:B:ALA:HB2	2:257:B:VAL:HG13	7	0.65
(1,3832)	2:214:B:VAL:HG11	2:213:B:ALA:HB2	2	0.65
(1,3832)	2:214:B:VAL:HG11	2:213:B:ALA:HB3	5	0.65
(1,3832)	2:214:B:VAL:HG11	2:213:B:ALA:HB2	10	0.65
(1,3795)	2:194:B:LEU:HD23	2:190:B:VAL:HG12	10	0.65
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	5	0.65
(1,3441)	2:227:B:VAL:HG21	1:100:A:ASN:HD21	13	0.65
(1,3441)	2:227:B:VAL:HG22	1:100:A:ASN:HD21	13	0.65
(1,3441)	2:227:B:VAL:HG23	1:100:A:ASN:HD21	13	0.65
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD3	3	0.65
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD3	3	0.65
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD3	3	0.65
(1,2811)	1:106:A:VAL:HG11	1:104:A:ASN:HB3	2	0.65
(1,2811)	1:106:A:VAL:HG12	1:104:A:ASN:HB3	2	0.65
(1,2811)	1:106:A:VAL:HG13	1:104:A:ASN:HB3	2	0.65
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	20	0.65
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	1	0.65
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	1	0.65
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	1	0.65
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG11	11	0.65
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG12	11	0.65
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG13	11	0.65
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG11	11	0.65
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG12	11	0.65
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG13	11	0.65
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG11	11	0.65
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG12	11	0.65
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG13	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,815)	2:253:B:PRO:HB2	2:256:B:GLN:HG3	20	0.65
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	1	0.65
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	1	0.65
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	1	0.65
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	9	0.65
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	9	0.65
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	9	0.65
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	1	0.65
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	1	0.65
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	1	0.65
(1,454)	2:202:B:LYS:HD3	2:211:B:GLU:HG2	13	0.65
(1,334)	2:259:B:GLY:HA2	2:190:B:VAL:HG21	14	0.65
(1,334)	2:259:B:GLY:HA2	2:190:B:VAL:HG22	14	0.65
(1,334)	2:259:B:GLY:HA2	2:190:B:VAL:HG23	14	0.65
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	19	0.65
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	19	0.65
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	19	0.65
(2,12)	2:288:B:LEU:HD21	2:157:B:LYS:H	8	0.64
(2,12)	2:288:B:LEU:HD22	2:157:B:LYS:H	8	0.64
(2,12)	2:288:B:LEU:HD23	2:157:B:LYS:H	8	0.64
(1,4639)	2:237:B:PHE:HE1	2:322:B:ALA:HB2	20	0.64
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	15	0.64
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG21	4	0.64
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	13	0.64
(1,4384)	2:169:B:VAL:HG21	1:109:A:GLU:HA	1	0.64
(1,4382)	2:168:B:LEU:HD13	1:108:A:PRO:HD3	9	0.64
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	13	0.64
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG23	16	0.64
(1,4324)	1:95:A:ILE:HG21	1:91:A:HIS:HB2	9	0.64
(1,4280)	2:290:B:TYR:HE2	1:81:A:LEU:HD22	13	0.64
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE2	11	0.64
(1,3843)	2:194:B:LEU:HD12	2:218:B:VAL:HG23	12	0.64
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB1	14	0.64
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	20	0.64
(1,2892)	2:268:B:VAL:HG21	1:108:A:PRO:HG3	19	0.64
(1,2892)	2:268:B:VAL:HG22	1:108:A:PRO:HG3	19	0.64
(1,2892)	2:268:B:VAL:HG23	1:108:A:PRO:HG3	19	0.64
(1,2683)	1:92:A:GLU:HG2	1:91:A:HIS:HB2	4	0.64
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB1	7	0.64
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB2	7	0.64
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB3	7	0.64
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB2	10	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB2	10	0.64
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB2	10	0.64
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	2	0.64
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	15	0.64
(1,1338)	2:162:B:GLU:HG3	2:162:B:GLU:H	6	0.64
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	3	0.64
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	3	0.64
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	3	0.64
(1,596)	2:234:B:LEU:HD21	2:230:B:GLY:HA3	20	0.64
(1,596)	2:234:B:LEU:HD22	2:230:B:GLY:HA3	20	0.64
(1,596)	2:234:B:LEU:HD23	2:230:B:GLY:HA3	20	0.64
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	8	0.64
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	8	0.64
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	8	0.64
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	4	0.63
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG22	18	0.63
(1,4442)	1:73:A:PRO:HD3	1:76:A:VAL:HG23	16	0.63
(1,4429)	1:73:A:PRO:HB2	1:76:A:VAL:HG11	16	0.63
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG23	3	0.63
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	7	0.63
(1,4024)	2:323:B:VAL:HG23	2:320:B:ARG:HA	17	0.63
(1,3990)	2:263:B:LEU:HD12	2:194:B:LEU:HD22	8	0.63
(1,3980)	2:164:B:LEU:HD22	2:295:B:LEU:HD21	20	0.63
(1,3945)	2:274:B:LEU:HD21	2:271:B:GLY:HA3	1	0.63
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	10	0.63
(1,3921)	2:221:B:ILE:HG22	2:263:B:LEU:HD21	19	0.63
(1,3920)	2:194:B:LEU:HD22	2:263:B:LEU:HD12	4	0.63
(1,3869)	2:232:B:GLN:HB3	2:233:B:LEU:HD21	3	0.63
(1,3766)	2:235:B:TYR:HD1	2:175:B:ILE:HD12	14	0.63
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	5	0.63
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	17	0.63
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	7	0.63
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	7	0.63
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	7	0.63
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD21	3	0.63
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD22	3	0.63
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD23	3	0.63
(1,1558)	2:189:B:ASN:HD21	2:191:B:ASP:H	12	0.63
(1,1054)	2:295:B:LEU:HD11	2:292:B:HIS:HA	3	0.63
(1,1054)	2:295:B:LEU:HD12	2:292:B:HIS:HA	3	0.63
(1,1054)	2:295:B:LEU:HD13	2:292:B:HIS:HA	3	0.63
(1,1054)	2:295:B:LEU:HD11	2:292:B:HIS:HA	16	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	2:295:B:LEU:HD12	2:292:B:HIS:HA	16	0.63
(1,1054)	2:295:B:LEU:HD13	2:292:B:HIS:HA	16	0.63
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	13	0.63
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	13	0.63
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	13	0.63
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	13	0.63
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	13	0.63
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	13	0.63
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	13	0.63
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	13	0.63
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	13	0.63
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	1	0.63
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	1	0.63
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	1	0.63
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	1	0.63
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	1	0.63
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	1	0.63
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	1	0.63
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	1	0.63
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	1	0.63
(1,718)	2:184:B:LEU:HD21	2:245:B:ILE:HG12	5	0.63
(1,718)	2:184:B:LEU:HD22	2:245:B:ILE:HG12	5	0.63
(1,718)	2:184:B:LEU:HD23	2:245:B:ILE:HG12	5	0.63
(1,387)	2:196:B:ASP:HA	2:195:B:GLU:HG3	20	0.63
(1,4604)	2:167:B:TRP:HD1	2:164:B:LEU:HD11	9	0.62
(1,4603)	2:225:B:PHE:HD1	2:266:B:LEU:HD13	12	0.62
(1,4555)	2:294:B:PHE:HD1	2:214:B:VAL:HG13	8	0.62
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	9	0.62
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	18	0.62
(1,4505)	2:311:B:TYR:HD1	2:181:B:LEU:HD22	8	0.62
(1,4418)	2:169:B:VAL:HG21	1:112:A:ILE:HG22	15	0.62
(1,4384)	2:169:B:VAL:HG23	1:109:A:GLU:HA	11	0.62
(1,4278)	1:84:A:MET:HE1	1:81:A:LEU:HD23	20	0.62
(1,4268)	1:76:A:VAL:HG21	1:78:A:TRP:HB2	19	0.62
(1,3950)	2:270:B:ILE:HG21	2:274:B:LEU:HD22	14	0.62
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE2	20	0.62
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG23	16	0.62
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	18	0.62
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	18	0.62
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	18	0.62
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	18	0.62
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	18	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	18	0.62
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	18	0.62
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	18	0.62
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	18	0.62
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	3	0.62
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	3	0.62
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	3	0.62
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	8	0.62
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB2	7	0.62
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB2	7	0.62
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB2	7	0.62
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	12	0.62
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	7	0.62
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	5	0.62
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	5	0.62
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	5	0.62
(1,1303)	2:155:B:GLU:HG2	2:155:B:GLU:H	5	0.62
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD11	19	0.62
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD12	19	0.62
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD13	19	0.62
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD11	19	0.62
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD12	19	0.62
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD13	19	0.62
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	4	0.62
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	4	0.62
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	4	0.62
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	4	0.62
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	4	0.62
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	4	0.62
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	4	0.62
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	4	0.62
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	4	0.62
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	11	0.62
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	11	0.62
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	11	0.62
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	13	0.62
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	13	0.62
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	13	0.62
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	15	0.62
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	15	0.62
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	15	0.62
(1,387)	2:196:B:ASP:HA	2:195:B:GLU:HG3	1	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	18	0.62
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	18	0.62
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	18	0.62
(1,4639)	2:212:B:TYR:HD1	2:213:B:ALA:HB2	7	0.61
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	3	0.61
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG21	2	0.61
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	5	0.61
(1,4327)	1:95:A:ILE:HD13	1:92:A:GLU:HB3	17	0.61
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD13	19	0.61
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG11	9	0.61
(1,4008)	2:170:B:ASP:HB3	2:169:B:VAL:HG12	11	0.61
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE1	7	0.61
(1,3843)	1:96:A:LEU:HD22	2:227:B:VAL:HG13	8	0.61
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB2	1	0.61
(1,2803)	2:232:B:GLN:HA	1:103:A:ARG:HD3	7	0.61
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	7	0.61
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	7	0.61
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	7	0.61
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	14	0.61
(1,1112)	2:300:B:LYS:HB2	2:300:B:LYS:HG3	4	0.61
(1,1112)	2:300:B:LYS:HB2	2:300:B:LYS:HG3	6	0.61
(1,1112)	2:300:B:LYS:HB2	2:300:B:LYS:HG3	10	0.61
(1,1112)	2:300:B:LYS:HB2	2:300:B:LYS:HG3	11	0.61
(1,1112)	2:300:B:LYS:HB2	2:300:B:LYS:HG3	12	0.61
(1,1112)	2:300:B:LYS:HB2	2:300:B:LYS:HG3	13	0.61
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	7	0.61
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	7	0.61
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	7	0.61
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	7	0.61
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	7	0.61
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	7	0.61
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	7	0.61
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	7	0.61
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	7	0.61
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	16	0.61
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	16	0.61
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	16	0.61
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	16	0.61
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	16	0.61
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	16	0.61
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	16	0.61
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	16	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	16	0.61
(1,815)	2:253:B:PRO:HG2	2:256:B:GLN:HG3	9	0.61
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	4	0.61
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	4	0.61
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	4	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	4	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	4	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	4	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	4	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	4	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	4	0.61
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	6	0.61
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	6	0.61
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	6	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	6	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	6	0.61
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	6	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	6	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	6	0.61
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	6	0.61
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	9	0.61
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	9	0.61
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	9	0.61
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	9	0.61
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	9	0.61
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	9	0.61
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	9	0.61
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	9	0.61
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	9	0.61
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	4	0.61
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	4	0.61
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	4	0.61
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	11	0.61
(1,309)	2:192:B:SER:HB2	2:188:B:LYS:HE2	1	0.61
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	7	0.6
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	12	0.6
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG22	17	0.6
(1,4429)	1:73:A:PRO:HB2	1:76:A:VAL:HG12	7	0.6
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD11	19	0.6
(1,4296)	1:90:A:LEU:HD12	1:87:A:MET:HE2	12	0.6
(1,4279)	1:84:A:MET:HG3	1:81:A:LEU:HD22	3	0.6
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD22	12	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3988)	2:295:B:LEU:HG	2:298:B:LEU:HD12	8	0.6
(1,3920)	2:194:B:LEU:HD22	2:263:B:LEU:HD13	19	0.6
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE3	14	0.6
(1,3857)	1:98:A:PHE:HE2	2:227:B:VAL:HG12	14	0.6
(1,3852)	2:218:B:VAL:HG22	2:202:B:LYS:HE3	8	0.6
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE3	15	0.6
(1,3832)	2:214:B:VAL:HG11	2:213:B:ALA:HB2	13	0.6
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	12	0.6
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE3	12	0.6
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE3	12	0.6
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	18	0.6
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	5	0.6
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	5	0.6
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	5	0.6
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	13	0.6
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	13	0.6
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	13	0.6
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	17	0.6
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	17	0.6
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	17	0.6
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB3	1	0.6
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB3	1	0.6
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB3	1	0.6
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	1	0.6
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	14	0.6
(1,1558)	2:189:B:ASN:HD21	2:191:B:ASP:H	20	0.6
(1,1338)	2:162:B:GLU:HG3	2:162:B:GLU:H	18	0.6
(1,1303)	2:155:B:GLU:HG2	2:155:B:GLU:H	3	0.6
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	16	0.6
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	16	0.6
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	16	0.6
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	10	0.6
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	10	0.6
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	10	0.6
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	10	0.6
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	10	0.6
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	10	0.6
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	10	0.6
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	10	0.6
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	10	0.6
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	5	0.6
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	5	0.6
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	10	0.6
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	10	0.6
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	10	0.6
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	11	0.6
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	11	0.6
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	11	0.6
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD21	16	0.6
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD22	16	0.6
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD23	16	0.6
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	5	0.6
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	17	0.6
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	17	0.6
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	17	0.6
(1,4639)	2:237:B:PHE:HE1	2:322:B:ALA:HB3	11	0.59
(1,4623)	2:306:B:PHE:HE2	2:298:B:LEU:HD12	2	0.59
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	7	0.59
(1,4520)	2:237:B:PHE:HE1	2:179:B:LYS:HE3	17	0.59
(1,4513)	2:235:B:TYR:HE2	2:175:B:ILE:HD13	5	0.59
(1,4505)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	13	0.59
(1,4462)	1:88:A:GLN:HB2	1:88:A:GLN:H	14	0.59
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG12	9	0.59
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	4	0.59
(1,4343)	1:74:A:SER:HB3	1:95:A:ILE:HD11	18	0.59
(1,4337)	1:73:A:PRO:HB3	1:74:A:SER:HB2	16	0.59
(1,4323)	2:279:B:LEU:HD22	1:91:A:HIS:HB3	2	0.59
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD23	9	0.59
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD22	16	0.59
(1,4030)	2:192:B:SER:HB3	2:188:B:LYS:HG2	3	0.59
(1,4024)	2:323:B:VAL:HG11	2:320:B:ARG:HA	18	0.59
(1,4001)	2:273:B:MET:HB3	2:274:B:LEU:HD12	10	0.59
(1,3999)	2:200:B:TYR:HE2	2:296:B:LYS:HE3	18	0.59
(1,3947)	2:269:B:ARG:HB3	2:273:B:MET:HE1	9	0.59
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE1	18	0.59
(1,3940)	2:274:B:LEU:HG	2:270:B:ILE:HD13	7	0.59
(1,3893)	2:252:B:ALA:HB3	2:245:B:ILE:HG23	11	0.59
(1,3812)	2:218:B:VAL:HG22	2:194:B:LEU:HD22	20	0.59
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	14	0.59
(1,3420)	2:236:B:LYS:HG2	1:104:A:ASN:HD22	17	0.59
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	13	0.59
(1,2653)	1:90:A:LEU:HD21	1:89:A:ALA:HA	1	0.59
(1,2653)	1:90:A:LEU:HD22	1:89:A:ALA:HA	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2653)	1:90:A:LEU:HD23	1:89:A:ALA:HA	1	0.59
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB2	16	0.59
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB2	16	0.59
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB2	16	0.59
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	7	0.59
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	7	0.59
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	7	0.59
(1,2420)	2:321:B:LYS:HB3	2:321:B:LYS:H	11	0.59
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	2	0.59
(1,1896)	2:239:B:ARG:HB2	2:239:B:ARG:H	5	0.59
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD11	7	0.59
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD12	7	0.59
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD13	7	0.59
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD11	7	0.59
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD12	7	0.59
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD13	7	0.59
(1,1120)	2:305:B:LEU:HD21	2:301:B:ASN:HB2	8	0.59
(1,1120)	2:305:B:LEU:HD22	2:301:B:ASN:HB2	8	0.59
(1,1120)	2:305:B:LEU:HD23	2:301:B:ASN:HB2	8	0.59
(1,815)	2:253:B:PRO:HB2	2:256:B:GLN:HG2	3	0.59
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	14	0.59
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	14	0.59
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	14	0.59
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD21	14	0.59
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD22	14	0.59
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD23	14	0.59
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	11	0.58
(1,4363)	2:235:B:TYR:HD1	1:106:A:VAL:HG22	6	0.58
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	20	0.58
(1,4312)	1:73:A:PRO:HB3	1:96:A:LEU:HD12	18	0.58
(1,3967)	2:224:B:TYR:HA	2:266:B:LEU:HD11	2	0.58
(1,3894)	2:254:B:MET:HE1	2:245:B:ILE:HG23	10	0.58
(1,3888)	2:244:B:GLU:HG2	2:245:B:ILE:HD13	3	0.58
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG22	18	0.58
(1,3843)	2:194:B:LEU:HD13	2:218:B:VAL:HG22	5	0.58
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB3	3	0.58
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	8	0.58
(1,3796)	2:260:B:ALA:HA	2:190:B:VAL:HG13	1	0.58
(1,3795)	2:194:B:LEU:HD23	2:190:B:VAL:HG13	12	0.58
(1,3766)	2:235:B:TYR:HD2	2:175:B:ILE:HD11	20	0.58
(1,3750)	2:160:B:ILE:HG23	2:165:B:LYS:HE2	2	0.58
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD21	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD22	10	0.58
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD23	10	0.58
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD21	10	0.58
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD22	10	0.58
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD23	10	0.58
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	13	0.58
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	13	0.58
(1,2945)	1:107:A:LEU:HD21	1:112:A:ILE:HG13	8	0.58
(1,2945)	1:107:A:LEU:HD22	1:112:A:ILE:HG13	8	0.58
(1,2945)	1:107:A:LEU:HD23	1:112:A:ILE:HG13	8	0.58
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	5	0.58
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	7	0.58
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	13	0.58
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	13	0.58
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	13	0.58
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	16	0.58
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	16	0.58
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	16	0.58
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	20	0.58
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	20	0.58
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	20	0.58
(1,2420)	2:321:B:LYS:HB3	2:321:B:LYS:H	1	0.58
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	3	0.58
(1,1558)	2:189:B:ASN:HD21	2:191:B:ASP:H	9	0.58
(1,1344)	2:163:B:GLU:HB2	2:163:B:GLU:H	5	0.58
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD21	17	0.58
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	15	0.58
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	15	0.58
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	15	0.58
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	15	0.58
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	15	0.58
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	15	0.58
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	15	0.58
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	15	0.58
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	15	0.58
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	12	0.58
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	12	0.58
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	12	0.58
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	12	0.58
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	12	0.58
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	12	0.58
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	12	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	12	0.58
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	12	0.58
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	16	0.58
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	16	0.58
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	16	0.58
(1,307)	2:193:B:ILE:HG12	2:188:B:LYS:HE3	10	0.58
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	11	0.58
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	11	0.58
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	11	0.58
(1,7)	2:300:B:LYS:HE2	2:300:B:LYS:HG2	20	0.58
(1,4612)	2:262:B:HIS:HD2	2:265:B:ARG:HG3	6	0.57
(1,4611)	2:290:B:TYR:HD2	2:286:B:LEU:HG	11	0.57
(1,4601)	2:267:B:PHE:HE2	2:263:B:LEU:HD21	16	0.57
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	16	0.57
(1,4462)	1:88:A:GLN:HB2	1:88:A:GLN:H	4	0.57
(1,4462)	1:88:A:GLN:HB2	1:88:A:GLN:H	6	0.57
(1,4462)	1:88:A:GLN:HB2	1:88:A:GLN:H	9	0.57
(1,4462)	1:88:A:GLN:HB2	1:88:A:GLN:H	18	0.57
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG11	16	0.57
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG22	7	0.57
(1,4390)	1:115:A:VAL:HG23	1:111:A:ILE:HA	7	0.57
(1,4390)	1:115:A:VAL:HG23	1:111:A:ILE:HA	12	0.57
(1,4357)	2:273:B:MET:HE2	1:100:A:ASN:HA	13	0.57
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD23	18	0.57
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	6	0.57
(1,3869)	2:232:B:GLN:HB2	2:233:B:LEU:HD23	10	0.57
(1,3845)	2:202:B:LYS:HE2	2:218:B:VAL:HG23	13	0.57
(1,3832)	2:214:B:VAL:HG13	2:213:B:ALA:HB3	6	0.57
(1,3768)	2:235:B:TYR:HE2	2:176:B:THR:HG23	6	0.57
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	1	0.57
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	14	0.57
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	8	0.57
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	13	0.57
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	16	0.57
(1,1520)	2:187:B:LYS:HB2	2:187:B:LYS:H	1	0.57
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD11	20	0.57
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD12	20	0.57
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD13	20	0.57
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	13	0.57
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	13	0.57
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	13	0.57
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	4	0.57
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	4	0.57
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD21	20	0.57
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD22	20	0.57
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD23	20	0.57
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD21	2	0.57
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD22	2	0.57
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD23	2	0.57
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD23	4	0.57
(1,4621)	2:267:B:PHE:HE2	2:298:B:LEU:HD13	16	0.56
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	16	0.56
(1,4472)	1:93:A:SER:HB2	1:95:A:ILE:H	11	0.56
(1,4424)	1:116:A:ARG:HG2	1:115:A:VAL:HG12	3	0.56
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG21	19	0.56
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	6	0.56
(1,4296)	2:279:B:LEU:HD12	1:87:A:MET:HE3	19	0.56
(1,4167)	2:279:B:LEU:HD11	2:280:B:ASP:H	4	0.56
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG13	6	0.56
(1,4008)	2:170:B:ASP:HB3	2:169:B:VAL:HG11	10	0.56
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD23	18	0.56
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG23	9	0.56
(1,3893)	2:252:B:ALA:HB1	2:245:B:ILE:HG22	18	0.56
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD22	14	0.56
(1,3768)	2:235:B:TYR:HE2	2:176:B:THR:HG22	16	0.56
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	17	0.56
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	17	0.56
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	17	0.56
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	9	0.56
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	18	0.56
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB3	19	0.56
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB3	19	0.56
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB3	19	0.56
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	5	0.56
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	10	0.56
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	10	0.56
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	10	0.56
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	10	0.56
(1,1228)	2:320:B:ARG:HG3	2:320:B:ARG:HA	10	0.56
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG3	10	0.56
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG3	10	0.56
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG3	10	0.56
(1,681)	2:234:B:LEU:HD21	2:239:B:ARG:HG2	5	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	2:234:B:LEU:HD22	2:239:B:ARG:HG2	5	0.56
(1,681)	2:234:B:LEU:HD23	2:239:B:ARG:HG2	5	0.56
(1,4612)	2:290:B:TYR:HE2	2:286:B:LEU:HG	3	0.55
(1,4611)	2:290:B:TYR:HD2	2:286:B:LEU:HG	19	0.55
(1,4555)	2:294:B:PHE:HD2	2:217:B:VAL:HG12	12	0.55
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG23	9	0.55
(1,4363)	2:172:B:TRP:HD1	1:106:A:VAL:HG22	15	0.55
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD13	2	0.55
(1,3936)	2:268:B:VAL:HG23	2:269:B:ARG:HD2	16	0.55
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG23	12	0.55
(1,3823)	2:211:B:GLU:HB3	2:202:B:LYS:HE2	12	0.55
(1,3776)	2:257:B:VAL:HG21	2:185:B:PRO:HB3	5	0.55
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD21	9	0.55
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD22	10	0.55
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD23	19	0.55
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	16	0.55
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	16	0.55
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	16	0.55
(1,2838)	2:268:B:VAL:HG21	1:107:A:LEU:HA	19	0.55
(1,2838)	2:268:B:VAL:HG22	1:107:A:LEU:HA	19	0.55
(1,2838)	2:268:B:VAL:HG23	1:107:A:LEU:HA	19	0.55
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	6	0.55
(1,2693)	1:92:A:GLU:HG3	1:93:A:SER:HA	18	0.55
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD21	1	0.55
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD22	1	0.55
(1,2572)	1:90:A:LEU:HA	1:90:A:LEU:HD23	1	0.55
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	2	0.55
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	2	0.55
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	2	0.55
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	1	0.55
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	7	0.55
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	4	0.55
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	15	0.55
(1,1338)	2:162:B:GLU:HG3	2:162:B:GLU:H	19	0.55
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD11	16	0.55
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD12	16	0.55
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD13	16	0.55
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	2	0.55
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	2	0.55
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	2	0.55
(1,671)	2:234:B:LEU:HD21	2:239:B:ARG:HD2	20	0.55
(1,671)	2:234:B:LEU:HD22	2:239:B:ARG:HD2	20	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	2:234:B:LEU:HD23	2:239:B:ARG:HD2	20	0.55
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	14	0.55
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	14	0.55
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	14	0.55
(1,510)	2:194:B:LEU:HD21	2:218:B:VAL:HG21	16	0.55
(1,510)	2:194:B:LEU:HD21	2:218:B:VAL:HG22	16	0.55
(1,510)	2:194:B:LEU:HD21	2:218:B:VAL:HG23	16	0.55
(1,510)	2:194:B:LEU:HD22	2:218:B:VAL:HG21	16	0.55
(1,510)	2:194:B:LEU:HD22	2:218:B:VAL:HG22	16	0.55
(1,510)	2:194:B:LEU:HD22	2:218:B:VAL:HG23	16	0.55
(1,510)	2:194:B:LEU:HD23	2:218:B:VAL:HG21	16	0.55
(1,510)	2:194:B:LEU:HD23	2:218:B:VAL:HG22	16	0.55
(1,510)	2:194:B:LEU:HD23	2:218:B:VAL:HG23	16	0.55
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD11	14	0.55
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD12	14	0.55
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD13	14	0.55
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD11	14	0.55
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD12	14	0.55
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD13	14	0.55
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD11	14	0.55
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD12	14	0.55
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD13	14	0.55
(1,313)	2:192:B:SER:HB2	2:188:B:LYS:HG3	19	0.55
(1,298)	2:192:B:SER:HB2	2:188:B:LYS:HD3	17	0.55
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	2	0.55
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	2	0.55
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	2	0.55
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	2	0.55
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	2	0.55
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	2	0.55
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	2	0.55
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	2	0.55
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	2	0.55
(1,4449)	2:290:B:TYR:HE1	1:81:A:LEU:HD13	8	0.54
(1,4418)	2:169:B:VAL:HG22	1:112:A:ILE:HG21	13	0.54
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	1	0.54
(1,4382)	2:168:B:LEU:HD12	1:108:A:PRO:HD3	14	0.54
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG21	20	0.54
(1,4310)	1:85:A:TYR:HD2	1:90:A:LEU:HB3	4	0.54
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE1	11	0.54
(1,4280)	2:290:B:TYR:HE1	1:81:A:LEU:HD23	8	0.54
(1,4002)	2:188:B:LYS:HE2	2:305:B:LEU:HD12	17	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD23	16	0.54
(1,3932)	1:107:A:LEU:HA	2:268:B:VAL:HG21	19	0.54
(1,3845)	2:202:B:LYS:HE2	2:218:B:VAL:HG21	12	0.54
(1,3843)	2:194:B:LEU:HD13	2:218:B:VAL:HG22	13	0.54
(1,3832)	2:214:B:VAL:HG12	2:213:B:ALA:HB1	7	0.54
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	15	0.54
(1,3776)	2:257:B:VAL:HG23	2:185:B:PRO:HB3	15	0.54
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE2	3	0.54
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE2	3	0.54
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE3	9	0.54
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE3	9	0.54
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	16	0.54
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	16	0.54
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	16	0.54
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	20	0.54
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	20	0.54
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	20	0.54
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	12	0.54
(1,2653)	1:90:A:LEU:HD21	1:89:A:ALA:HA	9	0.54
(1,2653)	1:90:A:LEU:HD22	1:89:A:ALA:HA	9	0.54
(1,2653)	1:90:A:LEU:HD23	1:89:A:ALA:HA	9	0.54
(1,2653)	1:90:A:LEU:HD21	1:89:A:ALA:HA	15	0.54
(1,2653)	1:90:A:LEU:HD22	1:89:A:ALA:HA	15	0.54
(1,2653)	1:90:A:LEU:HD23	1:89:A:ALA:HA	15	0.54
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	12	0.54
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	12	0.54
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	12	0.54
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG11	1	0.54
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG12	1	0.54
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG13	1	0.54
(1,2420)	2:321:B:LYS:HB3	2:321:B:LYS:H	18	0.54
(1,1899)	2:239:B:ARG:HG2	2:239:B:ARG:H	5	0.54
(1,1054)	2:295:B:LEU:HD11	2:292:B:HIS:HA	8	0.54
(1,1054)	2:295:B:LEU:HD12	2:292:B:HIS:HA	8	0.54
(1,1054)	2:295:B:LEU:HD13	2:292:B:HIS:HA	8	0.54
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD11	12	0.54
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD12	12	0.54
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD13	12	0.54
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD11	8	0.54
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD12	8	0.54
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD13	8	0.54
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD11	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	8	0.54
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD13	8	0.54
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD21	20	0.54
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD22	20	0.54
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD23	20	0.54
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD21	20	0.54
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD22	20	0.54
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD23	20	0.54
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD21	20	0.54
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD22	20	0.54
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD23	20	0.54
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	2	0.54
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	2	0.54
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	2	0.54
(1,432)	2:204:B:ARG:HA	2:204:B:ARG:HD3	19	0.54
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD21	8	0.54
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD22	8	0.54
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD23	8	0.54
(2,12)	2:288:B:LEU:HD21	2:157:B:LYS:H	1	0.53
(2,12)	2:288:B:LEU:HD22	2:157:B:LYS:H	1	0.53
(2,12)	2:288:B:LEU:HD23	2:157:B:LYS:H	1	0.53
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	5	0.53
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	5	0.53
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	5	0.53
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	5	0.53
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	5	0.53
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	5	0.53
(1,4620)	2:267:B:PHE:HD1	2:266:B:LEU:HD23	14	0.53
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	6	0.53
(1,4604)	2:225:B:PHE:HE1	2:266:B:LEU:HD11	3	0.53
(1,4575)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	14	0.53
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG23	3	0.53
(1,4511)	2:182:B:PHE:HD2	2:181:B:LEU:HG	18	0.53
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD23	4	0.53
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD13	19	0.53
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG22	18	0.53
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	11	0.53
(1,4265)	1:74:A:SER:HA	1:77:A:ILE:HB	18	0.53
(1,4222)	2:317:B:GLU:HB2	2:318:B:TYR:H	3	0.53
(1,4198)	2:164:B:LEU:HD21	2:299:B:ALA:H	16	0.53
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD11	16	0.53
(1,3976)	2:292:B:HIS:HA	2:295:B:LEU:HD13	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3966)	2:288:B:LEU:HD22	2:288:B:LEU:HA	2	0.53
(1,3950)	2:279:B:LEU:HD21	2:274:B:LEU:HD23	2	0.53
(1,3894)	2:254:B:MET:HE3	2:245:B:ILE:HG23	7	0.53
(1,3789)	2:193:B:ILE:HD12	2:188:B:LYS:HE2	16	0.53
(1,3768)	2:235:B:TYR:HE1	2:176:B:THR:HG23	20	0.53
(1,3408)	1:119:A:LYS:HB2	1:119:A:LYS:H	14	0.53
(1,2803)	2:232:B:GLN:HA	1:103:A:ARG:HD2	9	0.53
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	3	0.53
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	10	0.53
(1,2653)	1:90:A:LEU:HD21	1:89:A:ALA:HA	20	0.53
(1,2653)	1:90:A:LEU:HD22	1:89:A:ALA:HA	20	0.53
(1,2653)	1:90:A:LEU:HD23	1:89:A:ALA:HA	20	0.53
(1,2525)	1:78:A:TRP:HZ3	1:77:A:ILE:HA	6	0.53
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	4	0.53
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	4	0.53
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	4	0.53
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB3	11	0.53
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB3	11	0.53
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB3	11	0.53
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	15	0.53
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	15	0.53
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	15	0.53
(1,2420)	2:321:B:LYS:HB3	2:321:B:LYS:H	2	0.53
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	10	0.53
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	19	0.53
(1,1857)	2:320:B:ARG:HB2	2:320:B:ARG:H	10	0.53
(1,1661)	2:202:B:LYS:HG3	2:202:B:LYS:H	5	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD11	1	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD12	1	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD13	1	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD11	2	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD12	2	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD13	2	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD11	3	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD12	3	0.53
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD13	3	0.53
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD11	10	0.53
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD12	10	0.53
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD13	10	0.53
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD11	10	0.53
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD12	10	0.53
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD13	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	8	0.53
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	8	0.53
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	8	0.53
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	8	0.53
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	8	0.53
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	8	0.53
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	8	0.53
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	8	0.53
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	8	0.53
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	14	0.53
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	14	0.53
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	14	0.53
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	14	0.53
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	14	0.53
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	14	0.53
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	14	0.53
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	14	0.53
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	14	0.53
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	12	0.53
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	12	0.53
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	12	0.53
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	8	0.53
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	8	0.53
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	8	0.53
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD21	13	0.53
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD22	13	0.53
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD23	13	0.53
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD21	13	0.53
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD22	13	0.53
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD23	13	0.53
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD21	13	0.53
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD22	13	0.53
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD23	13	0.53
(1,432)	2:204:B:ARG:HA	2:204:B:ARG:HD3	17	0.53
(1,288)	2:187:B:LYS:HA	2:187:B:LYS:HG2	1	0.53
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HB3	13	0.52
(1,4425)	2:165:B:LYS:HA	1:115:A:VAL:HG13	2	0.52
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD11	3	0.52
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	1	0.52
(1,4384)	2:169:B:VAL:HG21	1:109:A:GLU:HA	6	0.52
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD13	18	0.52
(1,4324)	1:81:A:LEU:HD11	1:80:A:HIS:HB2	20	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	8	0.52
(1,4167)	2:279:B:LEU:HD13	2:280:B:ASP:H	9	0.52
(1,3980)	2:164:B:LEU:HD22	2:295:B:LEU:HD21	14	0.52
(1,3947)	2:272:B:ALA:HB1	2:273:B:MET:HE2	6	0.52
(1,3947)	2:269:B:ARG:HB3	2:273:B:MET:HE2	8	0.52
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	12	0.52
(1,3803)	2:194:B:LEU:HD21	2:193:B:ILE:HG23	12	0.52
(1,3776)	2:257:B:VAL:HG23	2:185:B:PRO:HB3	2	0.52
(1,3494)	2:237:B:PHE:HE1	2:181:B:LEU:HD21	14	0.52
(1,3494)	2:237:B:PHE:HE1	2:181:B:LEU:HD22	14	0.52
(1,3494)	2:237:B:PHE:HE1	2:181:B:LEU:HD23	14	0.52
(1,3494)	2:237:B:PHE:HE2	2:181:B:LEU:HD21	14	0.52
(1,3494)	2:237:B:PHE:HE2	2:181:B:LEU:HD22	14	0.52
(1,3494)	2:237:B:PHE:HE2	2:181:B:LEU:HD23	14	0.52
(1,3184)	1:90:A:LEU:HD21	1:89:A:ALA:H	4	0.52
(1,3184)	1:90:A:LEU:HD22	1:89:A:ALA:H	4	0.52
(1,3184)	1:90:A:LEU:HD23	1:89:A:ALA:H	4	0.52
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	19	0.52
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	19	0.52
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	19	0.52
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	14	0.52
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	14	0.52
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	14	0.52
(1,2803)	2:232:B:GLN:HA	1:103:A:ARG:HD2	1	0.52
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	19	0.52
(1,2341)	2:307:B:SER:HB3	2:309:B:SER:H	19	0.52
(1,1832)	2:233:B:LEU:HD11	2:230:B:GLY:H	20	0.52
(1,1832)	2:233:B:LEU:HD12	2:230:B:GLY:H	20	0.52
(1,1832)	2:233:B:LEU:HD13	2:230:B:GLY:H	20	0.52
(1,1459)	2:179:B:LYS:HG2	2:179:B:LYS:H	16	0.52
(1,1303)	2:155:B:GLU:HG3	2:155:B:GLU:H	13	0.52
(1,1120)	2:305:B:LEU:HD21	2:301:B:ASN:HB2	13	0.52
(1,1120)	2:305:B:LEU:HD22	2:301:B:ASN:HB2	13	0.52
(1,1120)	2:305:B:LEU:HD23	2:301:B:ASN:HB2	13	0.52
(1,1054)	2:295:B:LEU:HD11	2:292:B:HIS:HA	13	0.52
(1,1054)	2:295:B:LEU:HD12	2:292:B:HIS:HA	13	0.52
(1,1054)	2:295:B:LEU:HD13	2:292:B:HIS:HA	13	0.52
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD11	6	0.52
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD12	6	0.52
(1,1045)	2:291:B:LEU:HA	2:291:B:LEU:HD13	6	0.52
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	13	0.52
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	13	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	13	0.52
(1,432)	2:204:B:ARG:HA	2:204:B:ARG:HD3	20	0.52
(1,307)	2:193:B:ILE:HG12	2:188:B:LYS:HE3	13	0.52
(1,112)	1:105:A:PHE:HE1	2:168:B:LEU:HD11	11	0.52
(1,112)	1:105:A:PHE:HE1	2:168:B:LEU:HD12	11	0.52
(1,112)	1:105:A:PHE:HE1	2:168:B:LEU:HD13	11	0.52
(1,112)	1:105:A:PHE:HE2	2:168:B:LEU:HD11	11	0.52
(1,112)	1:105:A:PHE:HE2	2:168:B:LEU:HD12	11	0.52
(1,112)	1:105:A:PHE:HE2	2:168:B:LEU:HD13	11	0.52
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HB3	20	0.51
(1,4548)	2:200:B:TYR:HE2	2:201:B:LYS:HD2	2	0.51
(1,4546)	2:200:B:TYR:HE2	2:201:B:LYS:HB2	12	0.51
(1,4435)	1:75:A:LYS:HE3	1:92:A:GLU:HA	6	0.51
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	9	0.51
(1,4364)	1:111:A:ILE:HD12	1:107:A:LEU:HA	9	0.51
(1,4347)	1:97:A:PRO:HG3	1:95:A:ILE:HG22	9	0.51
(1,4329)	1:89:A:ALA:HB2	1:92:A:GLU:HG3	17	0.51
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD23	12	0.51
(1,4167)	1:90:A:LEU:HD11	2:280:B:ASP:H	12	0.51
(1,3966)	2:288:B:LEU:HD22	2:288:B:LEU:HA	3	0.51
(1,3966)	2:288:B:LEU:HD22	2:288:B:LEU:HA	20	0.51
(1,3920)	2:194:B:LEU:HD21	2:263:B:LEU:HD11	15	0.51
(1,3774)	2:245:B:ILE:HG12	2:184:B:LEU:HD21	17	0.51
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	3	0.51
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	3	0.51
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	3	0.51
(1,2812)	1:106:A:VAL:HG11	1:104:A:ASN:HB2	4	0.51
(1,2812)	1:106:A:VAL:HG12	1:104:A:ASN:HB2	4	0.51
(1,2812)	1:106:A:VAL:HG13	1:104:A:ASN:HB2	4	0.51
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	4	0.51
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	4	0.51
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	4	0.51
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	2	0.51
(1,2261)	2:164:B:LEU:HD11	2:298:B:LEU:H	9	0.51
(1,2261)	2:164:B:LEU:HD12	2:298:B:LEU:H	9	0.51
(1,2261)	2:164:B:LEU:HD13	2:298:B:LEU:H	9	0.51
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	3	0.51
(1,1120)	2:305:B:LEU:HD21	2:301:B:ASN:HB2	16	0.51
(1,1120)	2:305:B:LEU:HD22	2:301:B:ASN:HB2	16	0.51
(1,1120)	2:305:B:LEU:HD23	2:301:B:ASN:HB2	16	0.51
(1,1054)	2:295:B:LEU:HD11	2:292:B:HIS:HA	12	0.51
(1,1054)	2:295:B:LEU:HD12	2:292:B:HIS:HA	12	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	2:295:B:LEU:HD13	2:292:B:HIS:HA	12	0.51
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD21	19	0.51
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD22	19	0.51
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD23	19	0.51
(1,432)	2:204:B:ARG:HA	2:204:B:ARG:HD3	2	0.51
(1,420)	2:199:B:ASN:HA	2:202:B:LYS:HE3	8	0.51
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	7	0.51
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	7	0.51
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	7	0.51
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	7	0.51
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	7	0.51
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	7	0.51
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	7	0.51
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	7	0.51
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	7	0.51
(1,4644)	2:182:B:PHE:HD1	2:184:B:LEU:HB2	12	0.5
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD12	17	0.5
(1,4631)	2:167:B:TRP:HZ3	2:308:B:ALA:HB2	13	0.5
(1,4611)	2:237:B:PHE:HD2	2:175:B:ILE:HB	20	0.5
(1,4575)	2:167:B:TRP:HD1	2:164:B:LEU:HD22	2	0.5
(1,4545)	2:200:B:TYR:HD2	2:201:B:LYS:HD2	17	0.5
(1,4515)	2:172:B:TRP:HZ3	2:169:B:VAL:HG13	16	0.5
(1,4512)	2:235:B:TYR:HD1	2:175:B:ILE:HD13	16	0.5
(1,4511)	2:182:B:PHE:HD1	2:175:B:ILE:HD11	16	0.5
(1,4444)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	14	0.5
(1,4429)	1:73:A:PRO:HB2	1:76:A:VAL:HG12	8	0.5
(1,4418)	2:169:B:VAL:HG23	1:112:A:ILE:HG22	7	0.5
(1,4390)	1:115:A:VAL:HG22	1:111:A:ILE:HA	5	0.5
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD23	17	0.5
(1,4318)	2:279:B:LEU:HD22	1:91:A:HIS:HA	11	0.5
(1,4271)	2:212:B:TYR:HD1	1:81:A:LEU:HA	1	0.5
(1,4271)	2:212:B:TYR:HD1	1:81:A:LEU:HA	20	0.5
(1,3950)	2:270:B:ILE:HG21	2:274:B:LEU:HD21	7	0.5
(1,3949)	2:272:B:ALA:HA	2:274:B:LEU:HD13	12	0.5
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE3	2	0.5
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG23	19	0.5
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	11	0.5
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	11	0.5
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD11	8	0.5
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD12	8	0.5
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD13	8	0.5
(1,3064)	2:216:B:GLU:HG3	1:81:A:LEU:HD11	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3064)	2:216:B:GLU:HG3	1:81:A:LEU:HD12	2	0.5
(1,3064)	2:216:B:GLU:HG3	1:81:A:LEU:HD13	2	0.5
(1,3039)	2:231:B:THR:HA	1:102:A:GLU:HG3	2	0.5
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	8	0.5
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	8	0.5
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	8	0.5
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	12	0.5
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	12	0.5
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	12	0.5
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	15	0.5
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	15	0.5
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	15	0.5
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	17	0.5
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB1	9	0.5
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB2	9	0.5
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB3	9	0.5
(1,2604)	1:87:A:MET:HB2	1:85:A:TYR:HA	20	0.5
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	3	0.5
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	3	0.5
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	3	0.5
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	2	0.5
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	2	0.5
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	2	0.5
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	9	0.5
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	9	0.5
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	9	0.5
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	13	0.5
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	13	0.5
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	13	0.5
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	7	0.5
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	7	0.5
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	7	0.5
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	18	0.5
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	18	0.5
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	18	0.5
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	9	0.5
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	17	0.5
(1,1558)	2:189:B:ASN:HD21	2:191:B:ASP:H	2	0.5
(1,1558)	2:189:B:ASN:HD21	2:191:B:ASP:H	15	0.5
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	6	0.5
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	6	0.5
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	2:163:B:GLU:HB2	2:163:B:GLU:H	17	0.5
(1,1170)	2:180:B:GLN:HG2	2:313:B:VAL:HG21	13	0.5
(1,1170)	2:180:B:GLN:HG2	2:313:B:VAL:HG22	13	0.5
(1,1170)	2:180:B:GLN:HG2	2:313:B:VAL:HG23	13	0.5
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD21	2	0.5
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD22	2	0.5
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD23	2	0.5
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	7	0.5
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	7	0.5
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	7	0.5
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	18	0.5
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	7	0.5
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	7	0.5
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	7	0.5
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	7	0.5
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	7	0.5
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	7	0.5
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	7	0.5
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	7	0.5
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	7	0.5
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD2	18	0.5
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	19	0.49
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	19	0.49
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	19	0.49
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	19	0.49
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	19	0.49
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	19	0.49
(1,4623)	2:306:B:PHE:HE2	2:298:B:LEU:HD13	18	0.49
(1,4579)	2:242:B:TYR:HE1	2:254:B:MET:HE1	15	0.49
(1,4533)	2:183:B:TYR:HE2	2:321:B:LYS:HE3	13	0.49
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG22	10	0.49
(1,4364)	1:111:A:ILE:HD12	1:107:A:LEU:HA	17	0.49
(1,4334)	1:96:A:LEU:HD12	1:74:A:SER:HB3	19	0.49
(1,4316)	1:87:A:MET:HE1	1:90:A:LEU:HD23	9	0.49
(1,4296)	2:279:B:LEU:HD11	1:87:A:MET:HE2	16	0.49
(1,4031)	2:298:B:LEU:HB2	2:193:B:ILE:HD13	20	0.49
(1,3962)	2:281:B:GLU:HA	2:284:B:LEU:HD12	9	0.49
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD23	12	0.49
(1,3921)	2:221:B:ILE:HG21	2:263:B:LEU:HD23	15	0.49
(1,3837)	2:210:B:LYS:HG3	2:214:B:VAL:HG22	17	0.49
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	15	0.49
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	15	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3421)	2:236:B:LYS:HE3	1:104:A:ASN:HD22	5	0.49
(1,3409)	1:119:A:LYS:HG3	1:119:A:LYS:H	18	0.49
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	4	0.49
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	14	0.49
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	14	0.49
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	14	0.49
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	14	0.49
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	14	0.49
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	14	0.49
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	14	0.49
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	14	0.49
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	14	0.49
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	14	0.49
(1,2811)	1:106:A:VAL:HG11	1:104:A:ASN:HB3	3	0.49
(1,2811)	1:106:A:VAL:HG12	1:104:A:ASN:HB3	3	0.49
(1,2811)	1:106:A:VAL:HG13	1:104:A:ASN:HB3	3	0.49
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	8	0.49
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB1	1	0.49
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB2	1	0.49
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB3	1	0.49
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	13	0.49
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	13	0.49
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	13	0.49
(1,2040)	2:190:B:VAL:HG21	2:260:B:ALA:H	14	0.49
(1,2040)	2:190:B:VAL:HG22	2:260:B:ALA:H	14	0.49
(1,2040)	2:190:B:VAL:HG23	2:260:B:ALA:H	14	0.49
(1,2007)	2:226:B:ASN:HD21	2:255:B:SER:H	14	0.49
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	13	0.49
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	9	0.49
(1,1715)	2:214:B:VAL:HG21	2:214:B:VAL:H	12	0.49
(1,1715)	2:214:B:VAL:HG22	2:214:B:VAL:H	12	0.49
(1,1715)	2:214:B:VAL:HG23	2:214:B:VAL:H	12	0.49
(1,1702)	2:211:B:GLU:HB2	2:212:B:TYR:H	6	0.49
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	20	0.49
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	20	0.49
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	20	0.49
(1,1344)	2:163:B:GLU:HB2	2:163:B:GLU:H	6	0.49
(1,1344)	2:163:B:GLU:HB2	2:163:B:GLU:H	12	0.49
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	14	0.49
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	14	0.49
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	14	0.49
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	15	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	15	0.49
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	15	0.49
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	1	0.49
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	1	0.49
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	3	0.49
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	3	0.49
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	3	0.49
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	3	0.49
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	3	0.49
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	3	0.49
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	3	0.49
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	3	0.49
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	3	0.49
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	5	0.49
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	5	0.49
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	5	0.49
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	5	0.49
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	5	0.49
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	5	0.49
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	5	0.49
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	5	0.49
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	5	0.49
(1,4612)	2:290:B:TYR:HE2	2:286:B:LEU:HG	19	0.48
(1,4609)	2:224:B:TYR:HD2	2:223:B:GLU:HB3	3	0.48
(1,4567)	2:242:B:TYR:HE1	2:234:B:LEU:HD22	7	0.48
(1,4513)	2:235:B:TYR:HE1	2:175:B:ILE:HD13	14	0.48
(1,4511)	2:182:B:PHE:HD1	2:184:B:LEU:HB3	12	0.48
(1,4418)	2:169:B:VAL:HG23	1:112:A:ILE:HG22	18	0.48
(1,4417)	1:109:A:GLU:HG2	1:112:A:ILE:HG21	18	0.48
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG22	8	0.48
(1,4387)	1:112:A:ILE:HG21	1:109:A:GLU:HG2	18	0.48
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	8	0.48
(1,4334)	1:95:A:ILE:HG21	1:74:A:SER:HB3	20	0.48
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	9	0.48
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	8	0.48
(1,4198)	2:164:B:LEU:HD23	2:299:B:ALA:H	12	0.48
(1,4140)	2:254:B:MET:HE1	2:252:B:ALA:H	7	0.48
(1,4035)	2:162:B:GLU:HG3	2:163:B:GLU:H	20	0.48
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD21	4	0.48
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG21	10	0.48
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG21	1	0.48
(1,3795)	2:221:B:ILE:HG22	2:190:B:VAL:HG12	13	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3776)	2:257:B:VAL:HG23	2:185:B:PRO:HB3	4	0.48
(1,3774)	2:245:B:ILE:HG12	2:184:B:LEU:HD23	15	0.48
(1,3750)	1:111:A:ILE:HD11	2:165:B:LYS:HE2	9	0.48
(1,3732)	2:168:B:LEU:HD13	2:160:B:ILE:HD13	13	0.48
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	15	0.48
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	15	0.48
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	15	0.48
(1,3060)	1:79:A:ASP:HB3	1:76:A:VAL:HG11	4	0.48
(1,3060)	1:79:A:ASP:HB3	1:76:A:VAL:HG12	4	0.48
(1,3060)	1:79:A:ASP:HB3	1:76:A:VAL:HG13	4	0.48
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	15	0.48
(1,2653)	1:90:A:LEU:HD21	1:89:A:ALA:HA	4	0.48
(1,2653)	1:90:A:LEU:HD22	1:89:A:ALA:HA	4	0.48
(1,2653)	1:90:A:LEU:HD23	1:89:A:ALA:HA	4	0.48
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD11	15	0.48
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD12	15	0.48
(1,2565)	1:78:A:TRP:HB2	1:81:A:LEU:HD13	15	0.48
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB3	14	0.48
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB3	14	0.48
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB3	14	0.48
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	11	0.48
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	17	0.48
(1,1270)	2:193:B:ILE:HD11	2:188:B:LYS:HE3	12	0.48
(1,1270)	2:193:B:ILE:HD12	2:188:B:LYS:HE3	12	0.48
(1,1270)	2:193:B:ILE:HD13	2:188:B:LYS:HE3	12	0.48
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	10	0.48
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	10	0.48
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	10	0.48
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE1	15	0.48
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE2	15	0.48
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE3	15	0.48
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE1	15	0.48
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE2	15	0.48
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE3	15	0.48
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE1	15	0.48
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE2	15	0.48
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE3	15	0.48
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG21	11	0.48
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG22	11	0.48
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG23	11	0.48
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG21	11	0.48
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG22	11	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG23	11	0.48
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG21	11	0.48
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG22	11	0.48
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG23	11	0.48
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	2	0.48
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	2	0.48
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	6	0.48
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	6	0.48
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	6	0.48
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	6	0.48
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	6	0.48
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	6	0.48
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	6	0.48
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	6	0.48
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	6	0.48
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	4	0.48
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	4	0.48
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	4	0.48
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	4	0.48
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	4	0.48
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	4	0.48
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	4	0.48
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	4	0.48
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	4	0.48
(1,4631)	2:167:B:TRP:HZ3	2:308:B:ALA:HB3	1	0.47
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	5	0.47
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	8	0.47
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	17	0.47
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG21	18	0.47
(1,4513)	2:235:B:TYR:HE2	2:175:B:ILE:HD11	3	0.47
(1,4511)	2:182:B:PHE:HD2	2:184:B:LEU:HB3	15	0.47
(1,4492)	2:212:B:TYR:HE1	1:81:A:LEU:H	19	0.47
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	18	0.47
(1,4364)	1:111:A:ILE:HD12	1:107:A:LEU:HA	3	0.47
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG23	4	0.47
(1,4361)	2:235:B:TYR:HE1	1:106:A:VAL:HG12	19	0.47
(1,4318)	1:95:A:ILE:HG22	1:91:A:HIS:HA	19	0.47
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	3	0.47
(1,4140)	2:185:B:PRO:HB3	2:252:B:ALA:H	5	0.47
(1,4028)	1:96:A:LEU:HD13	2:277:B:THR:HB	1	0.47
(1,4001)	2:193:B:ILE:HG13	2:305:B:LEU:HD12	17	0.47
(1,3980)	2:164:B:LEU:HD21	2:295:B:LEU:HD22	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3971)	2:267:B:PHE:HE2	2:295:B:LEU:HD12	5	0.47
(1,3894)	2:254:B:MET:HE3	2:245:B:ILE:HG21	16	0.47
(1,3869)	2:232:B:GLN:HB3	2:233:B:LEU:HD21	18	0.47
(1,3812)	2:218:B:VAL:HG23	2:194:B:LEU:HD23	1	0.47
(1,3796)	2:255:B:SER:HB3	2:190:B:VAL:HG13	20	0.47
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD11	15	0.47
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD12	15	0.47
(1,3057)	2:227:B:VAL:HG11	1:96:A:LEU:HD13	15	0.47
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD11	15	0.47
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD12	15	0.47
(1,3057)	2:227:B:VAL:HG12	1:96:A:LEU:HD13	15	0.47
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD11	15	0.47
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD12	15	0.47
(1,3057)	2:227:B:VAL:HG13	1:96:A:LEU:HD13	15	0.47
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	10	0.47
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	10	0.47
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	10	0.47
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	1	0.47
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	1	0.47
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	1	0.47
(1,1703)	2:211:B:GLU:HG2	2:212:B:TYR:H	12	0.47
(1,1542)	2:188:B:LYS:HG2	2:189:B:ASN:H	18	0.47
(1,1450)	2:179:B:LYS:HD3	2:179:B:LYS:H	10	0.47
(1,1450)	2:179:B:LYS:HD3	2:179:B:LYS:H	17	0.47
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD21	3	0.47
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD22	3	0.47
(1,1000)	2:279:B:LEU:HB2	2:284:B:LEU:HD23	3	0.47
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG21	3	0.47
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG22	3	0.47
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG23	3	0.47
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG21	3	0.47
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG22	3	0.47
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG23	3	0.47
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG21	3	0.47
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG22	3	0.47
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG23	3	0.47
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD21	2	0.47
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD22	2	0.47
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD23	2	0.47
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD21	2	0.47
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD22	2	0.47
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD23	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD21	2	0.47
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD22	2	0.47
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD23	2	0.47
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	11	0.47
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	11	0.47
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	4	0.47
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	4	0.47
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	4	0.47
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	4	0.47
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	4	0.47
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	4	0.47
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	4	0.47
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	4	0.47
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	4	0.47
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	1	0.47
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	1	0.47
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	1	0.47
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	16	0.47
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	16	0.47
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	16	0.47
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	4	0.46
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	4	0.46
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	4	0.46
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	4	0.46
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	4	0.46
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	4	0.46
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD11	10	0.46
(1,4622)	2:267:B:PHE:HZ	2:298:B:LEU:HD12	17	0.46
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG21	3	0.46
(1,4511)	2:182:B:PHE:HD1	2:175:B:ILE:HD13	19	0.46
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	5	0.46
(1,4450)	1:72:A:VAL:HB	1:72:A:VAL:H	12	0.46
(1,4390)	1:115:A:VAL:HG23	1:111:A:ILE:HA	3	0.46
(1,4384)	2:169:B:VAL:HG22	1:109:A:GLU:HA	2	0.46
(1,4302)	1:91:A:HIS:HB2	1:88:A:GLN:HA	10	0.46
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	19	0.46
(1,4035)	2:162:B:GLU:HG3	2:163:B:GLU:H	10	0.46
(1,3901)	2:246:B:LEU:HD12	2:252:B:ALA:HB1	2	0.46
(1,3869)	2:228:B:MET:HE1	2:233:B:LEU:HD22	20	0.46
(1,3857)	1:98:A:PHE:HE2	2:227:B:VAL:HG12	15	0.46
(1,3824)	2:214:B:VAL:HG21	2:202:B:LYS:HE2	2	0.46
(1,3774)	2:245:B:ILE:HG12	2:184:B:LEU:HD21	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3750)	2:160:B:ILE:HG21	2:165:B:LYS:HE2	6	0.46
(1,3734)	2:161:B:PRO:HB2	2:160:B:ILE:HG23	7	0.46
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD12	20	0.46
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	6	0.46
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	6	0.46
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	16	0.46
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	16	0.46
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	10	0.46
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	10	0.46
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	10	0.46
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	17	0.46
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	17	0.46
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	17	0.46
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	6	0.46
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	6	0.46
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	6	0.46
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD23	20	0.46
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD11	6	0.46
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD12	6	0.46
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD13	6	0.46
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD11	6	0.46
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD12	6	0.46
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD13	6	0.46
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD21	20	0.46
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD22	20	0.46
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD23	20	0.46
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	12	0.46
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	18	0.46
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	18	0.46
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	18	0.46
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	15	0.46
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	15	0.46
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	15	0.46
(1,4622)	2:267:B:PHE:HZ	2:221:B:ILE:HG12	5	0.45
(1,4599)	2:294:B:PHE:HZ	2:263:B:LEU:HD12	3	0.45
(1,4599)	2:294:B:PHE:HZ	2:263:B:LEU:HD12	14	0.45
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	18	0.45
(1,4444)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	18	0.45
(1,4440)	2:223:B:GLU:HG3	1:77:A:ILE:HG21	5	0.45
(1,4396)	2:165:B:LYS:HE2	1:111:A:ILE:HD11	6	0.45
(1,4384)	2:169:B:VAL:HG21	1:109:A:GLU:HA	17	0.45
(1,4363)	2:235:B:TYR:HD2	1:106:A:VAL:HG23	16	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4343)	1:74:A:SER:HB2	1:95:A:ILE:HD12	20	0.45
(1,4324)	1:95:A:ILE:HG23	1:91:A:HIS:HB2	12	0.45
(1,4296)	1:90:A:LEU:HD13	1:87:A:MET:HE1	8	0.45
(1,4280)	2:290:B:TYR:HE2	1:81:A:LEU:HD21	16	0.45
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD11	19	0.45
(1,3966)	2:288:B:LEU:HD22	2:288:B:LEU:HA	6	0.45
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD23	13	0.45
(1,3947)	2:272:B:ALA:HB2	2:273:B:MET:HE3	15	0.45
(1,3789)	2:305:B:LEU:HD12	2:188:B:LYS:HE2	9	0.45
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD22	4	0.45
(1,3721)	2:154:B:ALA:HB1	2:156:B:VAL:HA	1	0.45
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	1	0.45
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	1	0.45
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD21	15	0.45
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD22	15	0.45
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD23	15	0.45
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD21	15	0.45
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD22	15	0.45
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD23	15	0.45
(1,2870)	2:172:B:TRP:HE3	1:107:A:LEU:HD21	15	0.45
(1,2870)	2:172:B:TRP:HE3	1:107:A:LEU:HD22	15	0.45
(1,2870)	2:172:B:TRP:HE3	1:107:A:LEU:HD23	15	0.45
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	16	0.45
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	6	0.45
(1,1734)	2:216:B:GLU:HG2	2:216:B:GLU:H	8	0.45
(1,1702)	2:211:B:GLU:HB2	2:212:B:TYR:H	3	0.45
(1,1067)	2:298:B:LEU:HD11	2:295:B:LEU:HA	17	0.45
(1,1067)	2:298:B:LEU:HD12	2:295:B:LEU:HA	17	0.45
(1,1067)	2:298:B:LEU:HD13	2:295:B:LEU:HA	17	0.45
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD11	14	0.45
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD12	14	0.45
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD13	14	0.45
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD11	14	0.45
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	14	0.45
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD13	14	0.45
(1,313)	2:192:B:SER:HB2	2:188:B:LYS:HG3	6	0.45
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD21	5	0.45
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD22	5	0.45
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD23	5	0.45
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD21	5	0.45
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD22	5	0.45
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD23	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD21	5	0.45
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD22	5	0.45
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD23	5	0.45
(1,4616)	2:267:B:PHE:HE1	2:291:B:LEU:HG	5	0.44
(1,4611)	2:290:B:TYR:HD2	2:286:B:LEU:HG	16	0.44
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	1	0.44
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	3	0.44
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG23	8	0.44
(1,4515)	2:172:B:TRP:HZ3	2:169:B:VAL:HG12	8	0.44
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	12	0.44
(1,4447)	2:232:B:GLN:HG3	1:103:A:ARG:HG2	15	0.44
(1,4435)	1:119:A:LYS:HE3	1:119:A:LYS:HA	1	0.44
(1,4429)	1:73:A:PRO:HB2	1:76:A:VAL:HG12	10	0.44
(1,4418)	2:169:B:VAL:HG21	1:112:A:ILE:HG21	1	0.44
(1,4417)	1:109:A:GLU:HG2	1:112:A:ILE:HG23	10	0.44
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG22	15	0.44
(1,4395)	2:165:B:LYS:HE3	1:111:A:ILE:HD13	11	0.44
(1,4390)	1:115:A:VAL:HG23	1:111:A:ILE:HA	15	0.44
(1,4387)	1:112:A:ILE:HG23	1:109:A:GLU:HG2	10	0.44
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	19	0.44
(1,4327)	2:279:B:LEU:HD21	1:94:A:GLU:HB3	19	0.44
(1,4296)	2:279:B:LEU:HD12	1:87:A:MET:HE2	14	0.44
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	17	0.44
(1,4237)	2:218:B:VAL:HG12	2:198:B:ALA:H	13	0.44
(1,4036)	2:160:B:ILE:HG21	2:164:B:LEU:H	20	0.44
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD23	15	0.44
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE3	16	0.44
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	7	0.44
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	19	0.44
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	19	0.44
(1,3408)	1:119:A:LYS:HB2	1:119:A:LYS:H	7	0.44
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	8	0.44
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	8	0.44
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	8	0.44
(1,2852)	1:108:A:PRO:HD2	1:107:A:LEU:HD11	8	0.44
(1,2852)	1:108:A:PRO:HD2	1:107:A:LEU:HD12	8	0.44
(1,2852)	1:108:A:PRO:HD2	1:107:A:LEU:HD13	8	0.44
(1,2775)	1:96:A:LEU:HD11	1:100:A:ASN:HB3	13	0.44
(1,2775)	1:96:A:LEU:HD12	1:100:A:ASN:HB3	13	0.44
(1,2775)	1:96:A:LEU:HD13	1:100:A:ASN:HB3	13	0.44
(1,2693)	1:92:A:GLU:HG2	1:93:A:SER:HA	11	0.44
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	11	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	11	0.44
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	11	0.44
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB2	2	0.44
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB2	2	0.44
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB2	2	0.44
(1,1450)	2:179:B:LYS:HD3	2:179:B:LYS:H	4	0.44
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD21	15	0.44
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD22	15	0.44
(1,881)	2:270:B:ILE:HD11	2:266:B:LEU:HD23	15	0.44
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD21	15	0.44
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD22	15	0.44
(1,881)	2:270:B:ILE:HD12	2:266:B:LEU:HD23	15	0.44
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD21	15	0.44
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD22	15	0.44
(1,881)	2:270:B:ILE:HD13	2:266:B:LEU:HD23	15	0.44
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	5	0.44
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	5	0.44
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	5	0.44
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	5	0.44
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	5	0.44
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	5	0.44
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	5	0.44
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	5	0.44
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	5	0.44
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	20	0.44
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	20	0.44
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	20	0.44
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD21	2	0.44
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD22	2	0.44
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD23	2	0.44
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD21	2	0.44
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD22	2	0.44
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD23	2	0.44
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD21	2	0.44
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD22	2	0.44
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD23	2	0.44
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD21	5	0.44
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD22	5	0.44
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD23	5	0.44
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD21	5	0.44
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD22	5	0.44
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD23	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD21	5	0.44
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD22	5	0.44
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD23	5	0.44
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	7	0.44
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	7	0.44
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	7	0.44
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	10	0.44
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	10	0.44
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	10	0.44
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	10	0.44
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	10	0.44
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	10	0.44
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	10	0.44
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	10	0.44
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	10	0.44
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD12	9	0.43
(1,4613)	2:197:B:TYR:HE2	2:214:B:VAL:HG13	6	0.43
(1,4613)	2:197:B:TYR:HE2	2:214:B:VAL:HG13	14	0.43
(1,4609)	2:224:B:TYR:HD1	2:273:B:MET:HE3	4	0.43
(1,4595)	2:182:B:PHE:HD2	2:262:B:HIS:HE1	2	0.43
(1,4575)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	8	0.43
(1,4574)	2:242:B:TYR:HD1	2:234:B:LEU:HD13	17	0.43
(1,4562)	2:242:B:TYR:HE2	2:246:B:LEU:HD12	11	0.43
(1,4555)	2:294:B:PHE:HD1	2:217:B:VAL:HG12	14	0.43
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	20	0.43
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG23	1	0.43
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG22	12	0.43
(1,4516)	2:237:B:PHE:HE2	2:175:B:ILE:HG23	16	0.43
(1,4511)	2:182:B:PHE:HD2	2:181:B:LEU:HG	2	0.43
(1,4506)	2:235:B:TYR:HD1	2:175:B:ILE:HB	2	0.43
(1,4327)	2:279:B:LEU:HD21	1:94:A:GLU:HB3	14	0.43
(1,4304)	1:86:A:ASP:HB2	1:89:A:ALA:HB3	20	0.43
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	15	0.43
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD11	9	0.43
(1,4243)	1:72:A:VAL:HG21	1:71:A:GLN:HB2	9	0.43
(1,4047)	2:235:B:TYR:HE1	2:172:B:TRP:HE1	2	0.43
(1,4008)	2:178:B:GLN:HB2	2:313:B:VAL:HG13	2	0.43
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG13	14	0.43
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD23	8	0.43
(1,3893)	2:252:B:ALA:HB3	2:245:B:ILE:HG23	7	0.43
(1,3824)	2:214:B:VAL:HG23	2:202:B:LYS:HE2	4	0.43
(1,3795)	2:194:B:LEU:HD21	2:190:B:VAL:HG12	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2945)	1:107:A:LEU:HD21	1:112:A:ILE:HG13	3	0.43
(1,2945)	1:107:A:LEU:HD22	1:112:A:ILE:HG13	3	0.43
(1,2945)	1:107:A:LEU:HD23	1:112:A:ILE:HG13	3	0.43
(1,2911)	1:114:A:GLU:HB3	1:111:A:ILE:HA	1	0.43
(1,2811)	1:106:A:VAL:HG11	1:104:A:ASN:HB3	12	0.43
(1,2811)	1:106:A:VAL:HG12	1:104:A:ASN:HB3	12	0.43
(1,2811)	1:106:A:VAL:HG13	1:104:A:ASN:HB3	12	0.43
(1,2776)	1:98:A:PHE:HD1	1:100:A:ASN:HB3	15	0.43
(1,2776)	1:98:A:PHE:HD2	1:100:A:ASN:HB3	15	0.43
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	1	0.43
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	1	0.43
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	1	0.43
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	1	0.43
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	1	0.43
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	1	0.43
(1,2593)	2:212:B:TYR:HD1	1:84:A:MET:HB3	14	0.43
(1,2593)	2:212:B:TYR:HD2	1:84:A:MET:HB3	14	0.43
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	9	0.43
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	9	0.43
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	9	0.43
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	10	0.43
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	7	0.43
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	7	0.43
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	7	0.43
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	5	0.43
(1,1626)	2:195:B:GLU:HG2	2:199:B:ASN:HD22	12	0.43
(1,1558)	2:189:B:ASN:HD21	2:191:B:ASP:H	4	0.43
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	4	0.43
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	4	0.43
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	4	0.43
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	15	0.43
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	15	0.43
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	15	0.43
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	15	0.43
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	15	0.43
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	15	0.43
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	15	0.43
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	15	0.43
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	15	0.43
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD21	17	0.43
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD22	17	0.43
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD23	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE1	17	0.43
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE2	17	0.43
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE3	17	0.43
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD21	19	0.43
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD22	19	0.43
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD23	19	0.43
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD21	19	0.43
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD22	19	0.43
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD23	19	0.43
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD21	19	0.43
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD22	19	0.43
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD23	19	0.43
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	8	0.43
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	8	0.43
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	8	0.43
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	11	0.43
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	11	0.43
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	11	0.43
(1,455)	2:211:B:GLU:HA	2:211:B:GLU:HG2	10	0.43
(1,309)	2:192:B:SER:HB2	2:188:B:LYS:HE2	13	0.43
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE3	9	0.43
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE3	9	0.43
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	18	0.43
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	18	0.43
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	18	0.43
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	18	0.43
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	18	0.43
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	18	0.43
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	18	0.43
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	18	0.43
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	18	0.43
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD2	4	0.43
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD3	9	0.43
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD21	6	0.43
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD22	6	0.43
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD23	6	0.43
(1,4447)	2:232:B:GLN:HG3	1:103:A:ARG:HG2	1	0.42
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG23	5	0.42
(1,4384)	2:169:B:VAL:HG22	1:109:A:GLU:HA	9	0.42
(1,4267)	2:219:B:ALA:HA	1:77:A:ILE:HG23	6	0.42
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG23	4	0.42
(1,3812)	2:218:B:VAL:HG21	2:194:B:LEU:HD21	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3733)	2:165:B:LYS:HB3	2:160:B:ILE:HG22	10	0.42
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	11	0.42
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	12	0.42
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	12	0.42
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	12	0.42
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD21	3	0.42
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD22	3	0.42
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD23	3	0.42
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	16	0.42
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	16	0.42
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	16	0.42
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	16	0.42
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	16	0.42
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	16	0.42
(1,2693)	1:92:A:GLU:HG3	1:93:A:SER:HA	20	0.42
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	19	0.42
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	19	0.42
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	19	0.42
(1,2458)	1:70:A:ARG:HG3	1:70:A:ARG:HA	15	0.42
(1,2458)	1:70:A:ARG:HG3	1:70:A:ARG:HA	19	0.42
(1,2341)	2:307:B:SER:HB3	2:309:B:SER:H	10	0.42
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	20	0.42
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	20	0.42
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	20	0.42
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	9	0.42
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	9	0.42
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	9	0.42
(1,2023)	2:257:B:VAL:HG11	2:256:B:GLN:H	20	0.42
(1,2023)	2:257:B:VAL:HG12	2:256:B:GLN:H	20	0.42
(1,2023)	2:257:B:VAL:HG13	2:256:B:GLN:H	20	0.42
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD11	8	0.42
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD12	8	0.42
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD13	8	0.42
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD11	8	0.42
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD12	8	0.42
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD13	8	0.42
(1,815)	2:253:B:PRO:HG2	2:256:B:GLN:HG2	19	0.42
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	19	0.42
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	19	0.42
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	19	0.42
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	6	0.42
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	6	0.42
(1,455)	2:211:B:GLU:HA	2:211:B:GLU:HG3	6	0.42
(1,342)	2:188:B:LYS:HG2	2:192:B:SER:HB2	1	0.42
(1,332)	2:255:B:SER:HA	2:190:B:VAL:HG21	14	0.42
(1,332)	2:255:B:SER:HA	2:190:B:VAL:HG22	14	0.42
(1,332)	2:255:B:SER:HA	2:190:B:VAL:HG23	14	0.42
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD21	9	0.42
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD22	9	0.42
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD23	9	0.42
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	2	0.41
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	2	0.41
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	2	0.41
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	2	0.41
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	2	0.41
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	2	0.41
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD13	13	0.41
(1,4575)	2:242:B:TYR:HE1	2:246:B:LEU:HD12	15	0.41
(1,4555)	2:294:B:PHE:HD2	2:264:B:LEU:HD13	20	0.41
(1,4545)	2:200:B:TYR:HD1	2:201:B:LYS:HD2	12	0.41
(1,4390)	1:115:A:VAL:HG23	1:111:A:ILE:HA	2	0.41
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD21	14	0.41
(1,4237)	2:218:B:VAL:HG12	2:198:B:ALA:H	6	0.41
(1,4031)	2:188:B:LYS:HG2	2:193:B:ILE:HD12	6	0.41
(1,4030)	2:192:B:SER:HB3	2:188:B:LYS:HG2	16	0.41
(1,3972)	2:291:B:LEU:HA	2:291:B:LEU:HD22	8	0.41
(1,3918)	2:298:B:LEU:HD12	2:263:B:LEU:HD12	3	0.41
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE3	3	0.41
(1,3851)	2:211:B:GLU:HA	2:202:B:LYS:HE2	17	0.41
(1,3817)	2:198:B:ALA:HB1	2:195:B:GLU:HG3	14	0.41
(1,3750)	1:111:A:ILE:HD13	2:165:B:LYS:HE2	18	0.41
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	1	0.41
(1,3219)	1:94:A:GLU:HG3	1:94:A:GLU:H	12	0.41
(1,2818)	2:233:B:LEU:HD21	1:105:A:PHE:HA	15	0.41
(1,2818)	2:233:B:LEU:HD22	1:105:A:PHE:HA	15	0.41
(1,2818)	2:233:B:LEU:HD23	1:105:A:PHE:HA	15	0.41
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	18	0.41
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	18	0.41
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	18	0.41
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	4	0.41
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	4	0.41
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	4	0.41
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	6	0.41
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	6	0.41
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	18	0.41
(1,1888)	2:238:B:GLU:HG3	2:238:B:GLU:H	6	0.41
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	18	0.41
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	18	0.41
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	18	0.41
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	4	0.41
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	4	0.41
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	4	0.41
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	9	0.41
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	9	0.41
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	9	0.41
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	7	0.41
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	7	0.41
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	7	0.41
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	4	0.41
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	4	0.41
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	4	0.41
(1,342)	2:188:B:LYS:HG2	2:192:B:SER:HB2	13	0.41
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD11	15	0.41
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD12	15	0.41
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD13	15	0.41
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD3	19	0.41
(1,4607)	2:267:B:PHE:HD1	2:270:B:ILE:HG22	5	0.4
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	3	0.4
(1,4511)	2:182:B:PHE:HD2	2:181:B:LEU:HG	13	0.4
(1,4418)	2:169:B:VAL:HG22	1:112:A:ILE:HG22	3	0.4
(1,4361)	2:235:B:TYR:HE1	1:106:A:VAL:HG12	6	0.4
(1,4318)	2:279:B:LEU:HD23	1:91:A:HIS:HA	8	0.4
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	3	0.4
(1,4237)	2:218:B:VAL:HG13	2:198:B:ALA:H	2	0.4
(1,4055)	2:175:B:ILE:HG22	2:180:B:GLN:H	13	0.4
(1,4036)	2:164:B:LEU:HD11	2:164:B:LEU:H	16	0.4
(1,3990)	2:263:B:LEU:HD11	2:298:B:LEU:HD21	10	0.4
(1,3947)	2:272:B:ALA:HB3	2:273:B:MET:HE3	19	0.4
(1,3776)	2:257:B:VAL:HG21	2:185:B:PRO:HB3	7	0.4
(1,3766)	2:235:B:TYR:HD2	2:175:B:ILE:HD11	8	0.4
(1,3766)	2:235:B:TYR:HD1	2:175:B:ILE:HD13	16	0.4
(1,3737)	2:163:B:GLU:HG2	2:163:B:GLU:HA	6	0.4
(1,3724)	2:271:B:GLY:HA3	2:156:B:VAL:HG11	9	0.4
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	13	0.4
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	13	0.4
(1,3409)	1:119:A:LYS:HG2	1:119:A:LYS:H	2	0.4
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD11	15	0.4
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD12	15	0.4
(1,3091)	2:268:B:VAL:HB	1:107:A:LEU:HD13	15	0.4
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	13	0.4
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	13	0.4
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	13	0.4
(1,2803)	2:232:B:GLN:HA	1:103:A:ARG:HD2	15	0.4
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD11	7	0.4
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD12	7	0.4
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD13	7	0.4
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD11	7	0.4
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD12	7	0.4
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD13	7	0.4
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	12	0.4
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	12	0.4
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	12	0.4
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	12	0.4
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	7	0.4
(1,1703)	2:211:B:GLU:HG3	2:212:B:TYR:H	20	0.4
(1,1542)	2:188:B:LYS:HG2	2:189:B:ASN:H	13	0.4
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB1	8	0.4
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB2	8	0.4
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB3	8	0.4
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB1	8	0.4
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB2	8	0.4
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB3	8	0.4
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB1	8	0.4
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB2	8	0.4
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB3	8	0.4
(1,1067)	2:298:B:LEU:HD11	2:295:B:LEU:HA	12	0.4
(1,1067)	2:298:B:LEU:HD12	2:295:B:LEU:HA	12	0.4
(1,1067)	2:298:B:LEU:HD13	2:295:B:LEU:HA	12	0.4
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	7	0.4
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD21	10	0.4
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD22	10	0.4
(1,943)	2:271:B:GLY:HA3	2:274:B:LEU:HD23	10	0.4
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE1	10	0.4
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE2	10	0.4
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE3	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	6	0.4
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	6	0.4
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	6	0.4
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	6	0.4
(1,422)	2:211:B:GLU:HG2	2:202:B:LYS:HE2	13	0.4
(1,409)	2:202:B:LYS:HD3	2:199:B:ASN:HA	5	0.4
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	1	0.4
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	1	0.4
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	1	0.4
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	1	0.4
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	1	0.4
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	1	0.4
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	1	0.4
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	1	0.4
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	1	0.4
(1,124)	1:107:A:LEU:HD21	2:169:B:VAL:HA	8	0.4
(1,124)	1:107:A:LEU:HD22	2:169:B:VAL:HA	8	0.4
(1,124)	1:107:A:LEU:HD23	2:169:B:VAL:HA	8	0.4
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG3	20	0.39
(1,4643)	2:225:B:PHE:HE2	2:190:B:VAL:HB	11	0.39
(1,4608)	2:290:B:TYR:HD1	2:217:B:VAL:HG21	17	0.39
(1,4384)	2:169:B:VAL:HG23	1:109:A:GLU:HA	7	0.39
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	3	0.39
(1,4364)	1:111:A:ILE:HD13	1:107:A:LEU:HA	16	0.39
(1,4327)	1:95:A:ILE:HD12	1:92:A:GLU:HB3	6	0.39
(1,4313)	1:87:A:MET:HE2	1:90:A:LEU:HD11	16	0.39
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	4	0.39
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	6	0.39
(1,4055)	2:175:B:ILE:HG22	2:180:B:GLN:H	18	0.39
(1,3999)	2:200:B:TYR:HE2	2:296:B:LYS:HE3	12	0.39
(1,3990)	2:263:B:LEU:HD11	2:298:B:LEU:HD23	5	0.39
(1,3942)	2:274:B:LEU:HD21	2:270:B:ILE:HG23	11	0.39
(1,3794)	2:194:B:LEU:HG	2:190:B:VAL:HG11	14	0.39
(1,3749)	2:160:B:ILE:HG23	2:165:B:LYS:HE3	2	0.39
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	18	0.39
(1,3219)	1:94:A:GLU:HG3	1:94:A:GLU:H	18	0.39
(1,3039)	2:231:B:THR:HA	1:102:A:GLU:HG3	5	0.39
(1,2893)	2:268:B:VAL:HG21	1:108:A:PRO:HG2	1	0.39
(1,2893)	2:268:B:VAL:HG22	1:108:A:PRO:HG2	1	0.39
(1,2893)	2:268:B:VAL:HG23	1:108:A:PRO:HG2	1	0.39
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	12	0.39
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	12	0.39
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG3	20	0.39
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	18	0.39
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	18	0.39
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	18	0.39
(1,1703)	2:211:B:GLU:HG3	2:212:B:TYR:H	15	0.39
(1,1249)	2:321:B:LYS:HG2	2:321:B:LYS:HE2	10	0.39
(1,1249)	2:321:B:LYS:HG2	2:321:B:LYS:HE2	20	0.39
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB1	17	0.39
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB2	17	0.39
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB3	17	0.39
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB1	17	0.39
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB2	17	0.39
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB3	17	0.39
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB1	17	0.39
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB2	17	0.39
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB3	17	0.39
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	6	0.39
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	6	0.39
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	6	0.39
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG3	7	0.39
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG3	7	0.39
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG3	7	0.39
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD21	10	0.39
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD22	10	0.39
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD23	10	0.39
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD21	10	0.39
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD22	10	0.39
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD23	10	0.39
(1,596)	2:234:B:LEU:HD21	2:230:B:GLY:HA3	15	0.39
(1,596)	2:234:B:LEU:HD22	2:230:B:GLY:HA3	15	0.39
(1,596)	2:234:B:LEU:HD23	2:230:B:GLY:HA3	15	0.39
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD21	9	0.39
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD22	9	0.39
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD23	9	0.39
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD21	9	0.39
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD22	9	0.39
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD23	9	0.39
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD21	9	0.39
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD22	9	0.39
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD23	9	0.39
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	15	0.39
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	15	0.39
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	7	0.39
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	7	0.39
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	7	0.39
(1,456)	2:245:B:ILE:HG21	2:244:B:GLU:HG2	14	0.39
(1,456)	2:245:B:ILE:HG22	2:244:B:GLU:HG2	14	0.39
(1,456)	2:245:B:ILE:HG23	2:244:B:GLU:HG2	14	0.39
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD21	8	0.39
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD22	8	0.39
(1,5)	2:283:B:SER:HA	2:286:B:LEU:HD23	8	0.39
(1,4599)	2:294:B:PHE:HZ	2:263:B:LEU:HD12	12	0.38
(1,4575)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	5	0.38
(1,4562)	2:225:B:PHE:HE1	2:233:B:LEU:HD13	13	0.38
(1,4556)	2:197:B:TYR:HE2	2:217:B:VAL:HG22	11	0.38
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	4	0.38
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	11	0.38
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	11	0.38
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	20	0.38
(1,4384)	2:169:B:VAL:HG23	1:109:A:GLU:HA	16	0.38
(1,4329)	1:89:A:ALA:HB2	1:92:A:GLU:HG2	3	0.38
(1,4324)	1:95:A:ILE:HG23	1:91:A:HIS:HB2	13	0.38
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	9	0.38
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD12	5	0.38
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	15	0.38
(1,4030)	2:187:B:LYS:HA	2:188:B:LYS:HG2	6	0.38
(1,3979)	2:160:B:ILE:HG22	2:295:B:LEU:HD21	2	0.38
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD21	1	0.38
(1,3940)	2:274:B:LEU:HG	2:270:B:ILE:HD11	20	0.38
(1,3893)	2:246:B:LEU:HB2	2:245:B:ILE:HG21	19	0.38
(1,3810)	2:222:B:LYS:HB3	2:194:B:LEU:HD12	12	0.38
(1,3689)	2:318:B:TYR:HE1	2:241:B:GLN:HG2	2	0.38
(1,3689)	2:318:B:TYR:HE2	2:241:B:GLN:HG2	2	0.38
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	18	0.38
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	18	0.38
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD21	2	0.38
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD22	2	0.38
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD23	2	0.38
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD21	2	0.38
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD22	2	0.38
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD23	2	0.38
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	9	0.38
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD21	3	0.38
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD22	3	0.38
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD23	3	0.38
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	16	0.38
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	16	0.38
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	16	0.38
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	11	0.38
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	12	0.38
(1,1249)	2:321:B:LYS:HG2	2:321:B:LYS:HE2	6	0.38
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	5	0.38
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	5	0.38
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	5	0.38
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	20	0.38
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	20	0.38
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	20	0.38
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE1	7	0.38
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE2	7	0.38
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE3	7	0.38
(1,923)	2:155:B:GLU:HG3	2:272:B:ALA:HA	1	0.38
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	8	0.38
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	8	0.38
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	8	0.38
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD21	15	0.38
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD22	15	0.38
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD23	15	0.38
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	20	0.38
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	20	0.38
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	20	0.38
(1,420)	2:199:B:ASN:HA	2:202:B:LYS:HE2	2	0.38
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD11	8	0.38
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD12	8	0.38
(1,356)	2:263:B:LEU:HD11	2:193:B:ILE:HD13	8	0.38
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD11	8	0.38
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD12	8	0.38
(1,356)	2:263:B:LEU:HD12	2:193:B:ILE:HD13	8	0.38
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD11	8	0.38
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD12	8	0.38
(1,356)	2:263:B:LEU:HD13	2:193:B:ILE:HD13	8	0.38
(1,299)	2:193:B:ILE:HD11	2:188:B:LYS:HD3	18	0.38
(1,299)	2:193:B:ILE:HD12	2:188:B:LYS:HD3	18	0.38
(1,299)	2:193:B:ILE:HD13	2:188:B:LYS:HD3	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE3	10	0.38
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE3	10	0.38
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD2	14	0.38
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD11	1	0.37
(1,4611)	2:290:B:TYR:HD2	2:286:B:LEU:HG	3	0.37
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	16	0.37
(1,4560)	2:225:B:PHE:HD1	2:233:B:LEU:HD12	3	0.37
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE2	3	0.37
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG23	9	0.37
(1,4445)	1:70:A:ARG:HA	1:72:A:VAL:HG11	14	0.37
(1,4384)	1:106:A:VAL:HG12	1:109:A:GLU:HA	3	0.37
(1,4364)	1:111:A:ILE:HD13	1:107:A:LEU:HA	13	0.37
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD12	14	0.37
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	18	0.37
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	7	0.37
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	19	0.37
(1,4182)	2:291:B:LEU:HD23	2:292:B:HIS:H	3	0.37
(1,4182)	2:291:B:LEU:HD21	2:292:B:HIS:H	16	0.37
(1,3942)	2:274:B:LEU:HD21	2:270:B:ILE:HG22	19	0.37
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	17	0.37
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	17	0.37
(1,3613)	2:276:B:TYR:HE2	2:273:B:MET:HB3	3	0.37
(1,3585)	2:249:B:HIS:HD2	2:248:B:ASP:HB2	15	0.37
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	17	0.37
(1,3395)	1:117:A:GLU:HG2	1:117:A:GLU:H	8	0.37
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD11	2	0.37
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD12	2	0.37
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD13	2	0.37
(1,2902)	1:112:A:ILE:HD11	1:109:A:GLU:HG3	2	0.37
(1,2902)	1:112:A:ILE:HD12	1:109:A:GLU:HG3	2	0.37
(1,2902)	1:112:A:ILE:HD13	1:109:A:GLU:HG3	2	0.37
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	8	0.37
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	8	0.37
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	8	0.37
(1,1310)	2:157:B:LYS:HG3	2:157:B:LYS:H	12	0.37
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD11	14	0.37
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD12	14	0.37
(1,1284)	2:267:B:PHE:HD1	2:264:B:LEU:HD13	14	0.37
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD11	14	0.37
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD12	14	0.37
(1,1284)	2:267:B:PHE:HD2	2:264:B:LEU:HD13	14	0.37
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	9	0.37
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	9	0.37
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	1	0.37
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD11	8	0.37
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD12	8	0.37
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD13	8	0.37
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD11	8	0.37
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD12	8	0.37
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD13	8	0.37
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	6	0.37
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	6	0.37
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	6	0.37
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	6	0.37
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	6	0.37
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	6	0.37
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	6	0.37
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	6	0.37
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	6	0.37
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG3	14	0.37
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG3	14	0.37
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG3	14	0.37
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD21	19	0.37
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD22	19	0.37
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD23	19	0.37
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD21	19	0.37
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD22	19	0.37
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD23	19	0.37
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD21	19	0.37
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD22	19	0.37
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD23	19	0.37
(1,456)	2:245:B:ILE:HG21	2:244:B:GLU:HG2	7	0.37
(1,456)	2:245:B:ILE:HG22	2:244:B:GLU:HG2	7	0.37
(1,456)	2:245:B:ILE:HG23	2:244:B:GLU:HG2	7	0.37
(1,299)	2:193:B:ILE:HD11	2:188:B:LYS:HD3	13	0.37
(1,299)	2:193:B:ILE:HD12	2:188:B:LYS:HD3	13	0.37
(1,299)	2:193:B:ILE:HD13	2:188:B:LYS:HD3	13	0.37
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	10	0.37
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	10	0.37
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	10	0.37
(1,45)	2:159:B:LYS:HA	2:159:B:LYS:HD3	16	0.37
(1,4564)	2:290:B:TYR:HE1	2:210:B:LYS:HG3	2	0.36
(1,4560)	2:225:B:PHE:HD1	2:233:B:LEU:HD11	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	4	0.36
(1,4507)	2:235:B:TYR:HE2	2:175:B:ILE:HB	20	0.36
(1,4490)	2:165:B:LYS:HB2	1:115:A:VAL:H	3	0.36
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	3	0.36
(1,4435)	1:119:A:LYS:HE3	1:119:A:LYS:HA	5	0.36
(1,4435)	1:119:A:LYS:HE3	1:119:A:LYS:HA	8	0.36
(1,4427)	1:114:A:GLU:HB3	1:115:A:VAL:HG21	6	0.36
(1,4390)	1:115:A:VAL:HG21	1:111:A:ILE:HA	19	0.36
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD21	13	0.36
(1,4357)	2:273:B:MET:HE1	1:100:A:ASN:HA	6	0.36
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	8	0.36
(1,4278)	1:84:A:MET:HE1	1:81:A:LEU:HD23	14	0.36
(1,4198)	2:164:B:LEU:HD22	2:299:B:ALA:H	6	0.36
(1,4054)	2:313:B:VAL:HG12	2:180:B:GLN:HE22	1	0.36
(1,3851)	2:211:B:GLU:HA	2:202:B:LYS:HE2	13	0.36
(1,3776)	2:257:B:VAL:HG22	2:185:B:PRO:HB3	1	0.36
(1,3776)	2:257:B:VAL:HG22	2:185:B:PRO:HB3	9	0.36
(1,3732)	2:168:B:LEU:HD11	2:160:B:ILE:HD13	14	0.36
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE3	6	0.36
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE3	6	0.36
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	14	0.36
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	14	0.36
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	14	0.36
(1,3039)	2:231:B:THR:HA	1:102:A:GLU:HG3	14	0.36
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB1	2	0.36
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB2	2	0.36
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB3	2	0.36
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	15	0.36
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	15	0.36
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	15	0.36
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	11	0.36
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	14	0.36
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	14	0.36
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	14	0.36
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	15	0.36
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	15	0.36
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	15	0.36
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	5	0.36
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	14	0.36
(1,1949)	2:246:B:LEU:HB2	2:247:B:ALA:H	18	0.36
(1,1888)	2:238:B:GLU:HG2	2:238:B:GLU:H	9	0.36
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	19	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	19	0.36
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	19	0.36
(1,1115)	2:297:B:TYR:HA	2:300:B:LYS:HD3	6	0.36
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	14	0.36
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	14	0.36
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	14	0.36
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	16	0.36
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	16	0.36
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	16	0.36
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	9	0.36
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	7	0.36
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	7	0.36
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	7	0.36
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	11	0.36
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	11	0.36
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	11	0.36
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	11	0.36
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	11	0.36
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	11	0.36
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	11	0.36
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	11	0.36
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	11	0.36
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD21	11	0.36
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD22	11	0.36
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD23	11	0.36
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	8	0.36
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	8	0.36
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	14	0.36
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	14	0.36
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	14	0.36
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	12	0.36
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	12	0.36
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	12	0.36
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	12	0.36
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	12	0.36
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	12	0.36
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	12	0.36
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	12	0.36
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	12	0.36
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD3	1	0.36
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD3	2	0.36
(1,4639)	2:237:B:PHE:HE1	2:322:B:ALA:HB1	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4599)	2:294:B:PHE:HZ	2:263:B:LEU:HD13	16	0.35
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG21	8	0.35
(1,4491)	1:118:A:GLY:HA3	1:117:A:GLU:H	20	0.35
(1,4448)	2:222:B:LYS:HB2	1:77:A:ILE:HD11	12	0.35
(1,4357)	2:273:B:MET:HE3	1:100:A:ASN:HA	8	0.35
(1,4328)	2:279:B:LEU:HD22	1:94:A:GLU:HB2	6	0.35
(1,4312)	1:94:A:GLU:HG3	1:90:A:LEU:HD11	6	0.35
(1,4308)	1:90:A:LEU:HD11	1:90:A:LEU:HB2	2	0.35
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	6	0.35
(1,4237)	2:218:B:VAL:HG11	2:198:B:ALA:H	10	0.35
(1,4182)	2:291:B:LEU:HD21	2:292:B:HIS:H	12	0.35
(1,4087)	2:202:B:LYS:HG2	2:202:B:LYS:H	8	0.35
(1,4036)	2:164:B:LEU:HD11	2:164:B:LEU:H	7	0.35
(1,4014)	2:181:B:LEU:HD12	2:314:B:ALA:HB2	18	0.35
(1,4009)	2:180:B:GLN:HG3	2:313:B:VAL:HG12	10	0.35
(1,3945)	2:274:B:LEU:HD21	2:271:B:GLY:HA3	20	0.35
(1,3920)	2:194:B:LEU:HD21	2:263:B:LEU:HD13	7	0.35
(1,3901)	2:257:B:VAL:HG22	2:252:B:ALA:HB2	9	0.35
(1,3869)	2:232:B:GLN:HB3	2:233:B:LEU:HD21	2	0.35
(1,3817)	2:198:B:ALA:HB1	2:195:B:GLU:HG3	5	0.35
(1,3817)	2:198:B:ALA:HB3	2:195:B:GLU:HG3	7	0.35
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD23	4	0.35
(1,3380)	1:116:A:ARG:HG3	1:116:A:ARG:H	11	0.35
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	3	0.35
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	16	0.35
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	16	0.35
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	16	0.35
(1,1703)	2:211:B:GLU:HG3	2:212:B:TYR:H	19	0.35
(1,1702)	2:211:B:GLU:HB3	2:212:B:TYR:H	9	0.35
(1,1626)	2:195:B:GLU:HG2	2:199:B:ASN:HD22	20	0.35
(1,1450)	2:179:B:LYS:HD3	2:179:B:LYS:H	12	0.35
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	12	0.35
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	12	0.35
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	12	0.35
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	6	0.35
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	19	0.35
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG3	19	0.35
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG3	19	0.35
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG3	19	0.35
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	7	0.35
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	7	0.35
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	7	0.35
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	7	0.35
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	7	0.35
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	7	0.35
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	7	0.35
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	7	0.35
(1,455)	2:211:B:GLU:HA	2:211:B:GLU:HG3	3	0.35
(1,309)	2:192:B:SER:HB2	2:188:B:LYS:HE2	19	0.35
(1,45)	2:159:B:LYS:HA	2:159:B:LYS:HD3	19	0.35
(1,45)	2:159:B:LYS:HA	2:159:B:LYS:HD3	20	0.35
(2,307)	2:279:B:LEU:HD11	1:87:A:MET:HA	6	0.34
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	8	0.34
(1,4597)	2:267:B:PHE:HE2	2:263:B:LEU:HG	15	0.34
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	6	0.34
(1,4491)	1:118:A:GLY:HA3	1:117:A:GLU:H	17	0.34
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	1	0.34
(1,4014)	2:179:B:LYS:HD2	2:314:B:ALA:HB3	20	0.34
(1,3817)	2:198:B:ALA:HB3	2:195:B:GLU:HG3	12	0.34
(1,3750)	2:160:B:ILE:HG23	2:165:B:LYS:HE2	14	0.34
(1,3250)	1:103:A:ARG:HD3	1:102:A:GLU:H	13	0.34
(1,2736)	1:96:A:LEU:HB3	1:97:A:PRO:HA	7	0.34
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD21	6	0.34
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD22	6	0.34
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD23	6	0.34
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	8	0.34
(1,2210)	2:288:B:LEU:HB2	2:289:B:ASN:H	3	0.34
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	19	0.34
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	19	0.34
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	19	0.34
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	8	0.34
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	8	0.34
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	8	0.34
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	18	0.34
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	4	0.34
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	4	0.34
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	4	0.34
(1,1310)	2:157:B:LYS:HG3	2:157:B:LYS:H	6	0.34
(1,1249)	2:321:B:LYS:HG3	2:321:B:LYS:HE2	13	0.34
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	17	0.34
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	17	0.34
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	17	0.34
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD11	14	0.34
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD12	14	0.34
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD13	14	0.34
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD11	14	0.34
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD12	14	0.34
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD13	14	0.34
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	1	0.34
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	1	0.34
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	1	0.34
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	2	0.34
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	2	0.34
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	2	0.34
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD21	11	0.34
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD22	11	0.34
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD23	11	0.34
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD21	10	0.34
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD22	10	0.34
(1,633)	2:230:B:GLY:HA2	2:234:B:LEU:HD23	10	0.34
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	14	0.34
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE1	1	0.34
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE2	1	0.34
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE3	1	0.34
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE1	1	0.34
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE2	1	0.34
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE3	1	0.34
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE1	1	0.34
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE2	1	0.34
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE3	1	0.34
(1,285)	2:187:B:LYS:HG3	2:187:B:LYS:HE2	13	0.34
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	20	0.34
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	20	0.34
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	20	0.34
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	20	0.34
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	20	0.34
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	20	0.34
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	20	0.34
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	20	0.34
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	20	0.34
(1,113)	1:105:A:PHE:HZ	2:168:B:LEU:HD11	11	0.34
(1,113)	1:105:A:PHE:HZ	2:168:B:LEU:HD12	11	0.34
(1,113)	1:105:A:PHE:HZ	2:168:B:LEU:HD13	11	0.34
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD13	18	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4634)	2:237:B:PHE:HE2	2:314:B:ALA:HB3	20	0.33
(1,4587)	2:306:B:PHE:HE2	2:305:B:LEU:HB3	2	0.33
(1,4575)	2:167:B:TRP:HD1	2:164:B:LEU:HD21	6	0.33
(1,4562)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	14	0.33
(1,4548)	2:200:B:TYR:HE2	2:204:B:ARG:HG3	13	0.33
(1,4547)	2:200:B:TYR:HD1	2:204:B:ARG:HD3	10	0.33
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	14	0.33
(1,4492)	2:212:B:TYR:HE2	1:81:A:LEU:H	11	0.33
(1,4472)	1:93:A:SER:HB2	1:95:A:ILE:H	16	0.33
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	18	0.33
(1,4382)	2:168:B:LEU:HD11	1:108:A:PRO:HD3	20	0.33
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD23	19	0.33
(1,4360)	2:235:B:TYR:HE1	1:106:A:VAL:HA	3	0.33
(1,4313)	1:87:A:MET:HE3	1:90:A:LEU:HD13	18	0.33
(1,4302)	1:91:A:HIS:HB2	1:92:A:GLU:HA	1	0.33
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	5	0.33
(1,4237)	2:218:B:VAL:HG13	2:198:B:ALA:H	19	0.33
(1,4014)	2:179:B:LYS:HD2	2:314:B:ALA:HB1	9	0.33
(1,3988)	2:295:B:LEU:HG	2:298:B:LEU:HD12	10	0.33
(1,3949)	2:302:B:SER:HB2	2:305:B:LEU:HD12	13	0.33
(1,3795)	2:194:B:LEU:HD23	2:190:B:VAL:HG12	17	0.33
(1,3732)	2:168:B:LEU:HD11	2:160:B:ILE:HD12	18	0.33
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD11	17	0.33
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	8	0.33
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	8	0.33
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE3	10	0.33
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE3	10	0.33
(1,3488)	2:237:B:PHE:HD1	2:179:B:LYS:HE2	18	0.33
(1,3488)	2:237:B:PHE:HD2	2:179:B:LYS:HE2	18	0.33
(1,3409)	1:119:A:LYS:HG2	1:119:A:LYS:H	8	0.33
(1,3408)	1:119:A:LYS:HB2	1:119:A:LYS:H	3	0.33
(1,3219)	1:94:A:GLU:HG3	1:94:A:GLU:H	5	0.33
(1,3004)	1:115:A:VAL:HG11	1:116:A:ARG:HD2	14	0.33
(1,3004)	1:115:A:VAL:HG12	1:116:A:ARG:HD2	14	0.33
(1,3004)	1:115:A:VAL:HG13	1:116:A:ARG:HD2	14	0.33
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	4	0.33
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	16	0.33
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	16	0.33
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	16	0.33
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	8	0.33
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	8	0.33
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	2:297:B:TYR:HA	2:300:B:LYS:HD3	10	0.33
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD21	18	0.33
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD22	18	0.33
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD23	18	0.33
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE1	8	0.33
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE2	8	0.33
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE3	8	0.33
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	16	0.33
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	3	0.33
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	3	0.33
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	3	0.33
(1,455)	2:211:B:GLU:HA	2:211:B:GLU:HG3	4	0.33
(1,344)	2:188:B:LYS:HE3	2:193:B:ILE:HA	3	0.33
(1,309)	2:192:B:SER:HB2	2:188:B:LYS:HE2	18	0.33
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	19	0.33
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	19	0.33
(1,175)	2:311:B:TYR:HE2	2:175:B:ILE:HD13	14	0.33
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD2	3	0.33
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	15	0.32
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG3	18	0.32
(1,4611)	2:290:B:TYR:HD1	2:210:B:LYS:HD2	18	0.32
(1,4579)	2:306:B:PHE:HD1	2:261:B:PRO:HG3	2	0.32
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	15	0.32
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG22	16	0.32
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	19	0.32
(1,4450)	1:72:A:VAL:HB	1:72:A:VAL:H	18	0.32
(1,4418)	2:169:B:VAL:HG22	1:112:A:ILE:HG21	20	0.32
(1,4364)	1:111:A:ILE:HD11	1:107:A:LEU:HA	14	0.32
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD12	11	0.32
(1,4317)	1:87:A:MET:HB2	1:90:A:LEU:HD22	10	0.32
(1,4314)	1:74:A:SER:HB3	1:96:A:LEU:HD23	11	0.32
(1,4308)	1:96:A:LEU:HD12	1:96:A:LEU:HB3	6	0.32
(1,4283)	1:82:A:SER:HA	1:84:A:MET:HE1	11	0.32
(1,4237)	2:218:B:VAL:HG12	2:198:B:ALA:H	1	0.32
(1,4031)	2:298:B:LEU:HB2	2:193:B:ILE:HD13	5	0.32
(1,3976)	2:264:B:LEU:HA	2:295:B:LEU:HD11	12	0.32
(1,3942)	2:274:B:LEU:HD22	2:270:B:ILE:HG21	14	0.32
(1,3927)	2:160:B:ILE:HD13	2:268:B:VAL:HG13	15	0.32
(1,3921)	2:221:B:ILE:HG21	2:263:B:LEU:HD23	9	0.32
(1,3893)	2:252:B:ALA:HB2	2:245:B:ILE:HG21	14	0.32
(1,3795)	2:194:B:LEU:HD22	2:190:B:VAL:HG11	8	0.32
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD12	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3443)	2:227:B:VAL:HG21	1:100:A:ASN:HD22	13	0.32
(1,3443)	2:227:B:VAL:HG22	1:100:A:ASN:HD22	13	0.32
(1,3443)	2:227:B:VAL:HG23	1:100:A:ASN:HD22	13	0.32
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	14	0.32
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	14	0.32
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	14	0.32
(1,2736)	1:96:A:LEU:HB3	1:97:A:PRO:HA	11	0.32
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD21	3	0.32
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD22	3	0.32
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD23	3	0.32
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	10	0.32
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	10	0.32
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	10	0.32
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	15	0.32
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG3	18	0.32
(1,2353)	2:310:B:ASP:HB2	2:310:B:ASP:H	13	0.32
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	9	0.32
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	16	0.32
(1,2184)	2:284:B:LEU:HD11	2:285:B:ALA:H	19	0.32
(1,2184)	2:284:B:LEU:HD12	2:285:B:ALA:H	19	0.32
(1,2184)	2:284:B:LEU:HD13	2:285:B:ALA:H	19	0.32
(1,1975)	2:246:B:LEU:HB2	2:249:B:HIS:H	19	0.32
(1,1090)	2:298:B:LEU:HD21	2:298:B:LEU:HA	1	0.32
(1,1090)	2:298:B:LEU:HD22	2:298:B:LEU:HA	1	0.32
(1,1090)	2:298:B:LEU:HD23	2:298:B:LEU:HA	1	0.32
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE1	5	0.32
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE2	5	0.32
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE3	5	0.32
(1,900)	2:269:B:ARG:HA	2:269:B:ARG:HD2	9	0.32
(1,900)	2:269:B:ARG:HA	2:269:B:ARG:HD3	16	0.32
(1,811)	2:257:B:VAL:HG11	2:256:B:GLN:HB3	20	0.32
(1,811)	2:257:B:VAL:HG12	2:256:B:GLN:HB3	20	0.32
(1,811)	2:257:B:VAL:HG13	2:256:B:GLN:HB3	20	0.32
(1,797)	2:257:B:VAL:HG11	2:254:B:MET:HA	11	0.32
(1,797)	2:257:B:VAL:HG12	2:254:B:MET:HA	11	0.32
(1,797)	2:257:B:VAL:HG13	2:254:B:MET:HA	11	0.32
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD21	20	0.32
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD22	20	0.32
(1,640)	2:239:B:ARG:HD3	2:234:B:LEU:HD23	20	0.32
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE1	17	0.32
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE2	17	0.32
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE3	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	2:192:B:SER:HA	2:195:B:GLU:HG2	19	0.32
(1,299)	2:193:B:ILE:HD11	2:188:B:LYS:HD3	10	0.32
(1,299)	2:193:B:ILE:HD12	2:188:B:LYS:HD3	10	0.32
(1,299)	2:193:B:ILE:HD13	2:188:B:LYS:HD3	10	0.32
(1,285)	2:187:B:LYS:HG3	2:187:B:LYS:HE2	18	0.32
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	8	0.32
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	8	0.32
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	8	0.32
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	8	0.32
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	8	0.32
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	8	0.32
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	8	0.32
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	8	0.32
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	8	0.32
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	13	0.32
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	13	0.32
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	13	0.32
(2,307)	2:279:B:LEU:HD12	1:94:A:GLU:HA	10	0.31
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD12	1	0.31
(1,4639)	2:237:B:PHE:HE1	2:322:B:ALA:HB1	14	0.31
(1,4627)	2:294:B:PHE:HZ	2:221:B:ILE:HG23	6	0.31
(1,4620)	2:182:B:PHE:HZ	2:184:B:LEU:HB2	20	0.31
(1,4497)	2:292:B:HIS:HE1	2:291:B:LEU:HD21	18	0.31
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	12	0.31
(1,4435)	1:119:A:LYS:HE2	1:119:A:LYS:HA	17	0.31
(1,4418)	2:169:B:VAL:HG23	1:112:A:ILE:HG21	19	0.31
(1,4384)	2:169:B:VAL:HG22	1:109:A:GLU:HA	5	0.31
(1,4382)	2:168:B:LEU:HD12	1:108:A:PRO:HD3	4	0.31
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	15	0.31
(1,4198)	2:164:B:LEU:HD23	2:299:B:ALA:H	1	0.31
(1,4167)	2:279:B:LEU:HD13	2:280:B:ASP:H	15	0.31
(1,4014)	2:181:B:LEU:HD13	2:314:B:ALA:HB2	19	0.31
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD21	20	0.31
(1,3851)	2:211:B:GLU:HA	2:202:B:LYS:HE2	12	0.31
(1,3817)	2:198:B:ALA:HB1	2:195:B:GLU:HG3	6	0.31
(1,3740)	2:317:B:GLU:HB2	2:317:B:GLU:HG3	12	0.31
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	2	0.31
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	2	0.31
(1,3495)	2:237:B:PHE:HZ	2:181:B:LEU:HD21	14	0.31
(1,3495)	2:237:B:PHE:HZ	2:181:B:LEU:HD22	14	0.31
(1,3495)	2:237:B:PHE:HZ	2:181:B:LEU:HD23	14	0.31
(1,3402)	1:117:A:GLU:HB3	1:119:A:LYS:H	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	2	0.31
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	2	0.31
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	2	0.31
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD21	2	0.31
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD22	2	0.31
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD23	2	0.31
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD21	6	0.31
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD22	6	0.31
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD23	6	0.31
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	2	0.31
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	4	0.31
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	6	0.31
(1,2051)	2:190:B:VAL:HG21	2:263:B:LEU:H	14	0.31
(1,2051)	2:190:B:VAL:HG22	2:263:B:LEU:H	14	0.31
(1,2051)	2:190:B:VAL:HG23	2:263:B:LEU:H	14	0.31
(1,1899)	2:239:B:ARG:HG2	2:239:B:ARG:H	15	0.31
(1,1832)	2:233:B:LEU:HD11	2:230:B:GLY:H	3	0.31
(1,1832)	2:233:B:LEU:HD12	2:230:B:GLY:H	3	0.31
(1,1832)	2:233:B:LEU:HD13	2:230:B:GLY:H	3	0.31
(1,1542)	2:188:B:LYS:HG2	2:189:B:ASN:H	17	0.31
(1,1505)	2:184:B:LEU:HD11	2:186:B:ALA:H	14	0.31
(1,1505)	2:184:B:LEU:HD12	2:186:B:ALA:H	14	0.31
(1,1505)	2:184:B:LEU:HD13	2:186:B:ALA:H	14	0.31
(1,1115)	2:297:B:TYR:HA	2:300:B:LYS:HD3	11	0.31
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG3	16	0.31
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG3	16	0.31
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG3	16	0.31
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	1	0.31
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	1	0.31
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	1	0.31
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	1	0.31
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	1	0.31
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	1	0.31
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	1	0.31
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	1	0.31
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	1	0.31
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD21	4	0.31
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD22	4	0.31
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD23	4	0.31
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD21	4	0.31
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD22	4	0.31
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD23	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE1	16	0.31
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE2	16	0.31
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE3	16	0.31
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	10	0.31
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	10	0.31
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	10	0.31
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB1	11	0.31
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB2	11	0.31
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB3	11	0.31
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB1	11	0.31
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB2	11	0.31
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB3	11	0.31
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB1	11	0.31
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB2	11	0.31
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB3	11	0.31
(1,455)	2:211:B:GLU:HA	2:211:B:GLU:HG3	9	0.31
(1,454)	2:202:B:LYS:HD3	2:211:B:GLU:HG3	12	0.31
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	19	0.3
(1,4631)	2:237:B:PHE:HE2	2:179:B:LYS:HB2	2	0.3
(1,4534)	2:183:B:TYR:HD1	2:238:B:GLU:HB2	13	0.3
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	11	0.3
(1,4527)	2:242:B:TYR:HE2	2:243:B:ALA:HB1	8	0.3
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG22	6	0.3
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	13	0.3
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	15	0.3
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	18	0.3
(1,4447)	2:232:B:GLN:HG2	1:103:A:ARG:HG2	2	0.3
(1,4413)	2:169:B:VAL:HG22	1:112:A:ILE:HB	5	0.3
(1,4364)	1:111:A:ILE:HD13	1:107:A:LEU:HA	8	0.3
(1,4364)	1:111:A:ILE:HD11	1:107:A:LEU:HA	18	0.3
(1,4317)	1:87:A:MET:HB2	1:90:A:LEU:HD23	3	0.3
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	19	0.3
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	13	0.3
(1,4280)	1:85:A:TYR:HE2	1:90:A:LEU:HD23	5	0.3
(1,4198)	2:164:B:LEU:HD22	2:299:B:ALA:H	10	0.3
(1,4087)	2:202:B:LYS:HG2	2:202:B:LYS:H	12	0.3
(1,3979)	2:160:B:ILE:HG23	2:295:B:LEU:HD23	15	0.3
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD3	11	0.3
(1,3928)	1:111:A:ILE:HD12	2:268:B:VAL:HG13	4	0.3
(1,3901)	2:257:B:VAL:HG21	2:252:B:ALA:HB2	1	0.3
(1,3824)	2:214:B:VAL:HG23	2:202:B:LYS:HE2	13	0.3
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	7	0.3
(1,3409)	1:119:A:LYS:HG3	1:119:A:LYS:H	20	0.3
(1,3392)	1:116:A:ARG:HB2	1:117:A:GLU:H	13	0.3
(1,2803)	2:232:B:GLN:HA	1:103:A:ARG:HD2	11	0.3
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD21	8	0.3
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD22	8	0.3
(1,2732)	1:96:A:LEU:HA	1:96:A:LEU:HD23	8	0.3
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	19	0.3
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB1	5	0.3
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB2	5	0.3
(1,2660)	1:92:A:GLU:HG2	1:89:A:ALA:HB3	5	0.3
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB1	10	0.3
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB2	10	0.3
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB3	10	0.3
(1,2505)	1:75:A:LYS:HD2	1:75:A:LYS:HA	13	0.3
(1,2466)	1:72:A:VAL:HG11	1:71:A:GLN:HA	16	0.3
(1,2466)	1:72:A:VAL:HG12	1:71:A:GLN:HA	16	0.3
(1,2466)	1:72:A:VAL:HG13	1:71:A:GLN:HA	16	0.3
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	18	0.3
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	7	0.3
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB1	3	0.3
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB2	3	0.3
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB3	3	0.3
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB1	3	0.3
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB2	3	0.3
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB3	3	0.3
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB1	3	0.3
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB2	3	0.3
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB3	3	0.3
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD11	2	0.3
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD12	2	0.3
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD13	2	0.3
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD11	2	0.3
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD12	2	0.3
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD13	2	0.3
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD21	12	0.3
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD22	12	0.3
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD23	12	0.3
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD21	18	0.3
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD22	18	0.3
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD23	18	0.3
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG11	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG12	11	0.3
(1,554)	2:224:B:TYR:HA	2:227:B:VAL:HG13	11	0.3
(1,385)	2:192:B:SER:HA	2:195:B:GLU:HG2	4	0.3
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	3	0.3
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	3	0.3
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	3	0.3
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD11	19	0.3
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD12	19	0.3
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD13	19	0.3
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	3	0.29
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG3	14	0.29
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	16	0.29
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD13	14	0.29
(1,4603)	2:224:B:TYR:HD1	2:266:B:LEU:HD11	13	0.29
(1,4589)	2:182:B:PHE:HD2	2:261:B:PRO:HD3	5	0.29
(1,4564)	2:290:B:TYR:HE1	2:210:B:LYS:HG3	13	0.29
(1,4560)	2:225:B:PHE:HD1	2:233:B:LEU:HD12	20	0.29
(1,4547)	2:200:B:TYR:HD1	2:204:B:ARG:HD2	8	0.29
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	7	0.29
(1,4520)	2:237:B:PHE:HE2	2:179:B:LYS:HE2	1	0.29
(1,4496)	2:267:B:PHE:HD2	2:263:B:LEU:HD21	15	0.29
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	16	0.29
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	1	0.29
(1,4413)	2:169:B:VAL:HG22	1:112:A:ILE:HB	13	0.29
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD21	9	0.29
(1,4343)	1:74:A:SER:HB2	1:95:A:ILE:HD12	15	0.29
(1,4310)	1:85:A:TYR:HD2	1:90:A:LEU:HB3	10	0.29
(1,4283)	1:82:A:SER:HA	1:84:A:MET:HE2	4	0.29
(1,4271)	2:212:B:TYR:HD2	1:81:A:LEU:HA	14	0.29
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	15	0.29
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG22	20	0.29
(1,3750)	1:111:A:ILE:HD11	2:165:B:LYS:HE2	15	0.29
(1,2996)	1:116:A:ARG:HD2	1:115:A:VAL:HG21	4	0.29
(1,2996)	1:116:A:ARG:HD2	1:115:A:VAL:HG22	4	0.29
(1,2996)	1:116:A:ARG:HD2	1:115:A:VAL:HG23	4	0.29
(1,2945)	1:107:A:LEU:HD21	1:112:A:ILE:HG13	15	0.29
(1,2945)	1:107:A:LEU:HD22	1:112:A:ILE:HG13	15	0.29
(1,2945)	1:107:A:LEU:HD23	1:112:A:ILE:HG13	15	0.29
(1,2900)	1:112:A:ILE:HD11	1:109:A:GLU:HB3	3	0.29
(1,2900)	1:112:A:ILE:HD12	1:109:A:GLU:HB3	3	0.29
(1,2900)	1:112:A:ILE:HD13	1:109:A:GLU:HB3	3	0.29
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG3	14	0.29
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	16	0.29
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	1	0.29
(1,2007)	2:226:B:ASN:HD21	2:255:B:SER:H	11	0.29
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	1	0.29
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	1	0.29
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	1	0.29
(1,1449)	2:178:B:GLN:HG2	2:178:B:GLN:H	11	0.29
(1,1310)	2:157:B:LYS:HG3	2:157:B:LYS:H	20	0.29
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	9	0.29
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	9	0.29
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	9	0.29
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	9	0.29
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	9	0.29
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	9	0.29
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	9	0.29
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	9	0.29
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	9	0.29
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	15	0.29
(1,1061)	2:296:B:LYS:HE3	2:294:B:PHE:HA	15	0.29
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	17	0.29
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD11	9	0.29
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD12	9	0.29
(1,1009)	2:290:B:TYR:HD1	2:286:B:LEU:HD13	9	0.29
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD11	9	0.29
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD12	9	0.29
(1,1009)	2:290:B:TYR:HD2	2:286:B:LEU:HD13	9	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	4	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	4	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	4	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	8	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	8	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	8	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	15	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	15	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	15	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	16	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	16	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	16	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	18	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	18	0.29
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	18	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	2:155:B:GLU:HG2	2:272:B:ALA:HA	8	0.29
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG2	8	0.29
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG2	8	0.29
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG2	8	0.29
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	10	0.29
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	10	0.29
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	10	0.29
(1,797)	2:257:B:VAL:HG11	2:254:B:MET:HA	20	0.29
(1,797)	2:257:B:VAL:HG12	2:254:B:MET:HA	20	0.29
(1,797)	2:257:B:VAL:HG13	2:254:B:MET:HA	20	0.29
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD21	14	0.29
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD22	14	0.29
(1,755)	2:254:B:MET:HE1	2:246:B:LEU:HD23	14	0.29
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD21	14	0.29
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD22	14	0.29
(1,755)	2:254:B:MET:HE2	2:246:B:LEU:HD23	14	0.29
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD21	14	0.29
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD22	14	0.29
(1,755)	2:254:B:MET:HE3	2:246:B:LEU:HD23	14	0.29
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD21	17	0.29
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD22	17	0.29
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD23	17	0.29
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD21	19	0.29
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD22	19	0.29
(1,753)	2:246:B:LEU:HB3	2:246:B:LEU:HD23	19	0.29
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	5	0.29
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	13	0.29
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE1	9	0.29
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE2	9	0.29
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE3	9	0.29
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE1	9	0.29
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE2	9	0.29
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE3	9	0.29
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE1	9	0.29
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE2	9	0.29
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE3	9	0.29
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	17	0.29
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	17	0.29
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	17	0.29
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB1	4	0.29
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB2	4	0.29
(1,465)	2:217:B:VAL:HG21	2:213:B:ALA:HB3	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB1	4	0.29
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB2	4	0.29
(1,465)	2:217:B:VAL:HG22	2:213:B:ALA:HB3	4	0.29
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB1	4	0.29
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB2	4	0.29
(1,465)	2:217:B:VAL:HG23	2:213:B:ALA:HB3	4	0.29
(1,285)	2:187:B:LYS:HG3	2:187:B:LYS:HE2	11	0.29
(1,45)	2:159:B:LYS:HA	2:159:B:LYS:HD3	9	0.29
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	11	0.28
(1,4620)	2:182:B:PHE:HZ	2:184:B:LEU:HB2	1	0.28
(1,4597)	2:267:B:PHE:HE2	2:263:B:LEU:HG	4	0.28
(1,4562)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	4	0.28
(1,4496)	2:267:B:PHE:HD2	2:263:B:LEU:HD21	2	0.28
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	11	0.28
(1,4444)	1:97:A:PRO:HG3	1:96:A:LEU:HD11	13	0.28
(1,4438)	2:166:B:PRO:HA	1:111:A:ILE:HG23	8	0.28
(1,4418)	2:169:B:VAL:HG23	1:112:A:ILE:HG21	10	0.28
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	18	0.28
(1,4347)	1:97:A:PRO:HG3	1:95:A:ILE:HG21	18	0.28
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	12	0.28
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	10	0.28
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD13	20	0.28
(1,4237)	2:218:B:VAL:HG11	2:198:B:ALA:H	18	0.28
(1,4063)	2:186:B:ALA:HB3	2:188:B:LYS:H	4	0.28
(1,4002)	2:188:B:LYS:HE2	2:305:B:LEU:HD13	16	0.28
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD3	5	0.28
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG23	1	0.28
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD23	7	0.28
(1,3920)	2:194:B:LEU:HD22	2:263:B:LEU:HD12	6	0.28
(1,3920)	2:194:B:LEU:HD23	2:263:B:LEU:HD12	11	0.28
(1,3920)	2:194:B:LEU:HD23	2:263:B:LEU:HD13	20	0.28
(1,3915)	2:305:B:LEU:HD21	2:260:B:ALA:HB3	1	0.28
(1,3898)	2:254:B:MET:HE1	2:252:B:ALA:HB1	19	0.28
(1,3749)	2:160:B:ILE:HG23	2:165:B:LYS:HE3	14	0.28
(1,3359)	1:114:A:GLU:HB3	1:114:A:GLU:H	17	0.28
(1,3039)	2:231:B:THR:HA	1:102:A:GLU:HG3	12	0.28
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	11	0.28
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD3	13	0.28
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	6	0.28
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	3	0.28
(1,2210)	2:288:B:LEU:HB2	2:289:B:ASN:H	10	0.28
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	20	0.28
(1,1739)	2:217:B:VAL:HB	2:218:B:VAL:H	11	0.28
(1,1539)	2:188:B:LYS:HD3	2:189:B:ASN:H	10	0.28
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD11	7	0.28
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD12	7	0.28
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD13	7	0.28
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	10	0.28
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	10	0.28
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	10	0.28
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	10	0.28
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	8	0.28
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	8	0.28
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	8	0.28
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	8	0.28
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	8	0.28
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	8	0.28
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	8	0.28
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	8	0.28
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	8	0.28
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD11	8	0.28
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD12	8	0.28
(1,962)	2:233:B:LEU:HD11	2:266:B:LEU:HD13	8	0.28
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD11	8	0.28
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD12	8	0.28
(1,962)	2:233:B:LEU:HD12	2:266:B:LEU:HD13	8	0.28
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD11	8	0.28
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD12	8	0.28
(1,962)	2:233:B:LEU:HD13	2:266:B:LEU:HD13	8	0.28
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE1	2	0.28
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE2	2	0.28
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE3	2	0.28
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE1	10	0.28
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE2	10	0.28
(1,938)	1:98:A:PHE:HB2	2:273:B:MET:HE3	10	0.28
(1,671)	2:234:B:LEU:HD21	2:239:B:ARG:HD2	10	0.28
(1,671)	2:234:B:LEU:HD22	2:239:B:ARG:HD2	10	0.28
(1,671)	2:234:B:LEU:HD23	2:239:B:ARG:HD2	10	0.28
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE1	2	0.28
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE2	2	0.28
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE3	2	0.28
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE1	2	0.28
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE2	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE3	2	0.28
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE1	2	0.28
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE2	2	0.28
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE3	2	0.28
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	9	0.28
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	9	0.28
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	9	0.28
(1,420)	2:199:B:ASN:HA	2:202:B:LYS:HE3	17	0.28
(1,313)	2:192:B:SER:HB3	2:188:B:LYS:HG3	16	0.28
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	19	0.27
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	19	0.27
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	19	0.27
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	19	0.27
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	19	0.27
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	19	0.27
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	19	0.27
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	19	0.27
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	19	0.27
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	19	0.27
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	19	0.27
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	19	0.27
(1,4634)	2:237:B:PHE:HE2	2:314:B:ALA:HB1	13	0.27
(1,4612)	2:290:B:TYR:HE2	2:286:B:LEU:HG	15	0.27
(1,4574)	2:242:B:TYR:HD1	2:246:B:LEU:HD11	14	0.27
(1,4547)	2:200:B:TYR:HD1	2:204:B:ARG:HD3	12	0.27
(1,4546)	2:224:B:TYR:HD1	2:270:B:ILE:HB	11	0.27
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	18	0.27
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	1	0.27
(1,4515)	2:172:B:TRP:HZ3	2:169:B:VAL:HG11	2	0.27
(1,4506)	2:172:B:TRP:HD1	2:175:B:ILE:HB	14	0.27
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	10	0.27
(1,4444)	2:273:B:MET:HB3	1:96:A:LEU:HD11	16	0.27
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	10	0.27
(1,4382)	2:168:B:LEU:HD13	1:108:A:PRO:HD3	2	0.27
(1,4357)	2:273:B:MET:HE3	1:100:A:ASN:HA	3	0.27
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	16	0.27
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD12	3	0.27
(1,4310)	1:91:A:HIS:HD2	1:90:A:LEU:HB3	1	0.27
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	15	0.27
(1,4133)	2:254:B:MET:HE1	2:246:B:LEU:H	10	0.27
(1,4133)	2:254:B:MET:HE3	2:246:B:LEU:H	16	0.27
(1,4054)	2:313:B:VAL:HG12	2:180:B:GLN:HE22	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4036)	2:160:B:ILE:HG23	2:164:B:LEU:H	5	0.27
(1,4030)	2:192:B:SER:HB2	2:188:B:LYS:HG2	19	0.27
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	11	0.27
(1,3990)	2:263:B:LEU:HD13	2:298:B:LEU:HD22	4	0.27
(1,3976)	2:264:B:LEU:HA	2:295:B:LEU:HD11	16	0.27
(1,3945)	2:274:B:LEU:HD23	2:271:B:GLY:HA3	8	0.27
(1,3940)	2:274:B:LEU:HG	2:270:B:ILE:HD11	15	0.27
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG23	11	0.27
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG3	3	0.27
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG3	9	0.27
(1,3395)	1:117:A:GLU:HG3	1:117:A:GLU:H	10	0.27
(1,2911)	1:114:A:GLU:HB3	1:111:A:ILE:HA	6	0.27
(1,2902)	1:112:A:ILE:HD11	1:109:A:GLU:HG2	12	0.27
(1,2902)	1:112:A:ILE:HD12	1:109:A:GLU:HG2	12	0.27
(1,2902)	1:112:A:ILE:HD13	1:109:A:GLU:HG2	12	0.27
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD11	11	0.27
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD12	11	0.27
(1,2671)	1:98:A:PHE:HD1	1:96:A:LEU:HD13	11	0.27
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD11	11	0.27
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD12	11	0.27
(1,2671)	1:98:A:PHE:HD2	1:96:A:LEU:HD13	11	0.27
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	12	0.27
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	12	0.27
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	12	0.27
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	20	0.27
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	20	0.27
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	20	0.27
(1,2440)	2:253:B:PRO:HG2	2:256:B:GLN:H	18	0.27
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	13	0.27
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	19	0.27
(1,2145)	2:280:B:ASP:HB2	2:280:B:ASP:H	1	0.27
(1,2040)	2:190:B:VAL:HG21	2:260:B:ALA:H	11	0.27
(1,2040)	2:190:B:VAL:HG22	2:260:B:ALA:H	11	0.27
(1,2040)	2:190:B:VAL:HG23	2:260:B:ALA:H	11	0.27
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	1	0.27
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	17	0.27
(1,1904)	2:241:B:GLN:HG2	2:241:B:GLN:H	13	0.27
(1,1702)	2:211:B:GLU:HB2	2:212:B:TYR:H	10	0.27
(1,1676)	2:204:B:ARG:HG3	2:204:B:ARG:H	14	0.27
(1,1539)	2:188:B:LYS:HD3	2:189:B:ASN:H	13	0.27
(1,1061)	2:296:B:LYS:HE3	2:294:B:PHE:HA	11	0.27
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD11	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD12	2	0.27
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD13	2	0.27
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD11	2	0.27
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	2	0.27
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD13	2	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	1	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	1	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	1	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	9	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	9	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	9	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	14	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	14	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	14	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	19	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	19	0.27
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	19	0.27
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG2	18	0.27
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG2	18	0.27
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG2	18	0.27
(1,815)	2:253:B:PRO:HG2	2:256:B:GLN:HG2	10	0.27
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD21	14	0.27
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD22	14	0.27
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD23	14	0.27
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD21	14	0.27
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD22	14	0.27
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD23	14	0.27
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD21	14	0.27
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD22	14	0.27
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD23	14	0.27
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG21	3	0.27
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG22	3	0.27
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG23	3	0.27
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG21	3	0.27
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG22	3	0.27
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG23	3	0.27
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG21	3	0.27
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG22	3	0.27
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG23	3	0.27
(1,327)	2:263:B:LEU:HD21	2:190:B:VAL:HG11	14	0.27
(1,327)	2:263:B:LEU:HD21	2:190:B:VAL:HG12	14	0.27
(1,327)	2:263:B:LEU:HD21	2:190:B:VAL:HG13	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	2:263:B:LEU:HD22	2:190:B:VAL:HG11	14	0.27
(1,327)	2:263:B:LEU:HD22	2:190:B:VAL:HG12	14	0.27
(1,327)	2:263:B:LEU:HD22	2:190:B:VAL:HG13	14	0.27
(1,327)	2:263:B:LEU:HD23	2:190:B:VAL:HG11	14	0.27
(1,327)	2:263:B:LEU:HD23	2:190:B:VAL:HG12	14	0.27
(1,327)	2:263:B:LEU:HD23	2:190:B:VAL:HG13	14	0.27
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD21	15	0.27
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD22	15	0.27
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD23	15	0.27
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	8	0.27
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD2	8	0.27
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	8	0.26
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	8	0.26
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	8	0.26
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	8	0.26
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	8	0.26
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	8	0.26
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	8	0.26
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	8	0.26
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	8	0.26
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	8	0.26
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	8	0.26
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	8	0.26
(2,69)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	7	0.26
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	1	0.26
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	1	0.26
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	1	0.26
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	1	0.26
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	1	0.26
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	1	0.26
(1,4511)	2:182:B:PHE:HD1	2:175:B:ILE:HD13	10	0.26
(1,4499)	2:306:B:PHE:HE1	2:298:B:LEU:HD23	17	0.26
(1,4476)	1:92:A:GLU:HG2	1:90:A:LEU:H	9	0.26
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	4	0.26
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	5	0.26
(1,4413)	2:169:B:VAL:HG21	1:112:A:ILE:HB	6	0.26
(1,4364)	1:111:A:ILE:HD11	1:107:A:LEU:HA	5	0.26
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD12	1	0.26
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	5	0.26
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG3	20	0.26
(1,4278)	1:84:A:MET:HE2	1:81:A:LEU:HD22	9	0.26
(1,4268)	1:76:A:VAL:HG23	1:78:A:TRP:HB2	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4243)	1:72:A:VAL:HG23	1:71:A:GLN:HB2	12	0.26
(1,4087)	2:202:B:LYS:HG2	2:202:B:LYS:H	4	0.26
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	18	0.26
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	14	0.26
(1,3961)	2:282:B:LYS:HG2	2:282:B:LYS:HD3	15	0.26
(1,3918)	2:298:B:LEU:HD12	2:263:B:LEU:HD11	17	0.26
(1,3915)	2:305:B:LEU:HD21	2:260:B:ALA:HB1	4	0.26
(1,3910)	2:257:B:VAL:HG21	2:256:B:GLN:HG2	9	0.26
(1,3901)	2:257:B:VAL:HG22	2:252:B:ALA:HB1	15	0.26
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE3	5	0.26
(1,3746)	2:306:B:PHE:HE1	2:298:B:LEU:HD23	17	0.26
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	16	0.26
(1,3454)	2:292:B:HIS:HE1	2:159:B:LYS:HG3	13	0.26
(1,3443)	2:227:B:VAL:HG21	1:100:A:ASN:HD22	16	0.26
(1,3443)	2:227:B:VAL:HG22	1:100:A:ASN:HD22	16	0.26
(1,3443)	2:227:B:VAL:HG23	1:100:A:ASN:HD22	16	0.26
(1,3359)	1:114:A:GLU:HG2	1:114:A:GLU:H	6	0.26
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD21	15	0.26
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD22	15	0.26
(1,3071)	2:172:B:TRP:HB3	1:107:A:LEU:HD23	15	0.26
(1,3069)	1:99:A:PRO:HB3	1:100:A:ASN:HA	2	0.26
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD11	17	0.26
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD12	17	0.26
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD13	17	0.26
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG21	8	0.26
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG22	8	0.26
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG23	8	0.26
(1,2690)	1:91:A:HIS:HD2	1:92:A:GLU:HG2	7	0.26
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	8	0.26
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	15	0.26
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	17	0.26
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	10	0.26
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	12	0.26
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	15	0.26
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	15	0.26
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	15	0.26
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	15	0.26
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	15	0.26
(1,1869)	2:235:B:TYR:HB3	2:236:B:LYS:H	20	0.26
(1,1554)	2:190:B:VAL:HG11	2:190:B:VAL:H	14	0.26
(1,1554)	2:190:B:VAL:HG12	2:190:B:VAL:H	14	0.26
(1,1554)	2:190:B:VAL:HG13	2:190:B:VAL:H	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1542)	2:188:B:LYS:HG2	2:189:B:ASN:H	11	0.26
(1,1529)	2:188:B:LYS:HB2	2:188:B:LYS:H	3	0.26
(1,1310)	2:157:B:LYS:HG2	2:157:B:LYS:H	4	0.26
(1,1101)	2:294:B:PHE:HZ	2:298:B:LEU:HD21	9	0.26
(1,1101)	2:294:B:PHE:HZ	2:298:B:LEU:HD22	9	0.26
(1,1101)	2:294:B:PHE:HZ	2:298:B:LEU:HD23	9	0.26
(1,1003)	2:288:B:LEU:HD11	2:285:B:ALA:HA	10	0.26
(1,1003)	2:288:B:LEU:HD12	2:285:B:ALA:HA	10	0.26
(1,1003)	2:288:B:LEU:HD13	2:285:B:ALA:HA	10	0.26
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	6	0.26
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	6	0.26
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	6	0.26
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	7	0.26
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	7	0.26
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	7	0.26
(1,677)	2:234:B:LEU:HD21	2:239:B:ARG:HG3	5	0.26
(1,677)	2:234:B:LEU:HD22	2:239:B:ARG:HG3	5	0.26
(1,677)	2:234:B:LEU:HD23	2:239:B:ARG:HG3	5	0.26
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD21	14	0.26
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD22	14	0.26
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD23	14	0.26
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE1	6	0.26
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE2	6	0.26
(1,563)	1:96:A:LEU:HD21	2:228:B:MET:HE3	6	0.26
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE1	6	0.26
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE2	6	0.26
(1,563)	1:96:A:LEU:HD22	2:228:B:MET:HE3	6	0.26
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE1	6	0.26
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE2	6	0.26
(1,563)	1:96:A:LEU:HD23	2:228:B:MET:HE3	6	0.26
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	6	0.26
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	6	0.26
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	6	0.26
(1,285)	2:187:B:LYS:HG3	2:187:B:LYS:HE2	2	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	10	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	10	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	10	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	10	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	10	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	10	0.26
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	10	0.26
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	10	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	12	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	12	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	12	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	12	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	12	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	12	0.26
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	12	0.26
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	12	0.26
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	12	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	19	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	19	0.26
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	19	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	19	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	19	0.26
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	19	0.26
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	19	0.26
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	19	0.26
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	19	0.26
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	2	0.25
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	2	0.25
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	2	0.25
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	2	0.25
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	2	0.25
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	2	0.25
(2,12)	2:288:B:LEU:HD21	2:157:B:LYS:H	14	0.25
(2,12)	2:288:B:LEU:HD22	2:157:B:LYS:H	14	0.25
(2,12)	2:288:B:LEU:HD23	2:157:B:LYS:H	14	0.25
(1,4600)	2:200:B:TYR:HE2	2:201:B:LYS:HG2	8	0.25
(1,4589)	2:182:B:PHE:HD2	2:259:B:GLY:HA2	17	0.25
(1,4548)	2:200:B:TYR:HE2	2:201:B:LYS:HD2	19	0.25
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	10	0.25
(1,4527)	2:242:B:TYR:HE2	2:243:B:ALA:HB3	16	0.25
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	6	0.25
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	14	0.25
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	2	0.25
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG12	9	0.25
(1,4363)	2:235:B:TYR:HD1	1:106:A:VAL:HG23	1	0.25
(1,4328)	2:279:B:LEU:HD22	1:94:A:GLU:HB2	5	0.25
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	16	0.25
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	11	0.25
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4009)	2:180:B:GLN:HG3	2:313:B:VAL:HG13	2	0.25
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG12	15	0.25
(1,3998)	2:300:B:LYS:HG2	2:300:B:LYS:HD3	13	0.25
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	16	0.25
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	17	0.25
(1,3965)	2:290:B:TYR:HE2	2:286:B:LEU:HG	1	0.25
(1,3950)	2:270:B:ILE:HG23	2:274:B:LEU:HD23	9	0.25
(1,3795)	2:194:B:LEU:HD23	2:190:B:VAL:HG11	2	0.25
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD23	7	0.25
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD21	12	0.25
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD22	12	0.25
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD23	12	0.25
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD21	12	0.25
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD22	12	0.25
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD23	12	0.25
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	19	0.25
(1,2874)	1:106:A:VAL:HG21	1:108:A:PRO:HA	4	0.25
(1,2874)	1:106:A:VAL:HG22	1:108:A:PRO:HA	4	0.25
(1,2874)	1:106:A:VAL:HG23	1:108:A:PRO:HA	4	0.25
(1,2210)	2:288:B:LEU:HB2	2:289:B:ASN:H	5	0.25
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	5	0.25
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	5	0.25
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	5	0.25
(1,2138)	2:279:B:LEU:HB3	2:279:B:LEU:H	18	0.25
(1,1270)	2:193:B:ILE:HD11	2:188:B:LYS:HE3	20	0.25
(1,1270)	2:193:B:ILE:HD12	2:188:B:LYS:HE3	20	0.25
(1,1270)	2:193:B:ILE:HD13	2:188:B:LYS:HE3	20	0.25
(1,1061)	2:296:B:LYS:HE3	2:294:B:PHE:HA	3	0.25
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE1	18	0.25
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE2	18	0.25
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE3	18	0.25
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE1	18	0.25
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE2	18	0.25
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE3	18	0.25
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE1	18	0.25
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE2	18	0.25
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE3	18	0.25
(1,547)	2:194:B:LEU:HD11	2:222:B:LYS:HE3	10	0.25
(1,547)	2:194:B:LEU:HD12	2:222:B:LYS:HE3	10	0.25
(1,547)	2:194:B:LEU:HD13	2:222:B:LYS:HE3	10	0.25
(1,547)	2:194:B:LEU:HD11	2:222:B:LYS:HE3	13	0.25
(1,547)	2:194:B:LEU:HD12	2:222:B:LYS:HE3	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	2:194:B:LEU:HD13	2:222:B:LYS:HE3	13	0.25
(1,432)	2:204:B:ARG:HA	2:204:B:ARG:HD3	15	0.25
(1,342)	2:188:B:LYS:HG2	2:192:B:SER:HB2	17	0.25
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	14	0.25
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	14	0.25
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	14	0.25
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	14	0.25
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	14	0.25
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	14	0.25
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	14	0.25
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	14	0.25
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	14	0.25
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD21	3	0.25
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD22	3	0.25
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD23	3	0.25
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD21	2	0.25
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD22	2	0.25
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD23	2	0.25
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	3	0.24
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	3	0.24
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	3	0.24
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	3	0.24
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	3	0.24
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	3	0.24
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	3	0.24
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	3	0.24
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	3	0.24
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	3	0.24
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	3	0.24
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	3	0.24
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	8	0.24
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	8	0.24
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	8	0.24
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	8	0.24
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	8	0.24
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	8	0.24
(1,4604)	2:225:B:PHE:HE1	2:266:B:LEU:HD11	18	0.24
(1,4603)	2:225:B:PHE:HD1	2:266:B:LEU:HD12	14	0.24
(1,4591)	2:258:B:TYR:HE2	2:230:B:GLY:HA3	18	0.24
(1,4554)	2:290:B:TYR:HD1	2:217:B:VAL:HG13	14	0.24
(1,4533)	2:262:B:HIS:HD2	2:258:B:TYR:HB2	15	0.24
(1,4496)	2:267:B:PHE:HD1	2:158:B:VAL:HG13	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4476)	1:92:A:GLU:HG2	1:90:A:LEU:H	2	0.24
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	6	0.24
(1,4435)	1:75:A:LYS:HE3	1:92:A:GLU:HA	2	0.24
(1,4385)	1:112:A:ILE:HG23	1:109:A:GLU:HB3	13	0.24
(1,4382)	2:168:B:LEU:HD12	1:108:A:PRO:HD3	16	0.24
(1,4376)	1:112:A:ILE:HG13	1:108:A:PRO:HA	1	0.24
(1,4328)	2:279:B:LEU:HD21	1:94:A:GLU:HB2	19	0.24
(1,4327)	2:279:B:LEU:HD22	1:94:A:GLU:HB3	2	0.24
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	11	0.24
(1,4283)	1:82:A:SER:HA	1:84:A:MET:HE2	19	0.24
(1,4055)	2:175:B:ILE:HG21	2:180:B:GLN:H	9	0.24
(1,3998)	2:300:B:LYS:HG2	2:300:B:LYS:HD3	12	0.24
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	14	0.24
(1,3976)	2:264:B:LEU:HA	2:295:B:LEU:HD11	8	0.24
(1,3961)	2:282:B:LYS:HG2	2:282:B:LYS:HD2	2	0.24
(1,3959)	2:210:B:LYS:HD3	2:210:B:LYS:HG2	7	0.24
(1,3959)	2:210:B:LYS:HD3	2:210:B:LYS:HG2	14	0.24
(1,3950)	2:270:B:ILE:HG22	2:274:B:LEU:HD23	3	0.24
(1,3915)	2:305:B:LEU:HD22	2:260:B:ALA:HB1	18	0.24
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	3	0.24
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	4	0.24
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB2	8	0.24
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	11	0.24
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	13	0.24
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	19	0.24
(1,3835)	2:156:B:VAL:HG13	2:156:B:VAL:HB	18	0.24
(1,3783)	2:160:B:ILE:HB	2:165:B:LYS:HE2	19	0.24
(1,3750)	1:111:A:ILE:HD11	2:165:B:LYS:HE2	3	0.24
(1,3740)	2:317:B:GLU:HB2	2:317:B:GLU:HG3	15	0.24
(1,3734)	2:161:B:PRO:HB2	2:160:B:ILE:HG21	1	0.24
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	5	0.24
(1,3663)	2:183:B:TYR:HE1	2:312:B:GLU:HB2	10	0.24
(1,3663)	2:183:B:TYR:HE2	2:312:B:GLU:HB2	10	0.24
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	5	0.24
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	5	0.24
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	5	0.24
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	5	0.24
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	5	0.24
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	5	0.24
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	3	0.24
(1,3250)	1:103:A:ARG:HD3	1:102:A:GLU:H	1	0.24
(1,2595)	1:83:A:THR:HG21	1:84:A:MET:HE1	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2595)	1:83:A:THR:HG21	1:84:A:MET:HE2	9	0.24
(1,2595)	1:83:A:THR:HG21	1:84:A:MET:HE3	9	0.24
(1,2595)	1:83:A:THR:HG22	1:84:A:MET:HE1	9	0.24
(1,2595)	1:83:A:THR:HG22	1:84:A:MET:HE2	9	0.24
(1,2595)	1:83:A:THR:HG22	1:84:A:MET:HE3	9	0.24
(1,2595)	1:83:A:THR:HG23	1:84:A:MET:HE1	9	0.24
(1,2595)	1:83:A:THR:HG23	1:84:A:MET:HE2	9	0.24
(1,2595)	1:83:A:THR:HG23	1:84:A:MET:HE3	9	0.24
(1,2593)	2:212:B:TYR:HD1	1:84:A:MET:HB2	20	0.24
(1,2593)	2:212:B:TYR:HD2	1:84:A:MET:HB2	20	0.24
(1,2440)	2:253:B:PRO:HB2	2:256:B:GLN:H	2	0.24
(1,2393)	2:317:B:GLU:HG3	2:317:B:GLU:H	9	0.24
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	11	0.24
(1,1904)	2:241:B:GLN:HG2	2:241:B:GLN:H	19	0.24
(1,1780)	2:223:B:GLU:HG2	2:223:B:GLU:H	6	0.24
(1,1739)	2:217:B:VAL:HB	2:218:B:VAL:H	4	0.24
(1,1581)	2:193:B:ILE:HG13	2:194:B:LEU:H	17	0.24
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	15	0.24
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	15	0.24
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	15	0.24
(1,1310)	2:157:B:LYS:HG2	2:157:B:LYS:H	1	0.24
(1,1102)	2:164:B:LEU:HD21	2:299:B:ALA:HA	5	0.24
(1,1102)	2:164:B:LEU:HD22	2:299:B:ALA:HA	5	0.24
(1,1102)	2:164:B:LEU:HD23	2:299:B:ALA:HA	5	0.24
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD2	3	0.24
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	4	0.24
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	10	0.24
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD2	12	0.24
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	13	0.24
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	15	0.24
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	19	0.24
(1,1061)	2:296:B:LYS:HE3	2:294:B:PHE:HA	12	0.24
(1,1061)	2:296:B:LYS:HE3	2:294:B:PHE:HA	14	0.24
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD21	7	0.24
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD22	7	0.24
(1,616)	1:105:A:PHE:HE1	2:233:B:LEU:HD23	7	0.24
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD21	7	0.24
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD22	7	0.24
(1,616)	1:105:A:PHE:HE2	2:233:B:LEU:HD23	7	0.24
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	15	0.24
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	18	0.24
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD21	13	0.24
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD22	13	0.24
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD23	13	0.24
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	2	0.24
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	3	0.24
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	4	0.24
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	2	0.24
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	3	0.24
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	9	0.24
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	12	0.24
(2,261)	2:227:B:VAL:HG22	1:98:A:PHE:HD1	17	0.23
(2,259)	2:227:B:VAL:HG22	1:98:A:PHE:HD1	17	0.23
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	4	0.23
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	4	0.23
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	4	0.23
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	4	0.23
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	4	0.23
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	4	0.23
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	4	0.23
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	4	0.23
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	4	0.23
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	4	0.23
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	4	0.23
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	4	0.23
(2,45)	1:85:A:TYR:HD1	1:81:A:LEU:HG	8	0.23
(2,45)	1:85:A:TYR:HD2	1:81:A:LEU:HG	8	0.23
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD13	3	0.23
(1,4591)	2:258:B:TYR:HE2	2:230:B:GLY:HA3	6	0.23
(1,4589)	2:182:B:PHE:HD2	2:261:B:PRO:HD3	7	0.23
(1,4575)	2:167:B:TRP:HD1	2:164:B:LEU:HD23	18	0.23
(1,4573)	2:249:B:HIS:HD2	2:245:B:ILE:HG22	8	0.23
(1,4571)	2:318:B:TYR:HE2	2:241:B:GLN:HA	4	0.23
(1,4562)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	7	0.23
(1,4562)	2:242:B:TYR:HE1	2:246:B:LEU:HD11	8	0.23
(1,4532)	2:183:B:TYR:HD2	2:184:B:LEU:HA	5	0.23
(1,4513)	2:235:B:TYR:HE1	2:175:B:ILE:HD13	17	0.23
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	4	0.23
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	5	0.23
(1,4436)	1:119:A:LYS:HD3	1:119:A:LYS:HG2	11	0.23
(1,4436)	1:75:A:LYS:HD2	1:75:A:LYS:HG3	19	0.23
(1,4413)	2:169:B:VAL:HG22	1:112:A:ILE:HB	3	0.23
(1,4343)	1:74:A:SER:HB3	1:95:A:ILE:HD12	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	5	0.23
(1,4278)	1:84:A:MET:HE2	1:81:A:LEU:HD21	15	0.23
(1,4179)	2:288:B:LEU:HG	2:288:B:LEU:H	20	0.23
(1,4140)	2:254:B:MET:HE2	2:252:B:ALA:H	12	0.23
(1,4055)	2:175:B:ILE:HG22	2:180:B:GLN:H	12	0.23
(1,4036)	2:164:B:LEU:HD13	2:164:B:LEU:H	1	0.23
(1,4028)	1:96:A:LEU:HD11	2:277:B:THR:HB	3	0.23
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	6	0.23
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	8	0.23
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	16	0.23
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	1	0.23
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	6	0.23
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	8	0.23
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	16	0.23
(1,3928)	1:111:A:ILE:HD13	2:268:B:VAL:HG13	15	0.23
(1,3921)	2:221:B:ILE:HG21	2:263:B:LEU:HD22	17	0.23
(1,3916)	2:263:B:LEU:HD21	2:263:B:LEU:HA	12	0.23
(1,3916)	2:263:B:LEU:HD23	2:263:B:LEU:HA	16	0.23
(1,3852)	2:218:B:VAL:HG22	2:202:B:LYS:HE3	6	0.23
(1,3846)	2:219:B:ALA:HA	2:219:B:ALA:HB1	1	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB2	2	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB2	5	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB1	6	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB2	10	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB1	12	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	14	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	15	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB1	16	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB3	17	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB1	18	0.23
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB2	20	0.23
(1,3835)	2:156:B:VAL:HG21	2:156:B:VAL:HB	1	0.23
(1,3835)	2:156:B:VAL:HG21	2:156:B:VAL:HB	5	0.23
(1,3835)	2:214:B:VAL:HG23	2:214:B:VAL:HB	7	0.23
(1,3835)	2:156:B:VAL:HG23	2:156:B:VAL:HB	9	0.23
(1,3835)	2:214:B:VAL:HG21	2:214:B:VAL:HB	13	0.23
(1,3835)	2:156:B:VAL:HG12	2:156:B:VAL:HB	17	0.23
(1,3835)	2:214:B:VAL:HG23	2:214:B:VAL:HB	19	0.23
(1,3835)	2:214:B:VAL:HG21	2:214:B:VAL:HB	20	0.23
(1,3795)	2:194:B:LEU:HD22	2:190:B:VAL:HG11	6	0.23
(1,3749)	2:160:B:ILE:HG21	2:165:B:LYS:HE3	6	0.23
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD23	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3740)	2:317:B:GLU:HB3	2:317:B:GLU:HG3	5	0.23
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD11	15	0.23
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	19	0.23
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	19	0.23
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	19	0.23
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	19	0.23
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	19	0.23
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	19	0.23
(1,3541)	2:200:B:TYR:HE1	2:204:B:ARG:HD2	16	0.23
(1,3541)	2:200:B:TYR:HE2	2:204:B:ARG:HD2	16	0.23
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	3	0.23
(1,3250)	1:103:A:ARG:HD3	1:102:A:GLU:H	16	0.23
(1,2902)	1:112:A:ILE:HD11	1:109:A:GLU:HG3	6	0.23
(1,2902)	1:112:A:ILE:HD12	1:109:A:GLU:HG3	6	0.23
(1,2902)	1:112:A:ILE:HD13	1:109:A:GLU:HG3	6	0.23
(1,2900)	1:112:A:ILE:HD11	1:109:A:GLU:HB3	10	0.23
(1,2900)	1:112:A:ILE:HD12	1:109:A:GLU:HB3	10	0.23
(1,2900)	1:112:A:ILE:HD13	1:109:A:GLU:HB3	10	0.23
(1,2900)	1:112:A:ILE:HD11	1:109:A:GLU:HB3	20	0.23
(1,2900)	1:112:A:ILE:HD12	1:109:A:GLU:HB3	20	0.23
(1,2900)	1:112:A:ILE:HD13	1:109:A:GLU:HB3	20	0.23
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	5	0.23
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	5	0.23
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	5	0.23
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	14	0.23
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	14	0.23
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	14	0.23
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	20	0.23
(1,2145)	2:280:B:ASP:HB2	2:280:B:ASP:H	20	0.23
(1,2068)	2:265:B:ARG:HB2	2:265:B:ARG:H	13	0.23
(1,1904)	2:241:B:GLN:HG2	2:241:B:GLN:H	18	0.23
(1,1555)	2:190:B:VAL:HG21	2:190:B:VAL:H	14	0.23
(1,1555)	2:190:B:VAL:HG22	2:190:B:VAL:H	14	0.23
(1,1555)	2:190:B:VAL:HG23	2:190:B:VAL:H	14	0.23
(1,1505)	2:184:B:LEU:HD11	2:186:B:ALA:H	20	0.23
(1,1505)	2:184:B:LEU:HD12	2:186:B:ALA:H	20	0.23
(1,1505)	2:184:B:LEU:HD13	2:186:B:ALA:H	20	0.23
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	7	0.23
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	9	0.23
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG2	3	0.23
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG2	3	0.23
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	17	0.23
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE1	3	0.23
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE2	3	0.23
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE3	3	0.23
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE1	3	0.23
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE2	3	0.23
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE3	3	0.23
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE1	3	0.23
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE2	3	0.23
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE3	3	0.23
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	10	0.23
(1,427)	2:204:B:ARG:HG2	2:204:B:ARG:HA	7	0.23
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	8	0.23
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	12	0.23
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	13	0.23
(1,344)	2:188:B:LYS:HE3	2:193:B:ILE:HA	4	0.23
(1,342)	2:188:B:LYS:HG2	2:192:B:SER:HB2	11	0.23
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD11	9	0.23
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD12	9	0.23
(1,118)	2:268:B:VAL:HG11	2:168:B:LEU:HD13	9	0.23
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD11	9	0.23
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD12	9	0.23
(1,118)	2:268:B:VAL:HG12	2:168:B:LEU:HD13	9	0.23
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD11	9	0.23
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD12	9	0.23
(1,118)	2:268:B:VAL:HG13	2:168:B:LEU:HD13	9	0.23
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	14	0.23
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	20	0.23
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	4	0.23
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	5	0.23
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	8	0.23
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	15	0.23
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	20	0.23
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	1	0.23
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	14	0.23
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	16	0.23
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	18	0.23
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	14	0.22
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	3	0.22
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	9	0.22
(1,4442)	1:74:A:SER:HB3	1:76:A:VAL:HG23	12	0.22
(1,4436)	1:119:A:LYS:HD2	1:119:A:LYS:HG3	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4436)	1:119:A:LYS:HD3	1:119:A:LYS:HG2	15	0.22
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG13	12	0.22
(1,4413)	2:169:B:VAL:HG21	1:112:A:ILE:HB	1	0.22
(1,4373)	2:172:B:TRP:HB2	1:107:A:LEU:HD22	15	0.22
(1,4357)	2:273:B:MET:HE2	1:100:A:ASN:HA	12	0.22
(1,4318)	2:279:B:LEU:HD11	1:91:A:HIS:HA	3	0.22
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	8	0.22
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	9	0.22
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	12	0.22
(1,4275)	2:224:B:TYR:HE2	1:81:A:LEU:HD13	17	0.22
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD13	18	0.22
(1,4198)	2:164:B:LEU:HD21	2:299:B:ALA:H	9	0.22
(1,4198)	2:164:B:LEU:HD23	2:299:B:ALA:H	14	0.22
(1,4167)	1:90:A:LEU:HD11	2:280:B:ASP:H	5	0.22
(1,4153)	2:298:B:LEU:HD11	2:264:B:LEU:H	20	0.22
(1,4024)	2:323:B:VAL:HG23	2:320:B:ARG:HA	5	0.22
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	4	0.22
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	8	0.22
(1,3961)	2:282:B:LYS:HG2	2:282:B:LYS:HD3	1	0.22
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	4	0.22
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	13	0.22
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	18	0.22
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	19	0.22
(1,3960)	2:282:B:LYS:HB3	2:282:B:LYS:HD3	9	0.22
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	4	0.22
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	13	0.22
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	18	0.22
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	19	0.22
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD23	5	0.22
(1,3934)	1:108:A:PRO:HD2	2:268:B:VAL:HG21	7	0.22
(1,3910)	2:257:B:VAL:HG23	2:256:B:GLN:HG3	10	0.22
(1,3846)	2:247:B:ALA:HA	2:247:B:ALA:HB2	7	0.22
(1,3835)	2:156:B:VAL:HG21	2:156:B:VAL:HB	2	0.22
(1,3835)	2:214:B:VAL:HG23	2:214:B:VAL:HB	4	0.22
(1,3835)	2:156:B:VAL:HG12	2:156:B:VAL:HB	15	0.22
(1,3835)	2:214:B:VAL:HG22	2:214:B:VAL:HB	16	0.22
(1,3795)	2:194:B:LEU:HD22	2:190:B:VAL:HG13	19	0.22
(1,3774)	2:187:B:LYS:HG2	2:184:B:LEU:HD22	8	0.22
(1,3740)	2:317:B:GLU:HB2	2:317:B:GLU:HG3	1	0.22
(1,3740)	2:317:B:GLU:HB3	2:317:B:GLU:HG3	13	0.22
(1,3740)	2:281:B:GLU:HB3	2:281:B:GLU:HG3	17	0.22
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG2	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3734)	2:164:B:LEU:HB3	2:160:B:ILE:HG22	10	0.22
(1,3541)	2:200:B:TYR:HE1	2:204:B:ARG:HD2	19	0.22
(1,3541)	2:200:B:TYR:HE2	2:204:B:ARG:HD2	19	0.22
(1,3399)	1:117:A:GLU:HB3	1:118:A:GLY:H	10	0.22
(1,3172)	1:88:A:GLN:HB2	1:88:A:GLN:HE21	7	0.22
(1,2803)	2:232:B:GLN:HA	1:103:A:ARG:HD2	12	0.22
(1,2775)	1:96:A:LEU:HD11	1:100:A:ASN:HB3	8	0.22
(1,2775)	1:96:A:LEU:HD12	1:100:A:ASN:HB3	8	0.22
(1,2775)	1:96:A:LEU:HD13	1:100:A:ASN:HB3	8	0.22
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB1	6	0.22
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB2	6	0.22
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB3	6	0.22
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	10	0.22
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	10	0.22
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	10	0.22
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	10	0.22
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	10	0.22
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	10	0.22
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	10	0.22
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	10	0.22
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	10	0.22
(1,2623)	1:90:A:LEU:HD11	1:87:A:MET:HA	14	0.22
(1,2623)	1:90:A:LEU:HD12	1:87:A:MET:HA	14	0.22
(1,2623)	1:90:A:LEU:HD13	1:87:A:MET:HA	14	0.22
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	1	0.22
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	1	0.22
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	1	0.22
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	4	0.22
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	4	0.22
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	4	0.22
(1,2605)	1:87:A:MET:HB2	1:85:A:TYR:HA	8	0.22
(1,2604)	1:87:A:MET:HB2	1:85:A:TYR:HA	8	0.22
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD3	15	0.22
(1,2504)	1:77:A:ILE:HD11	1:74:A:SER:HB3	5	0.22
(1,2504)	1:77:A:ILE:HD12	1:74:A:SER:HB3	5	0.22
(1,2504)	1:77:A:ILE:HD13	1:74:A:SER:HB3	5	0.22
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	1	0.22
(1,2341)	2:307:B:SER:HB3	2:309:B:SER:H	4	0.22
(1,2252)	2:296:B:LYS:HD3	2:296:B:LYS:H	14	0.22
(1,2210)	2:288:B:LEU:HB2	2:289:B:ASN:H	20	0.22
(1,2135)	2:278:B:PRO:HA	2:279:B:LEU:H	3	0.22
(1,2119)	2:274:B:LEU:HD11	2:275:B:ALA:H	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2119)	2:274:B:LEU:HD12	2:275:B:ALA:H	17	0.22
(1,2119)	2:274:B:LEU:HD13	2:275:B:ALA:H	17	0.22
(1,2029)	2:257:B:VAL:HG11	2:257:B:VAL:H	20	0.22
(1,2029)	2:257:B:VAL:HG12	2:257:B:VAL:H	20	0.22
(1,2029)	2:257:B:VAL:HG13	2:257:B:VAL:H	20	0.22
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	8	0.22
(1,1904)	2:241:B:GLN:HG2	2:241:B:GLN:H	3	0.22
(1,1844)	2:232:B:GLN:HG3	2:232:B:GLN:H	9	0.22
(1,1676)	2:204:B:ARG:HG3	2:204:B:ARG:H	16	0.22
(1,1503)	2:184:B:LEU:HD11	2:184:B:LEU:H	15	0.22
(1,1503)	2:184:B:LEU:HD12	2:184:B:LEU:H	15	0.22
(1,1503)	2:184:B:LEU:HD13	2:184:B:LEU:H	15	0.22
(1,1503)	2:184:B:LEU:HD11	2:184:B:LEU:H	17	0.22
(1,1503)	2:184:B:LEU:HD12	2:184:B:LEU:H	17	0.22
(1,1503)	2:184:B:LEU:HD13	2:184:B:LEU:H	17	0.22
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	4	0.22
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB1	15	0.22
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB2	15	0.22
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB3	15	0.22
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB1	15	0.22
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB2	15	0.22
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB3	15	0.22
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB1	15	0.22
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB2	15	0.22
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB3	15	0.22
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	1	0.22
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	5	0.22
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	6	0.22
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD2	14	0.22
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	16	0.22
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	18	0.22
(1,978)	2:282:B:LYS:HD3	2:282:B:LYS:HB3	2	0.22
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD21	2	0.22
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD22	2	0.22
(1,942)	2:156:B:VAL:HB	2:274:B:LEU:HD23	2	0.22
(1,818)	2:257:B:VAL:HG11	2:256:B:GLN:HG2	13	0.22
(1,818)	2:257:B:VAL:HG12	2:256:B:GLN:HG2	13	0.22
(1,818)	2:257:B:VAL:HG13	2:256:B:GLN:HG2	13	0.22
(1,681)	2:234:B:LEU:HD21	2:239:B:ARG:HG2	11	0.22
(1,681)	2:234:B:LEU:HD22	2:239:B:ARG:HG2	11	0.22
(1,681)	2:234:B:LEU:HD23	2:239:B:ARG:HG2	11	0.22
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE1	14	0.22
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE2	14	0.22
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE3	14	0.22
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE1	14	0.22
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE2	14	0.22
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE3	14	0.22
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE1	14	0.22
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE2	14	0.22
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE3	14	0.22
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB2	2	0.22
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	4	0.22
(1,342)	2:188:B:LYS:HG2	2:192:B:SER:HB2	18	0.22
(1,301)	2:192:B:SER:HB3	2:188:B:LYS:HD2	14	0.22
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD11	11	0.22
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD12	11	0.22
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD13	11	0.22
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	6	0.22
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	16	0.22
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	3	0.22
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	8	0.22
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD21	4	0.22
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD22	4	0.22
(1,2)	1:87:A:MET:HE1	2:286:B:LEU:HD23	4	0.22
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD21	4	0.22
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD22	4	0.22
(1,2)	1:87:A:MET:HE2	2:286:B:LEU:HD23	4	0.22
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD21	4	0.22
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD22	4	0.22
(1,2)	1:87:A:MET:HE3	2:286:B:LEU:HD23	4	0.22
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	19	0.21
(1,4639)	2:212:B:TYR:HD1	2:213:B:ALA:HB1	5	0.21
(1,4620)	2:267:B:PHE:HD2	2:298:B:LEU:HD13	9	0.21
(1,4597)	2:267:B:PHE:HE2	2:263:B:LEU:HG	2	0.21
(1,4589)	2:182:B:PHE:HD2	2:259:B:GLY:HA2	20	0.21
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	2	0.21
(1,4527)	2:242:B:TYR:HE2	2:243:B:ALA:HB3	3	0.21
(1,4496)	2:267:B:PHE:HD1	2:158:B:VAL:HG13	11	0.21
(1,4496)	2:267:B:PHE:HD2	2:263:B:LEU:HD23	18	0.21
(1,4450)	1:72:A:VAL:HB	1:72:A:VAL:H	3	0.21
(1,4444)	1:97:A:PRO:HG3	1:96:A:LEU:HD11	3	0.21
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	7	0.21
(1,4424)	1:116:A:ARG:HG2	1:115:A:VAL:HG11	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4363)	2:235:B:TYR:HD1	1:106:A:VAL:HG22	5	0.21
(1,4328)	2:279:B:LEU:HD23	1:94:A:GLU:HB2	7	0.21
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	17	0.21
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	18	0.21
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	19	0.21
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	16	0.21
(1,4271)	2:212:B:TYR:HD2	1:81:A:LEU:HA	11	0.21
(1,4179)	2:288:B:LEU:HG	2:288:B:LEU:H	2	0.21
(1,4167)	1:90:A:LEU:HD13	2:280:B:ASP:H	10	0.21
(1,4087)	2:202:B:LYS:HG2	2:202:B:LYS:H	2	0.21
(1,4055)	2:175:B:ILE:HG22	2:180:B:GLN:H	19	0.21
(1,4036)	2:160:B:ILE:HG22	2:164:B:LEU:H	10	0.21
(1,4024)	2:323:B:VAL:HG11	2:320:B:ARG:HA	6	0.21
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	20	0.21
(1,3993)	2:296:B:LYS:HA	2:299:B:ALA:HB2	1	0.21
(1,3988)	2:263:B:LEU:HD12	2:298:B:LEU:HD12	3	0.21
(1,3961)	2:282:B:LYS:HG2	2:282:B:LYS:HD3	7	0.21
(1,3959)	2:210:B:LYS:HD3	2:210:B:LYS:HG2	5	0.21
(1,3846)	2:219:B:ALA:HA	2:219:B:ALA:HB1	9	0.21
(1,3835)	2:214:B:VAL:HG23	2:214:B:VAL:HB	6	0.21
(1,3835)	2:214:B:VAL:HG21	2:214:B:VAL:HB	8	0.21
(1,3835)	2:214:B:VAL:HG21	2:214:B:VAL:HB	11	0.21
(1,3835)	2:214:B:VAL:HG23	2:214:B:VAL:HB	12	0.21
(1,3795)	2:194:B:LEU:HD21	2:190:B:VAL:HG13	15	0.21
(1,3749)	2:160:B:ILE:HG21	2:165:B:LYS:HE3	15	0.21
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD21	7	0.21
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD22	7	0.21
(1,3656)	2:225:B:PHE:HE1	2:233:B:LEU:HD23	7	0.21
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD21	7	0.21
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD22	7	0.21
(1,3656)	2:225:B:PHE:HE2	2:233:B:LEU:HD23	7	0.21
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	8	0.21
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB3	13	0.21
(1,3395)	1:117:A:GLU:HG3	1:117:A:GLU:H	11	0.21
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	2	0.21
(1,3039)	2:231:B:THR:HA	1:102:A:GLU:HG3	15	0.21
(1,2900)	1:112:A:ILE:HD11	1:109:A:GLU:HB3	18	0.21
(1,2900)	1:112:A:ILE:HD12	1:109:A:GLU:HB3	18	0.21
(1,2900)	1:112:A:ILE:HD13	1:109:A:GLU:HB3	18	0.21
(1,2864)	1:108:A:PRO:HD2	1:107:A:LEU:HD21	15	0.21
(1,2864)	1:108:A:PRO:HD2	1:107:A:LEU:HD22	15	0.21
(1,2864)	1:108:A:PRO:HD2	1:107:A:LEU:HD23	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	18	0.21
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	18	0.21
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	18	0.21
(1,2526)	1:80:A:HIS:HB2	1:77:A:ILE:HA	19	0.21
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	13	0.21
(1,2171)	2:282:B:LYS:HG2	2:283:B:SER:H	17	0.21
(1,2138)	2:279:B:LEU:HG	2:279:B:LEU:H	3	0.21
(1,2138)	2:279:B:LEU:HB3	2:279:B:LEU:H	11	0.21
(1,2138)	2:279:B:LEU:HB3	2:279:B:LEU:H	12	0.21
(1,1975)	2:246:B:LEU:HG	2:249:B:HIS:H	11	0.21
(1,1561)	2:190:B:VAL:HB	2:191:B:ASP:H	14	0.21
(1,1542)	2:188:B:LYS:HG2	2:189:B:ASN:H	10	0.21
(1,1505)	2:184:B:LEU:HD11	2:186:B:ALA:H	1	0.21
(1,1505)	2:184:B:LEU:HD12	2:186:B:ALA:H	1	0.21
(1,1505)	2:184:B:LEU:HD13	2:186:B:ALA:H	1	0.21
(1,1458)	2:179:B:LYS:HG3	2:179:B:LYS:H	16	0.21
(1,1270)	2:193:B:ILE:HD11	2:188:B:LYS:HE3	3	0.21
(1,1270)	2:193:B:ILE:HD12	2:188:B:LYS:HE3	3	0.21
(1,1270)	2:193:B:ILE:HD13	2:188:B:LYS:HE3	3	0.21
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	19	0.21
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	2	0.21
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	11	0.21
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD21	3	0.21
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD22	3	0.21
(1,1001)	2:284:B:LEU:HA	2:284:B:LEU:HD23	3	0.21
(1,548)	2:222:B:LYS:HB2	2:222:B:LYS:HE3	14	0.21
(1,547)	2:194:B:LEU:HD11	2:222:B:LYS:HE3	4	0.21
(1,547)	2:194:B:LEU:HD12	2:222:B:LYS:HE3	4	0.21
(1,547)	2:194:B:LEU:HD13	2:222:B:LYS:HE3	4	0.21
(1,547)	2:194:B:LEU:HD11	2:222:B:LYS:HE3	14	0.21
(1,547)	2:194:B:LEU:HD12	2:222:B:LYS:HE3	14	0.21
(1,547)	2:194:B:LEU:HD13	2:222:B:LYS:HE3	14	0.21
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB2	16	0.21
(1,427)	2:204:B:ARG:HG2	2:204:B:ARG:HA	1	0.21
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	3	0.21
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	6	0.21
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	9	0.21
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	19	0.21
(1,300)	2:188:B:LYS:HA	2:188:B:LYS:HD2	17	0.21
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE2	17	0.21
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE2	17	0.21
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD11	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD12	4	0.21
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD13	4	0.21
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	5	0.21
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	6	0.21
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	13	0.21
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	19	0.21
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB3	4	0.21
(3,2)	1:77:A:ILE:O	1:81:A:LEU:N	19	0.2
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	7	0.2
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	7	0.2
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	7	0.2
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	7	0.2
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	7	0.2
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	7	0.2
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	7	0.2
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	7	0.2
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	7	0.2
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	7	0.2
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	7	0.2
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	7	0.2
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	10	0.2
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	10	0.2
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	10	0.2
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	10	0.2
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	10	0.2
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	10	0.2
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	10	0.2
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	10	0.2
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	10	0.2
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	10	0.2
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	10	0.2
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	10	0.2
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	15	0.2
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	15	0.2
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	15	0.2
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	15	0.2
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	15	0.2
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	15	0.2
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	15	0.2
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	15	0.2
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	15	0.2
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	15	0.2
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	15	0.2
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	17	0.2
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	17	0.2
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	17	0.2
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	17	0.2
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	17	0.2
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	17	0.2
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	17	0.2
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	17	0.2
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	17	0.2
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	17	0.2
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	17	0.2
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	17	0.2
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	6	0.2
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	6	0.2
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	6	0.2
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	6	0.2
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	6	0.2
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	6	0.2
(1,4613)	2:197:B:TYR:HE2	2:214:B:VAL:HG11	10	0.2
(1,4611)	2:290:B:TYR:HD2	2:286:B:LEU:HG	17	0.2
(1,4597)	2:267:B:PHE:HE2	2:263:B:LEU:HG	18	0.2
(1,4579)	2:242:B:TYR:HE1	2:254:B:MET:HE3	3	0.2
(1,4574)	2:242:B:TYR:HD1	2:246:B:LEU:HD11	6	0.2
(1,4534)	2:183:B:TYR:HD1	2:238:B:GLU:HB2	3	0.2
(1,4491)	1:118:A:GLY:HA2	1:117:A:GLU:H	1	0.2
(1,4457)	1:84:A:MET:HA	1:85:A:TYR:H	20	0.2
(1,4451)	1:72:A:VAL:HA	1:72:A:VAL:H	16	0.2
(1,4436)	1:119:A:LYS:HD3	1:119:A:LYS:HG2	1	0.2
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	6	0.2
(1,4418)	2:169:B:VAL:HG21	1:112:A:ILE:HG22	6	0.2
(1,4352)	1:96:A:LEU:HD23	1:97:A:PRO:HG3	18	0.2
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	2	0.2
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	3	0.2
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	7	0.2
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	15	0.2
(1,4283)	1:82:A:SER:HA	1:84:A:MET:HE2	8	0.2
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	1	0.2
(1,4182)	2:291:B:LEU:HD21	2:292:B:HIS:H	9	0.2
(1,4063)	2:186:B:ALA:HB2	2:188:B:LYS:H	13	0.2
(1,4054)	2:313:B:VAL:HG11	2:180:B:GLN:HE22	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4033)	2:161:B:PRO:HB2	2:163:B:GLU:H	11	0.2
(1,4028)	2:279:B:LEU:HD23	2:277:B:THR:HB	20	0.2
(1,3998)	2:300:B:LYS:HG2	2:300:B:LYS:HD3	5	0.2
(1,3990)	2:263:B:LEU:HD13	2:298:B:LEU:HD22	9	0.2
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	9	0.2
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD3	10	0.2
(1,3960)	2:282:B:LYS:HB3	2:282:B:LYS:HD3	13	0.2
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	9	0.2
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG2	10	0.2
(1,3953)	2:317:B:GLU:HB3	2:317:B:GLU:HG2	16	0.2
(1,3942)	2:274:B:LEU:HD21	2:270:B:ILE:HG21	7	0.2
(1,3894)	2:254:B:MET:HE2	2:245:B:ILE:HG23	8	0.2
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE3	9	0.2
(1,3835)	2:214:B:VAL:HG21	2:214:B:VAL:HB	3	0.2
(1,3835)	2:214:B:VAL:HG23	2:214:B:VAL:HB	14	0.2
(1,3752)	2:160:B:ILE:HG21	2:165:B:LYS:HG3	1	0.2
(1,3740)	2:317:B:GLU:HB2	2:317:B:GLU:HG3	11	0.2
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	1	0.2
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD21	13	0.2
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD22	13	0.2
(1,3641)	2:294:B:PHE:HD1	2:295:B:LEU:HD23	13	0.2
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD21	13	0.2
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD22	13	0.2
(1,3641)	2:294:B:PHE:HD2	2:295:B:LEU:HD23	13	0.2
(1,3591)	2:182:B:PHE:HZ	2:261:B:PRO:HG2	12	0.2
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD11	20	0.2
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD12	20	0.2
(1,3562)	2:235:B:TYR:HD1	2:234:B:LEU:HD13	20	0.2
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD11	20	0.2
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD12	20	0.2
(1,3562)	2:235:B:TYR:HD2	2:234:B:LEU:HD13	20	0.2
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	9	0.2
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	7	0.2
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	20	0.2
(1,3250)	1:103:A:ARG:HD2	1:102:A:GLU:H	2	0.2
(1,3219)	1:94:A:GLU:HG2	1:94:A:GLU:H	20	0.2
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	1	0.2
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD21	15	0.2
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD22	15	0.2
(1,2869)	2:172:B:TRP:HD1	1:107:A:LEU:HD23	15	0.2
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	11	0.2
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	11	0.2
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD21	11	0.2
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD22	11	0.2
(1,2735)	1:97:A:PRO:HD2	1:96:A:LEU:HD23	11	0.2
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG21	5	0.2
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG22	5	0.2
(1,2523)	1:77:A:ILE:HG13	1:76:A:VAL:HG23	5	0.2
(1,2320)	2:305:B:LEU:HB3	2:306:B:PHE:H	7	0.2
(1,2320)	2:305:B:LEU:HB3	2:306:B:PHE:H	17	0.2
(1,2206)	2:286:B:LEU:HD21	2:289:B:ASN:HD22	8	0.2
(1,2206)	2:286:B:LEU:HD22	2:289:B:ASN:HD22	8	0.2
(1,2206)	2:286:B:LEU:HD23	2:289:B:ASN:HD22	8	0.2
(1,2152)	2:281:B:GLU:HB3	2:281:B:GLU:H	10	0.2
(1,1904)	2:241:B:GLN:HG2	2:241:B:GLN:H	2	0.2
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	9	0.2
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD11	11	0.2
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD12	11	0.2
(1,1134)	2:188:B:LYS:HE3	2:305:B:LEU:HD13	11	0.2
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	8	0.2
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD11	9	0.2
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD12	9	0.2
(1,1010)	2:290:B:TYR:HE1	2:286:B:LEU:HD13	9	0.2
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD11	9	0.2
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	9	0.2
(1,1010)	2:290:B:TYR:HE2	2:286:B:LEU:HD13	9	0.2
(1,923)	2:155:B:GLU:HG2	2:272:B:ALA:HA	10	0.2
(1,814)	2:257:B:VAL:HG11	2:256:B:GLN:HB2	18	0.2
(1,814)	2:257:B:VAL:HG12	2:256:B:GLN:HB2	18	0.2
(1,814)	2:257:B:VAL:HG13	2:256:B:GLN:HB2	18	0.2
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD11	12	0.2
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD12	12	0.2
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD13	12	0.2
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD11	12	0.2
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD12	12	0.2
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD13	12	0.2
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD11	12	0.2
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD12	12	0.2
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD13	12	0.2
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD21	3	0.2
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD22	3	0.2
(1,588)	2:234:B:LEU:HD21	2:229:B:LEU:HD23	3	0.2
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD21	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD22	3	0.2
(1,588)	2:234:B:LEU:HD22	2:229:B:LEU:HD23	3	0.2
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD21	3	0.2
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD22	3	0.2
(1,588)	2:234:B:LEU:HD23	2:229:B:LEU:HD23	3	0.2
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	2	0.2
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	2	0.2
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	2	0.2
(1,453)	2:211:B:GLU:HG3	2:211:B:GLU:HB2	1	0.2
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	7	0.2
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	12	0.2
(1,307)	2:193:B:ILE:HG12	2:188:B:LYS:HE3	18	0.2
(1,28)	2:157:B:LYS:HA	2:157:B:LYS:HG3	3	0.2
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	1	0.2
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	17	0.2
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	10	0.2
(2,307)	2:279:B:LEU:HD12	1:94:A:GLU:HA	18	0.19
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	14	0.19
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	14	0.19
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	14	0.19
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	14	0.19
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	14	0.19
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	14	0.19
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	14	0.19
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	14	0.19
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	14	0.19
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	14	0.19
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	14	0.19
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	14	0.19
(1,4564)	2:290:B:TYR:HE1	2:210:B:LYS:HG3	5	0.19
(1,4556)	2:290:B:TYR:HE1	2:217:B:VAL:HG21	1	0.19
(1,4522)	2:225:B:PHE:HE1	2:225:B:PHE:HA	17	0.19
(1,4499)	2:306:B:PHE:HE1	2:298:B:LEU:HD21	5	0.19
(1,4499)	2:306:B:PHE:HE2	2:298:B:LEU:HD23	18	0.19
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	12	0.19
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	2	0.19
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	10	0.19
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	17	0.19
(1,4385)	1:112:A:ILE:HG22	1:109:A:GLU:HB3	12	0.19
(1,4286)	1:78:A:TRP:HZ3	1:84:A:MET:HE2	4	0.19
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	14	0.19
(1,4179)	2:286:B:LEU:HG	2:288:B:LEU:H	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4153)	2:298:B:LEU:HD11	2:264:B:LEU:H	8	0.19
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	1	0.19
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	19	0.19
(1,3993)	2:296:B:LYS:HA	2:299:B:ALA:HB2	5	0.19
(1,3976)	2:264:B:LEU:HA	2:295:B:LEU:HD13	3	0.19
(1,3959)	2:210:B:LYS:HD3	2:210:B:LYS:HG2	2	0.19
(1,3959)	2:210:B:LYS:HD3	2:210:B:LYS:HG2	11	0.19
(1,3953)	2:281:B:GLU:HB3	2:281:B:GLU:HG2	7	0.19
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD21	11	0.19
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG23	12	0.19
(1,3901)	2:257:B:VAL:HG23	2:252:B:ALA:HB1	12	0.19
(1,3859)	2:270:B:ILE:HG12	2:228:B:MET:HE1	1	0.19
(1,3837)	2:210:B:LYS:HG3	2:214:B:VAL:HG21	6	0.19
(1,3837)	2:198:B:ALA:HB1	2:214:B:VAL:HG21	12	0.19
(1,3817)	2:198:B:ALA:HB3	2:195:B:GLU:HG2	1	0.19
(1,3795)	2:221:B:ILE:HG22	2:190:B:VAL:HG13	4	0.19
(1,3789)	2:193:B:ILE:HD11	2:188:B:LYS:HE2	7	0.19
(1,3746)	2:306:B:PHE:HE1	2:298:B:LEU:HD21	5	0.19
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG3	16	0.19
(1,3740)	2:317:B:GLU:HB3	2:317:B:GLU:HG3	19	0.19
(1,3689)	2:318:B:TYR:HE1	2:241:B:GLN:HG2	16	0.19
(1,3689)	2:318:B:TYR:HE2	2:241:B:GLN:HG2	16	0.19
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD21	9	0.19
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD22	9	0.19
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD23	9	0.19
(1,3395)	1:117:A:GLU:HG3	1:117:A:GLU:H	13	0.19
(1,3395)	1:117:A:GLU:HG3	1:117:A:GLU:H	16	0.19
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	19	0.19
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	19	0.19
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	19	0.19
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	19	0.19
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	19	0.19
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	19	0.19
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	19	0.19
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	19	0.19
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	19	0.19
(1,2623)	1:90:A:LEU:HD11	1:87:A:MET:HA	2	0.19
(1,2623)	1:90:A:LEU:HD12	1:87:A:MET:HA	2	0.19
(1,2623)	1:90:A:LEU:HD13	1:87:A:MET:HA	2	0.19
(1,2286)	2:301:B:ASN:HD22	2:301:B:ASN:H	1	0.19
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	3	0.19
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	3	0.19
(1,2138)	2:279:B:LEU:HB3	2:279:B:LEU:H	2	0.19
(1,2003)	2:254:B:MET:HG2	2:254:B:MET:H	10	0.19
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	9	0.19
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	13	0.19
(1,1503)	2:184:B:LEU:HD11	2:184:B:LEU:H	16	0.19
(1,1503)	2:184:B:LEU:HD12	2:184:B:LEU:H	16	0.19
(1,1503)	2:184:B:LEU:HD13	2:184:B:LEU:H	16	0.19
(1,1437)	2:174:B:LEU:HD11	2:178:B:GLN:HE22	11	0.19
(1,1437)	2:174:B:LEU:HD12	2:178:B:GLN:HE22	11	0.19
(1,1437)	2:174:B:LEU:HD13	2:178:B:GLN:HE22	11	0.19
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	7	0.19
(1,1228)	2:320:B:ARG:HG2	2:320:B:ARG:HA	5	0.19
(1,1083)	2:296:B:LYS:HG3	2:296:B:LYS:HD3	20	0.19
(1,1061)	2:296:B:LYS:HE2	2:294:B:PHE:HA	13	0.19
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD21	1	0.19
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD22	1	0.19
(1,999)	2:274:B:LEU:HD21	2:284:B:LEU:HD23	1	0.19
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD21	1	0.19
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD22	1	0.19
(1,999)	2:274:B:LEU:HD22	2:284:B:LEU:HD23	1	0.19
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD21	1	0.19
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD22	1	0.19
(1,999)	2:274:B:LEU:HD23	2:284:B:LEU:HD23	1	0.19
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	4	0.19
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	4	0.19
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	4	0.19
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	5	0.19
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	5	0.19
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	5	0.19
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	6	0.19
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	6	0.19
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	6	0.19
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	8	0.19
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	8	0.19
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	8	0.19
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	14	0.19
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	14	0.19
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	14	0.19
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	20	0.19
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	20	0.19
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG21	17	0.19
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG22	17	0.19
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG23	17	0.19
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD21	15	0.19
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD22	15	0.19
(1,642)	2:242:B:TYR:HE1	2:234:B:LEU:HD23	15	0.19
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD21	15	0.19
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD22	15	0.19
(1,642)	2:242:B:TYR:HE2	2:234:B:LEU:HD23	15	0.19
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	19	0.19
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	19	0.19
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	19	0.19
(1,432)	2:204:B:ARG:HA	2:204:B:ARG:HD3	18	0.19
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	10	0.19
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	14	0.19
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	17	0.19
(1,335)	2:263:B:LEU:HB3	2:190:B:VAL:HG21	11	0.19
(1,335)	2:263:B:LEU:HB3	2:190:B:VAL:HG22	11	0.19
(1,335)	2:263:B:LEU:HB3	2:190:B:VAL:HG23	11	0.19
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD21	17	0.19
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD22	17	0.19
(1,244)	2:314:B:ALA:HA	2:181:B:LEU:HD23	17	0.19
(1,158)	2:311:B:TYR:HD2	2:174:B:LEU:HD22	13	0.19
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	1	0.19
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	1	0.19
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	17	0.19
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	7	0.19
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	5	0.19
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	6	0.18
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	6	0.18
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	6	0.18
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	6	0.18
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	6	0.18
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	6	0.18
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	6	0.18
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	6	0.18
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	6	0.18
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	6	0.18
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	6	0.18
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	6	0.18
(1,4634)	2:237:B:PHE:HE2	2:314:B:ALA:HB1	10	0.18
(1,4611)	2:290:B:TYR:HD1	2:210:B:LYS:HD2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4591)	2:182:B:PHE:HD1	2:261:B:PRO:HD2	2	0.18
(1,4574)	2:242:B:TYR:HD1	2:246:B:LEU:HD13	16	0.18
(1,4527)	2:242:B:TYR:HE2	2:243:B:ALA:HB1	20	0.18
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG23	5	0.18
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	10	0.18
(1,4451)	1:71:A:GLN:HA	1:72:A:VAL:H	13	0.18
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	3	0.18
(1,4436)	1:75:A:LYS:HD2	1:75:A:LYS:HG3	14	0.18
(1,4436)	1:75:A:LYS:HD2	1:75:A:LYS:HG3	16	0.18
(1,4436)	1:75:A:LYS:HD2	1:75:A:LYS:HG3	20	0.18
(1,4433)	2:169:B:VAL:HG23	1:116:A:ARG:HG3	14	0.18
(1,4418)	2:169:B:VAL:HG21	1:112:A:ILE:HG21	17	0.18
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG3	1	0.18
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	13	0.18
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	14	0.18
(1,4279)	1:84:A:MET:HG2	1:81:A:LEU:HD22	1	0.18
(1,4279)	1:88:A:GLN:HG3	1:90:A:LEU:HD22	13	0.18
(1,4237)	2:218:B:VAL:HG11	2:198:B:ALA:H	3	0.18
(1,4153)	2:298:B:LEU:HD12	2:264:B:LEU:H	16	0.18
(1,4140)	2:254:B:MET:HE1	2:252:B:ALA:H	16	0.18
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	2	0.18
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	7	0.18
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	10	0.18
(1,3993)	2:296:B:LYS:HA	2:299:B:ALA:HB2	6	0.18
(1,3990)	2:263:B:LEU:HD12	2:194:B:LEU:HD22	6	0.18
(1,3990)	2:263:B:LEU:HD12	2:194:B:LEU:HD23	11	0.18
(1,3990)	2:263:B:LEU:HD13	2:194:B:LEU:HD23	20	0.18
(1,3979)	2:164:B:LEU:HD11	2:295:B:LEU:HD23	16	0.18
(1,3960)	2:282:B:LYS:HB3	2:282:B:LYS:HD3	6	0.18
(1,3959)	2:210:B:LYS:HD3	2:210:B:LYS:HG2	15	0.18
(1,3956)	2:282:B:LYS:HE2	2:282:B:LYS:HA	8	0.18
(1,3951)	2:270:B:ILE:HG12	2:274:B:LEU:HD22	6	0.18
(1,3915)	2:305:B:LEU:HD21	2:260:B:ALA:HB2	9	0.18
(1,3857)	2:224:B:TYR:HD1	2:227:B:VAL:HG13	4	0.18
(1,3789)	2:305:B:LEU:HD12	2:188:B:LYS:HE2	3	0.18
(1,3740)	2:317:B:GLU:HB2	2:317:B:GLU:HG3	7	0.18
(1,3660)	2:311:B:TYR:HD1	2:308:B:ALA:HA	12	0.18
(1,3560)	2:242:B:TYR:HD1	2:229:B:LEU:HD21	6	0.18
(1,3560)	2:242:B:TYR:HD1	2:229:B:LEU:HD22	6	0.18
(1,3560)	2:242:B:TYR:HD1	2:229:B:LEU:HD23	6	0.18
(1,3560)	2:242:B:TYR:HD2	2:229:B:LEU:HD21	6	0.18
(1,3560)	2:242:B:TYR:HD2	2:229:B:LEU:HD22	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3560)	2:242:B:TYR:HD2	2:229:B:LEU:HD23	6	0.18
(1,3541)	2:200:B:TYR:HE1	2:204:B:ARG:HD2	15	0.18
(1,3541)	2:200:B:TYR:HE2	2:204:B:ARG:HD2	15	0.18
(1,3420)	2:236:B:LYS:HG2	1:104:A:ASN:HD22	15	0.18
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	10	0.18
(1,2902)	1:112:A:ILE:HD11	1:109:A:GLU:HG2	18	0.18
(1,2902)	1:112:A:ILE:HD12	1:109:A:GLU:HG2	18	0.18
(1,2902)	1:112:A:ILE:HD13	1:109:A:GLU:HG2	18	0.18
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	16	0.18
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	16	0.18
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	16	0.18
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	16	0.18
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	16	0.18
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	16	0.18
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	16	0.18
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	16	0.18
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	16	0.18
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	18	0.18
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	18	0.18
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	18	0.18
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	18	0.18
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	18	0.18
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	18	0.18
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	18	0.18
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	18	0.18
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	18	0.18
(1,2640)	1:87:A:MET:HB2	1:87:A:MET:HG2	6	0.18
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE1	18	0.18
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE2	18	0.18
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE3	18	0.18
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE1	18	0.18
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE2	18	0.18
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE3	18	0.18
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE1	18	0.18
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE2	18	0.18
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE3	18	0.18
(1,2623)	1:90:A:LEU:HD11	1:87:A:MET:HA	13	0.18
(1,2623)	1:90:A:LEU:HD12	1:87:A:MET:HA	13	0.18
(1,2623)	1:90:A:LEU:HD13	1:87:A:MET:HA	13	0.18
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG11	1	0.18
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG12	1	0.18
(1,2520)	1:77:A:ILE:HG13	1:76:A:VAL:HG13	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	16	0.18
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	3	0.18
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	3	0.18
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	3	0.18
(1,2463)	1:70:A:ARG:HB3	1:70:A:ARG:HD3	16	0.18
(1,2246)	2:295:B:LEU:HG	2:295:B:LEU:H	3	0.18
(1,2246)	2:295:B:LEU:HG	2:295:B:LEU:H	8	0.18
(1,2206)	2:286:B:LEU:HD21	2:289:B:ASN:HD22	10	0.18
(1,2206)	2:286:B:LEU:HD22	2:289:B:ASN:HD22	10	0.18
(1,2206)	2:286:B:LEU:HD23	2:289:B:ASN:HD22	10	0.18
(1,2171)	2:282:B:LYS:HG2	2:283:B:SER:H	7	0.18
(1,2171)	2:282:B:LYS:HG2	2:283:B:SER:H	18	0.18
(1,2135)	2:278:B:PRO:HA	2:279:B:LEU:H	17	0.18
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	2	0.18
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	3	0.18
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	6	0.18
(1,1908)	2:241:B:GLN:HG2	2:242:B:TYR:H	4	0.18
(1,1904)	2:241:B:GLN:HG3	2:241:B:GLN:H	17	0.18
(1,1676)	2:204:B:ARG:HG3	2:204:B:ARG:H	3	0.18
(1,1676)	2:204:B:ARG:HG3	2:204:B:ARG:H	4	0.18
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	11	0.18
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	11	0.18
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	11	0.18
(1,1316)	2:157:B:LYS:HB3	2:157:B:LYS:H	8	0.18
(1,1302)	2:155:B:GLU:HB2	2:155:B:GLU:H	13	0.18
(1,1228)	2:320:B:ARG:HG2	2:320:B:ARG:HA	19	0.18
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	13	0.18
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	13	0.18
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	13	0.18
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	16	0.18
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	16	0.18
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	16	0.18
(1,874)	2:270:B:ILE:HD11	2:266:B:LEU:HD11	13	0.18
(1,874)	2:270:B:ILE:HD11	2:266:B:LEU:HD12	13	0.18
(1,874)	2:270:B:ILE:HD11	2:266:B:LEU:HD13	13	0.18
(1,874)	2:270:B:ILE:HD12	2:266:B:LEU:HD11	13	0.18
(1,874)	2:270:B:ILE:HD12	2:266:B:LEU:HD12	13	0.18
(1,874)	2:270:B:ILE:HD12	2:266:B:LEU:HD13	13	0.18
(1,874)	2:270:B:ILE:HD13	2:266:B:LEU:HD11	13	0.18
(1,874)	2:270:B:ILE:HD13	2:266:B:LEU:HD12	13	0.18
(1,874)	2:270:B:ILE:HD13	2:266:B:LEU:HD13	13	0.18
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG21	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG22	8	0.18
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG23	8	0.18
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG21	8	0.18
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG22	8	0.18
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG23	8	0.18
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG21	8	0.18
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG22	8	0.18
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG23	8	0.18
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	9	0.18
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	9	0.18
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	9	0.18
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE1	16	0.18
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE2	16	0.18
(1,563)	1:96:A:LEU:HD11	2:228:B:MET:HE3	16	0.18
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE1	16	0.18
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE2	16	0.18
(1,563)	1:96:A:LEU:HD12	2:228:B:MET:HE3	16	0.18
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE1	16	0.18
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE2	16	0.18
(1,563)	1:96:A:LEU:HD13	2:228:B:MET:HE3	16	0.18
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	18	0.18
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	18	0.18
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	18	0.18
(1,471)	2:197:B:TYR:HE1	2:214:B:VAL:HG11	12	0.18
(1,471)	2:197:B:TYR:HE1	2:214:B:VAL:HG12	12	0.18
(1,471)	2:197:B:TYR:HE1	2:214:B:VAL:HG13	12	0.18
(1,471)	2:197:B:TYR:HE2	2:214:B:VAL:HG11	12	0.18
(1,471)	2:197:B:TYR:HE2	2:214:B:VAL:HG12	12	0.18
(1,471)	2:197:B:TYR:HE2	2:214:B:VAL:HG13	12	0.18
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	6	0.18
(1,437)	2:201:B:LYS:HA	2:204:B:ARG:HG3	17	0.18
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	2	0.18
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	5	0.18
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	11	0.18
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	18	0.18
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD11	9	0.18
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD12	9	0.18
(1,258)	2:186:B:ALA:HB1	2:184:B:LEU:HD13	9	0.18
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD11	9	0.18
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD12	9	0.18
(1,258)	2:186:B:ALA:HB2	2:184:B:LEU:HD13	9	0.18
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD11	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD12	9	0.18
(1,258)	2:186:B:ALA:HB3	2:184:B:LEU:HD13	9	0.18
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD21	1	0.18
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD22	1	0.18
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD23	1	0.18
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD11	20	0.18
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD12	20	0.18
(1,151)	2:180:B:GLN:HG3	2:174:B:LEU:HD13	20	0.18
(1,40)	2:159:B:LYS:HD2	2:159:B:LYS:HG2	16	0.18
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	19	0.18
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	20	0.18
(1,4)	2:213:B:ALA:HB1	2:286:B:LEU:HD11	20	0.18
(1,4)	2:213:B:ALA:HB1	2:286:B:LEU:HD12	20	0.18
(1,4)	2:213:B:ALA:HB1	2:286:B:LEU:HD13	20	0.18
(1,4)	2:213:B:ALA:HB2	2:286:B:LEU:HD11	20	0.18
(1,4)	2:213:B:ALA:HB2	2:286:B:LEU:HD12	20	0.18
(1,4)	2:213:B:ALA:HB2	2:286:B:LEU:HD13	20	0.18
(1,4)	2:213:B:ALA:HB3	2:286:B:LEU:HD11	20	0.18
(1,4)	2:213:B:ALA:HB3	2:286:B:LEU:HD12	20	0.18
(1,4)	2:213:B:ALA:HB3	2:286:B:LEU:HD13	20	0.18
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	11	0.17
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	11	0.17
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	11	0.17
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	11	0.17
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	11	0.17
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	11	0.17
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	11	0.17
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	11	0.17
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	11	0.17
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	11	0.17
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	11	0.17
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	11	0.17
(1,4555)	2:294:B:PHE:HD2	2:217:B:VAL:HG12	5	0.17
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	2	0.17
(1,4534)	2:183:B:TYR:HD1	2:310:B:ASP:HB3	6	0.17
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG21	4	0.17
(1,4490)	2:165:B:LYS:HB2	1:115:A:VAL:H	15	0.17
(1,4490)	2:165:B:LYS:HB2	1:115:A:VAL:H	18	0.17
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	13	0.17
(1,4433)	2:169:B:VAL:HG21	1:116:A:ARG:HG3	16	0.17
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	19	0.17
(1,4281)	1:86:A:ASP:HB2	1:83:A:THR:HA	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD12	2	0.17
(1,4233)	2:321:B:LYS:HA	2:323:B:VAL:H	2	0.17
(1,4222)	2:317:B:GLU:HB2	2:318:B:TYR:H	6	0.17
(1,4179)	2:288:B:LEU:HG	2:288:B:LEU:H	3	0.17
(1,4115)	2:233:B:LEU:HB3	2:232:B:GLN:H	9	0.17
(1,4063)	2:186:B:ALA:HB3	2:188:B:LYS:H	19	0.17
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	6	0.17
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	12	0.17
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	12	0.17
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	20	0.17
(1,3953)	2:317:B:GLU:HB3	2:317:B:GLU:HG2	1	0.17
(1,3947)	2:269:B:ARG:HB3	2:273:B:MET:HE1	1	0.17
(1,3893)	2:252:B:ALA:HB2	2:245:B:ILE:HG23	9	0.17
(1,3843)	1:96:A:LEU:HD21	2:227:B:VAL:HG11	4	0.17
(1,3835)	2:214:B:VAL:HG23	2:214:B:VAL:HB	10	0.17
(1,3765)	2:181:B:LEU:HD21	2:175:B:ILE:HD11	2	0.17
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG3	8	0.17
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG2	10	0.17
(1,3733)	2:165:B:LYS:HB3	2:160:B:ILE:HG21	1	0.17
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD12	4	0.17
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG3	20	0.17
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG3	20	0.17
(1,3496)	2:318:B:TYR:HD1	2:181:B:LEU:HD21	14	0.17
(1,3496)	2:318:B:TYR:HD1	2:181:B:LEU:HD22	14	0.17
(1,3496)	2:318:B:TYR:HD1	2:181:B:LEU:HD23	14	0.17
(1,3496)	2:318:B:TYR:HD2	2:181:B:LEU:HD21	14	0.17
(1,3496)	2:318:B:TYR:HD2	2:181:B:LEU:HD22	14	0.17
(1,3496)	2:318:B:TYR:HD2	2:181:B:LEU:HD23	14	0.17
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	2	0.17
(1,3403)	1:117:A:GLU:HA	1:119:A:LYS:H	16	0.17
(1,3399)	1:117:A:GLU:HB2	1:118:A:GLY:H	15	0.17
(1,3399)	1:117:A:GLU:HB2	1:118:A:GLY:H	17	0.17
(1,3395)	1:117:A:GLU:HG2	1:117:A:GLU:H	7	0.17
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	1	0.17
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	13	0.17
(1,3172)	1:88:A:GLN:HB2	1:88:A:GLN:HE21	14	0.17
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD11	14	0.17
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD12	14	0.17
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD13	14	0.17
(1,3035)	2:172:B:TRP:HZ2	1:112:A:ILE:HD13	6	0.17
(1,2812)	1:106:A:VAL:HG11	1:104:A:ASN:HB2	3	0.17
(1,2812)	1:106:A:VAL:HG12	1:104:A:ASN:HB2	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2812)	1:106:A:VAL:HG13	1:104:A:ASN:HB2	3	0.17
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	3	0.17
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	3	0.17
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	3	0.17
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	3	0.17
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	3	0.17
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	3	0.17
(1,2623)	1:90:A:LEU:HD11	1:87:A:MET:HA	17	0.17
(1,2623)	1:90:A:LEU:HD12	1:87:A:MET:HA	17	0.17
(1,2623)	1:90:A:LEU:HD13	1:87:A:MET:HA	17	0.17
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	8	0.17
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	8	0.17
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	8	0.17
(1,2440)	2:253:B:PRO:HG2	2:256:B:GLN:H	1	0.17
(1,2440)	2:253:B:PRO:HB2	2:256:B:GLN:H	4	0.17
(1,2440)	2:253:B:PRO:HG2	2:256:B:GLN:H	7	0.17
(1,2440)	2:253:B:PRO:HB2	2:256:B:GLN:H	12	0.17
(1,2261)	2:164:B:LEU:HD11	2:298:B:LEU:H	14	0.17
(1,2261)	2:164:B:LEU:HD12	2:298:B:LEU:H	14	0.17
(1,2261)	2:164:B:LEU:HD13	2:298:B:LEU:H	14	0.17
(1,2210)	2:288:B:LEU:HB2	2:289:B:ASN:H	2	0.17
(1,2029)	2:257:B:VAL:HG11	2:257:B:VAL:H	11	0.17
(1,2029)	2:257:B:VAL:HG12	2:257:B:VAL:H	11	0.17
(1,2029)	2:257:B:VAL:HG13	2:257:B:VAL:H	11	0.17
(1,1505)	2:184:B:LEU:HD11	2:186:B:ALA:H	3	0.17
(1,1505)	2:184:B:LEU:HD12	2:186:B:ALA:H	3	0.17
(1,1505)	2:184:B:LEU:HD13	2:186:B:ALA:H	3	0.17
(1,1494)	2:183:B:TYR:HB2	2:183:B:TYR:H	7	0.17
(1,1324)	2:158:B:VAL:HG21	2:158:B:VAL:H	10	0.17
(1,1324)	2:158:B:VAL:HG22	2:158:B:VAL:H	10	0.17
(1,1324)	2:158:B:VAL:HG23	2:158:B:VAL:H	10	0.17
(1,1310)	2:157:B:LYS:HG2	2:157:B:LYS:H	14	0.17
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	5	0.17
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	13	0.17
(1,1130)	2:305:B:LEU:HD11	2:305:B:LEU:HA	12	0.17
(1,1130)	2:305:B:LEU:HD12	2:305:B:LEU:HA	12	0.17
(1,1130)	2:305:B:LEU:HD13	2:305:B:LEU:HA	12	0.17
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD21	5	0.17
(1,1061)	2:296:B:LYS:HE3	2:294:B:PHE:HA	18	0.17
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	9	0.17
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	9	0.17
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	15	0.17
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	15	0.17
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	15	0.17
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	19	0.17
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	19	0.17
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	19	0.17
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	9	0.17
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	13	0.17
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	18	0.17
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD11	18	0.17
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD12	18	0.17
(1,752)	2:254:B:MET:HE1	2:246:B:LEU:HD13	18	0.17
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD11	18	0.17
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD12	18	0.17
(1,752)	2:254:B:MET:HE2	2:246:B:LEU:HD13	18	0.17
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD11	18	0.17
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD12	18	0.17
(1,752)	2:254:B:MET:HE3	2:246:B:LEU:HD13	18	0.17
(1,722)	2:185:B:PRO:HA	2:245:B:ILE:HD11	3	0.17
(1,722)	2:185:B:PRO:HA	2:245:B:ILE:HD12	3	0.17
(1,722)	2:185:B:PRO:HA	2:245:B:ILE:HD13	3	0.17
(1,715)	2:184:B:LEU:HD21	2:245:B:ILE:HG13	11	0.17
(1,715)	2:184:B:LEU:HD22	2:245:B:ILE:HG13	11	0.17
(1,715)	2:184:B:LEU:HD23	2:245:B:ILE:HG13	11	0.17
(1,628)	2:229:B:LEU:HD11	2:234:B:LEU:HD11	5	0.17
(1,628)	2:229:B:LEU:HD11	2:234:B:LEU:HD12	5	0.17
(1,628)	2:229:B:LEU:HD11	2:234:B:LEU:HD13	5	0.17
(1,628)	2:229:B:LEU:HD12	2:234:B:LEU:HD11	5	0.17
(1,628)	2:229:B:LEU:HD12	2:234:B:LEU:HD12	5	0.17
(1,628)	2:229:B:LEU:HD12	2:234:B:LEU:HD13	5	0.17
(1,628)	2:229:B:LEU:HD13	2:234:B:LEU:HD11	5	0.17
(1,628)	2:229:B:LEU:HD13	2:234:B:LEU:HD12	5	0.17
(1,628)	2:229:B:LEU:HD13	2:234:B:LEU:HD13	5	0.17
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD21	11	0.17
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD22	11	0.17
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD23	11	0.17
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD21	11	0.17
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD22	11	0.17
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD23	11	0.17
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD21	11	0.17
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD22	11	0.17
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD23	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD21	3	0.17
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD22	3	0.17
(1,586)	2:234:B:LEU:HG	2:229:B:LEU:HD23	3	0.17
(1,427)	2:204:B:ARG:HG2	2:204:B:ARG:HA	5	0.17
(1,384)	2:195:B:GLU:HG2	2:195:B:GLU:HB3	7	0.17
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	16	0.17
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG21	17	0.17
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG22	17	0.17
(1,331)	2:193:B:ILE:HD11	2:190:B:VAL:HG23	17	0.17
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG21	17	0.17
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG22	17	0.17
(1,331)	2:193:B:ILE:HD12	2:190:B:VAL:HG23	17	0.17
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG21	17	0.17
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG22	17	0.17
(1,331)	2:193:B:ILE:HD13	2:190:B:VAL:HG23	17	0.17
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD21	17	0.17
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD22	17	0.17
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD23	17	0.17
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD21	15	0.17
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD22	15	0.17
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD23	15	0.17
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD11	14	0.17
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD12	14	0.17
(1,150)	2:178:B:GLN:HB3	2:174:B:LEU:HD13	14	0.17
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	11	0.17
(1,40)	2:159:B:LYS:HD2	2:159:B:LYS:HG2	19	0.17
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	7	0.17
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	12	0.17
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	16	0.17
(1,37)	2:159:B:LYS:HA	2:159:B:LYS:HG3	12	0.17
(1,26)	2:157:B:LYS:HG3	2:157:B:LYS:HD2	14	0.17
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	13	0.17
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	9	0.16
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	9	0.16
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	9	0.16
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	9	0.16
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	9	0.16
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	9	0.16
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	9	0.16
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	9	0.16
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	9	0.16
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	9	0.16
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	9	0.16
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	19	0.16
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	19	0.16
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	19	0.16
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	19	0.16
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	19	0.16
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	19	0.16
(1,4613)	2:290:B:TYR:HE2	2:286:B:LEU:HD12	12	0.16
(1,4575)	2:242:B:TYR:HE1	2:234:B:LEU:HD13	11	0.16
(1,4564)	2:197:B:TYR:HE2	2:198:B:ALA:HB2	14	0.16
(1,4527)	2:242:B:TYR:HE2	2:243:B:ALA:HB1	6	0.16
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	3	0.16
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	4	0.16
(1,4440)	2:223:B:GLU:HG3	1:77:A:ILE:HG22	7	0.16
(1,4436)	1:119:A:LYS:HD3	1:119:A:LYS:HG2	12	0.16
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG13	17	0.16
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	8	0.16
(1,4396)	2:165:B:LYS:HE2	1:111:A:ILE:HD12	16	0.16
(1,4385)	1:112:A:ILE:HG23	1:109:A:GLU:HB3	20	0.16
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD23	7	0.16
(1,4304)	1:86:A:ASP:HB2	1:89:A:ALA:HB2	14	0.16
(1,4179)	2:288:B:LEU:HG	2:288:B:LEU:H	10	0.16
(1,4055)	2:175:B:ILE:HG22	2:180:B:GLN:H	7	0.16
(1,4024)	2:323:B:VAL:HG11	2:320:B:ARG:HA	8	0.16
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	3	0.16
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	9	0.16
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	3	0.16
(1,3961)	2:210:B:LYS:HG3	2:210:B:LYS:HD2	17	0.16
(1,3961)	2:282:B:LYS:HG2	2:282:B:LYS:HD3	20	0.16
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	3	0.16
(1,3959)	2:210:B:LYS:HD2	2:210:B:LYS:HG3	17	0.16
(1,3956)	2:282:B:LYS:HE2	2:282:B:LYS:HA	10	0.16
(1,3776)	2:257:B:VAL:HG23	2:185:B:PRO:HB3	12	0.16
(1,3768)	2:235:B:TYR:HE1	2:176:B:THR:HG21	2	0.16
(1,3730)	2:267:B:PHE:HB3	2:158:B:VAL:HG11	18	0.16
(1,3541)	2:200:B:TYR:HE1	2:204:B:ARG:HD3	12	0.16
(1,3541)	2:200:B:TYR:HE2	2:204:B:ARG:HD3	12	0.16
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD21	13	0.16
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD22	13	0.16
(1,3522)	2:292:B:HIS:HD2	2:295:B:LEU:HD23	13	0.16
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	5	0.16
(1,3419)	2:236:B:LYS:HD2	1:104:A:ASN:HD22	12	0.16
(1,3399)	1:117:A:GLU:HB2	1:118:A:GLY:H	14	0.16
(1,3380)	1:116:A:ARG:HG3	1:116:A:ARG:H	16	0.16
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	2	0.16
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	17	0.16
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	19	0.16
(1,3172)	1:88:A:GLN:HB2	1:88:A:GLN:HE21	1	0.16
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD11	6	0.16
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD12	6	0.16
(1,3068)	1:87:A:MET:HB2	1:90:A:LEU:HD13	6	0.16
(1,2979)	1:114:A:GLU:HA	1:114:A:GLU:HG2	13	0.16
(1,2902)	1:112:A:ILE:HD11	1:109:A:GLU:HG2	10	0.16
(1,2902)	1:112:A:ILE:HD12	1:109:A:GLU:HG2	10	0.16
(1,2902)	1:112:A:ILE:HD13	1:109:A:GLU:HG2	10	0.16
(1,2847)	1:107:A:LEU:HA	1:107:A:LEU:HD11	8	0.16
(1,2847)	1:107:A:LEU:HA	1:107:A:LEU:HD12	8	0.16
(1,2847)	1:107:A:LEU:HA	1:107:A:LEU:HD13	8	0.16
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	7	0.16
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	7	0.16
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	7	0.16
(1,2775)	1:96:A:LEU:HD21	1:100:A:ASN:HB3	20	0.16
(1,2775)	1:96:A:LEU:HD22	1:100:A:ASN:HB3	20	0.16
(1,2775)	1:96:A:LEU:HD23	1:100:A:ASN:HB3	20	0.16
(1,2770)	1:98:A:PHE:HD1	1:100:A:ASN:HA	12	0.16
(1,2770)	1:98:A:PHE:HD2	1:100:A:ASN:HA	12	0.16
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	8	0.16
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	8	0.16
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	8	0.16
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	8	0.16
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	8	0.16
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	8	0.16
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	8	0.16
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	8	0.16
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	8	0.16
(1,2593)	2:212:B:TYR:HD1	1:84:A:MET:HB2	1	0.16
(1,2593)	2:212:B:TYR:HD2	1:84:A:MET:HB2	1	0.16
(1,2561)	1:84:A:MET:HE1	1:81:A:LEU:HA	9	0.16
(1,2561)	1:84:A:MET:HE2	1:81:A:LEU:HA	9	0.16
(1,2561)	1:84:A:MET:HE3	1:81:A:LEU:HA	9	0.16
(1,2246)	2:295:B:LEU:HG	2:295:B:LEU:H	13	0.16
(1,2158)	2:281:B:GLU:HB2	2:282:B:LYS:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2147)	2:280:B:ASP:HB3	2:281:B:GLU:H	18	0.16
(1,2138)	2:279:B:LEU:HB3	2:279:B:LEU:H	10	0.16
(1,1985)	2:251:B:ASP:HB2	2:251:B:ASP:H	18	0.16
(1,1906)	2:234:B:LEU:HD21	2:242:B:TYR:H	20	0.16
(1,1906)	2:234:B:LEU:HD22	2:242:B:TYR:H	20	0.16
(1,1906)	2:234:B:LEU:HD23	2:242:B:TYR:H	20	0.16
(1,1904)	2:241:B:GLN:HG2	2:241:B:GLN:H	16	0.16
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	10	0.16
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	10	0.16
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	10	0.16
(1,1306)	2:155:B:GLU:HB3	2:156:B:VAL:H	3	0.16
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD11	2	0.16
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD12	2	0.16
(1,1285)	2:295:B:LEU:HD21	2:264:B:LEU:HD13	2	0.16
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD11	2	0.16
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD12	2	0.16
(1,1285)	2:295:B:LEU:HD22	2:264:B:LEU:HD13	2	0.16
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD11	2	0.16
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD12	2	0.16
(1,1285)	2:295:B:LEU:HD23	2:264:B:LEU:HD13	2	0.16
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	16	0.16
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	8	0.16
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	10	0.16
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB1	1	0.16
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB2	1	0.16
(1,1177)	2:181:B:LEU:HD21	2:314:B:ALA:HB3	1	0.16
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB1	1	0.16
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB2	1	0.16
(1,1177)	2:181:B:LEU:HD22	2:314:B:ALA:HB3	1	0.16
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB1	1	0.16
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB2	1	0.16
(1,1177)	2:181:B:LEU:HD23	2:314:B:ALA:HB3	1	0.16
(1,1119)	2:305:B:LEU:HD21	2:301:B:ASN:HB3	14	0.16
(1,1119)	2:305:B:LEU:HD22	2:301:B:ASN:HB3	14	0.16
(1,1119)	2:305:B:LEU:HD23	2:301:B:ASN:HB3	14	0.16
(1,960)	2:279:B:LEU:HD11	2:279:B:LEU:HA	7	0.16
(1,960)	2:279:B:LEU:HD12	2:279:B:LEU:HA	7	0.16
(1,960)	2:279:B:LEU:HD13	2:279:B:LEU:HA	7	0.16
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE1	15	0.16
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE2	15	0.16
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE3	15	0.16
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD21	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD22	10	0.16
(1,639)	2:239:B:ARG:HA	2:234:B:LEU:HD23	10	0.16
(1,618)	2:225:B:PHE:HD1	2:233:B:LEU:HD21	14	0.16
(1,618)	2:225:B:PHE:HD1	2:233:B:LEU:HD22	14	0.16
(1,618)	2:225:B:PHE:HD1	2:233:B:LEU:HD23	14	0.16
(1,618)	2:225:B:PHE:HD2	2:233:B:LEU:HD21	14	0.16
(1,618)	2:225:B:PHE:HD2	2:233:B:LEU:HD22	14	0.16
(1,618)	2:225:B:PHE:HD2	2:233:B:LEU:HD23	14	0.16
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE1	3	0.16
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE2	3	0.16
(1,569)	2:273:B:MET:HG2	2:228:B:MET:HE3	3	0.16
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE1	17	0.16
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE2	17	0.16
(1,566)	2:233:B:LEU:HD21	2:228:B:MET:HE3	17	0.16
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE1	17	0.16
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE2	17	0.16
(1,566)	2:233:B:LEU:HD22	2:228:B:MET:HE3	17	0.16
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE1	17	0.16
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE2	17	0.16
(1,566)	2:233:B:LEU:HD23	2:228:B:MET:HE3	17	0.16
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG11	1	0.16
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG12	1	0.16
(1,504)	2:194:B:LEU:HB3	2:218:B:VAL:HG13	1	0.16
(1,386)	2:195:B:GLU:HA	2:195:B:GLU:HG3	5	0.16
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	1	0.16
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD21	7	0.16
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD22	7	0.16
(1,157)	2:308:B:ALA:HA	2:174:B:LEU:HD23	7	0.16
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	9	0.16
(1,40)	2:159:B:LYS:HB2	2:159:B:LYS:HG2	12	0.16
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	11	0.16
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	15	0.16
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	11	0.16
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	6	0.16
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	1	0.15
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	1	0.15
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	1	0.15
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	1	0.15
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	1	0.15
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	1	0.15
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	1	0.15
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	1	0.15
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	1	0.15
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	1	0.15
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	1	0.15
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD11	7	0.15
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD12	7	0.15
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD13	7	0.15
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD21	7	0.15
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD22	7	0.15
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD23	7	0.15
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD11	7	0.15
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD12	7	0.15
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD13	7	0.15
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD21	7	0.15
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD22	7	0.15
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD23	7	0.15
(2,42)	1:78:A:TRP:HD1	1:81:A:LEU:HB2	9	0.15
(2,42)	1:78:A:TRP:HD1	1:81:A:LEU:HB3	9	0.15
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	17	0.15
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	17	0.15
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	17	0.15
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	17	0.15
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	17	0.15
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	17	0.15
(1,4624)	2:267:B:PHE:HE1	2:221:B:ILE:HG21	11	0.15
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD12	15	0.15
(1,4573)	2:249:B:HIS:HD2	2:245:B:ILE:HG22	17	0.15
(1,4564)	2:197:B:TYR:HE2	2:198:B:ALA:HB2	6	0.15
(1,4548)	2:200:B:TYR:HE2	2:201:B:LYS:HD2	17	0.15
(1,4527)	2:242:B:TYR:HE2	2:243:B:ALA:HB1	15	0.15
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG23	7	0.15
(1,4511)	2:182:B:PHE:HD1	2:175:B:ILE:HD12	6	0.15
(1,4493)	1:90:A:LEU:HD12	1:90:A:LEU:H	12	0.15
(1,4460)	1:86:A:ASP:HB2	1:87:A:MET:H	9	0.15
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	11	0.15
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	19	0.15
(1,4447)	2:232:B:GLN:HG3	1:103:A:ARG:HG2	9	0.15
(1,4418)	2:169:B:VAL:HG22	1:112:A:ILE:HG23	5	0.15
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	16	0.15
(1,4362)	1:73:A:PRO:HB3	1:76:A:VAL:HG23	5	0.15
(1,4340)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	18	0.15
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4208)	2:305:B:LEU:HG	2:305:B:LEU:H	13	0.15
(1,4173)	2:281:B:GLU:HA	2:285:B:ALA:H	17	0.15
(1,4009)	2:180:B:GLN:HG3	2:313:B:VAL:HG12	15	0.15
(1,3998)	2:187:B:LYS:HG2	2:187:B:LYS:HD3	15	0.15
(1,3953)	2:281:B:GLU:HB3	2:281:B:GLU:HG2	6	0.15
(1,3953)	2:317:B:GLU:HB3	2:317:B:GLU:HG2	15	0.15
(1,3936)	2:268:B:VAL:HG23	2:269:B:ARG:HD2	1	0.15
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD21	4	0.15
(1,3912)	2:185:B:PRO:HB3	2:257:B:VAL:HG23	10	0.15
(1,3745)	2:302:B:SER:HA	2:164:B:LEU:HD23	12	0.15
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG2	2	0.15
(1,3724)	2:271:B:GLY:HA3	2:156:B:VAL:HG12	2	0.15
(1,3541)	2:200:B:TYR:HE1	2:204:B:ARG:HD2	2	0.15
(1,3541)	2:200:B:TYR:HE2	2:204:B:ARG:HD2	2	0.15
(1,3440)	2:231:B:THR:HG21	1:100:A:ASN:HD21	16	0.15
(1,3440)	2:231:B:THR:HG22	1:100:A:ASN:HD21	16	0.15
(1,3440)	2:231:B:THR:HG23	1:100:A:ASN:HD21	16	0.15
(1,3380)	1:116:A:ARG:HG3	1:116:A:ARG:H	14	0.15
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	5	0.15
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	9	0.15
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	16	0.15
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	3	0.15
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	8	0.15
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	12	0.15
(1,3170)	1:88:A:GLN:HB3	1:88:A:GLN:HE21	19	0.15
(1,3060)	1:79:A:ASP:HB2	1:76:A:VAL:HG11	10	0.15
(1,3060)	1:79:A:ASP:HB2	1:76:A:VAL:HG12	10	0.15
(1,3060)	1:79:A:ASP:HB2	1:76:A:VAL:HG13	10	0.15
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD11	10	0.15
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD12	10	0.15
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD13	10	0.15
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD11	10	0.15
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD12	10	0.15
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD13	10	0.15
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD11	14	0.15
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD12	14	0.15
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD13	14	0.15
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD11	14	0.15
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD12	14	0.15
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD13	14	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG21	1	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG22	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG23	1	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG21	8	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG22	8	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG23	8	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG21	11	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG22	11	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG23	11	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG21	16	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG22	16	0.15
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG23	16	0.15
(1,2812)	1:106:A:VAL:HG11	1:104:A:ASN:HB2	2	0.15
(1,2812)	1:106:A:VAL:HG12	1:104:A:ASN:HB2	2	0.15
(1,2812)	1:106:A:VAL:HG13	1:104:A:ASN:HB2	2	0.15
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	13	0.15
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	13	0.15
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	13	0.15
(1,2721)	1:97:A:PRO:HD2	1:96:A:LEU:HA	7	0.15
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	10	0.15
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	10	0.15
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	10	0.15
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	10	0.15
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	10	0.15
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	10	0.15
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	9	0.15
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	9	0.15
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	9	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	9	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	9	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	9	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	9	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	9	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	9	0.15
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	12	0.15
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	12	0.15
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	12	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	12	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	12	0.15
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	12	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	12	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	12	0.15
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	12	0.15
(1,2623)	1:90:A:LEU:HD11	1:87:A:MET:HA	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:90:A:LEU:HD12	1:87:A:MET:HA	6	0.15
(1,2623)	1:90:A:LEU:HD13	1:87:A:MET:HA	6	0.15
(1,2623)	1:90:A:LEU:HD11	1:87:A:MET:HA	7	0.15
(1,2623)	1:90:A:LEU:HD12	1:87:A:MET:HA	7	0.15
(1,2623)	1:90:A:LEU:HD13	1:87:A:MET:HA	7	0.15
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	9	0.15
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	9	0.15
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	9	0.15
(1,2581)	1:86:A:ASP:HB3	1:83:A:THR:HA	9	0.15
(1,2514)	1:78:A:TRP:HD1	1:75:A:LYS:HD2	17	0.15
(1,2246)	2:295:B:LEU:HG	2:295:B:LEU:H	12	0.15
(1,2246)	2:295:B:LEU:HG	2:295:B:LEU:H	16	0.15
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	11	0.15
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	11	0.15
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	11	0.15
(1,2147)	2:280:B:ASP:HB3	2:281:B:GLU:H	4	0.15
(1,1985)	2:251:B:ASP:HB2	2:251:B:ASP:H	14	0.15
(1,1703)	2:211:B:GLU:HG2	2:212:B:TYR:H	18	0.15
(1,1460)	2:174:B:LEU:HD11	2:180:B:GLN:HE21	9	0.15
(1,1460)	2:174:B:LEU:HD12	2:180:B:GLN:HE21	9	0.15
(1,1460)	2:174:B:LEU:HD13	2:180:B:GLN:HE21	9	0.15
(1,1270)	2:193:B:ILE:HD11	2:188:B:LYS:HE3	2	0.15
(1,1270)	2:193:B:ILE:HD12	2:188:B:LYS:HE3	2	0.15
(1,1270)	2:193:B:ILE:HD13	2:188:B:LYS:HE3	2	0.15
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	1	0.15
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	11	0.15
(1,1115)	2:297:B:TYR:HA	2:300:B:LYS:HD3	12	0.15
(1,1061)	2:296:B:LYS:HE3	2:294:B:PHE:HA	20	0.15
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE1	2	0.15
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE2	2	0.15
(1,932)	2:228:B:MET:HG2	2:273:B:MET:HE3	2	0.15
(1,714)	2:246:B:LEU:HD21	2:245:B:ILE:HB	20	0.15
(1,714)	2:246:B:LEU:HD22	2:245:B:ILE:HB	20	0.15
(1,714)	2:246:B:LEU:HD23	2:245:B:ILE:HB	20	0.15
(1,696)	2:246:B:LEU:HD11	2:243:B:ALA:HA	20	0.15
(1,696)	2:246:B:LEU:HD12	2:243:B:ALA:HA	20	0.15
(1,696)	2:246:B:LEU:HD13	2:243:B:ALA:HA	20	0.15
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD21	15	0.15
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD22	15	0.15
(1,641)	2:242:B:TYR:HB2	2:234:B:LEU:HD23	15	0.15
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD21	9	0.15
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD22	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	2:234:B:LEU:HD11	2:229:B:LEU:HD23	9	0.15
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD21	9	0.15
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD22	9	0.15
(1,587)	2:234:B:LEU:HD12	2:229:B:LEU:HD23	9	0.15
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD21	9	0.15
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD22	9	0.15
(1,587)	2:234:B:LEU:HD13	2:229:B:LEU:HD23	9	0.15
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	10	0.15
(1,507)	2:197:B:TYR:HE1	2:218:B:VAL:HG11	4	0.15
(1,507)	2:197:B:TYR:HE1	2:218:B:VAL:HG12	4	0.15
(1,507)	2:197:B:TYR:HE1	2:218:B:VAL:HG13	4	0.15
(1,507)	2:197:B:TYR:HE2	2:218:B:VAL:HG11	4	0.15
(1,507)	2:197:B:TYR:HE2	2:218:B:VAL:HG12	4	0.15
(1,507)	2:197:B:TYR:HE2	2:218:B:VAL:HG13	4	0.15
(1,453)	2:211:B:GLU:HG3	2:211:B:GLU:HB2	13	0.15
(1,453)	2:211:B:GLU:HG3	2:211:B:GLU:HB2	15	0.15
(1,453)	2:211:B:GLU:HG3	2:211:B:GLU:HB2	17	0.15
(1,453)	2:211:B:GLU:HG3	2:211:B:GLU:HB2	19	0.15
(1,453)	2:211:B:GLU:HG3	2:211:B:GLU:HB2	20	0.15
(1,384)	2:195:B:GLU:HG3	2:195:B:GLU:HB2	20	0.15
(1,342)	2:188:B:LYS:HG2	2:192:B:SER:HB2	10	0.15
(1,298)	2:192:B:SER:HB2	2:188:B:LYS:HD3	1	0.15
(1,284)	1:85:A:TYR:HE1	2:280:B:ASP:HB2	2	0.15
(1,284)	1:85:A:TYR:HE2	2:280:B:ASP:HB2	2	0.15
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD21	15	0.15
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD22	15	0.15
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD23	15	0.15
(1,64)	2:267:B:PHE:HB2	2:160:B:ILE:HD11	4	0.15
(1,64)	2:267:B:PHE:HB2	2:160:B:ILE:HD12	4	0.15
(1,64)	2:267:B:PHE:HB2	2:160:B:ILE:HD13	4	0.15
(1,40)	2:159:B:LYS:HD3	2:159:B:LYS:HG2	14	0.15
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	18	0.15
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	7	0.15
(3,13)	1:89:A:ALA:O	1:93:A:SER:H	8	0.14
(3,7)	1:80:A:HIS:O	1:84:A:MET:H	9	0.14
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	17	0.14
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	2	0.14
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	2	0.14
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	2	0.14
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	2	0.14
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	2	0.14
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	2	0.14
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	2	0.14
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	2	0.14
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	2	0.14
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	2	0.14
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	2	0.14
(2,256)	2:227:B:VAL:HG11	1:97:A:PRO:HA	9	0.14
(2,256)	2:227:B:VAL:HG12	1:97:A:PRO:HA	9	0.14
(2,256)	2:227:B:VAL:HG13	1:97:A:PRO:HA	9	0.14
(2,256)	2:227:B:VAL:HG21	1:97:A:PRO:HA	9	0.14
(2,256)	2:227:B:VAL:HG22	1:97:A:PRO:HA	9	0.14
(2,256)	2:227:B:VAL:HG23	1:97:A:PRO:HA	9	0.14
(2,45)	1:85:A:TYR:HD1	1:81:A:LEU:HG	19	0.14
(2,45)	1:85:A:TYR:HD2	1:81:A:LEU:HG	19	0.14
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	5	0.14
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	5	0.14
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	5	0.14
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	5	0.14
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	5	0.14
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	5	0.14
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD11	18	0.14
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD12	18	0.14
(2,22)	2:224:B:TYR:HD1	1:81:A:LEU:HD13	18	0.14
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD11	18	0.14
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD12	18	0.14
(2,22)	2:224:B:TYR:HD2	1:81:A:LEU:HD13	18	0.14
(1,4624)	2:267:B:PHE:HE1	2:221:B:ILE:HG21	8	0.14
(1,4624)	2:267:B:PHE:HE1	2:221:B:ILE:HG22	15	0.14
(1,4574)	2:242:B:TYR:HD1	2:246:B:LEU:HD11	7	0.14
(1,4571)	2:318:B:TYR:HE1	2:241:B:GLN:HA	13	0.14
(1,4554)	2:290:B:TYR:HD2	2:217:B:VAL:HG13	8	0.14
(1,4499)	2:306:B:PHE:HE1	2:298:B:LEU:HD21	8	0.14
(1,4492)	2:212:B:TYR:HE1	1:81:A:LEU:H	1	0.14
(1,4457)	1:82:A:SER:HA	1:85:A:TYR:H	8	0.14
(1,4436)	1:75:A:LYS:HD3	1:75:A:LYS:HG2	9	0.14
(1,4357)	2:273:B:MET:HE3	1:100:A:ASN:HA	18	0.14
(1,4326)	1:94:A:GLU:HG2	1:94:A:GLU:HB3	6	0.14
(1,4326)	1:92:A:GLU:HG3	1:92:A:GLU:HB3	7	0.14
(1,4326)	1:94:A:GLU:HG2	1:94:A:GLU:HB3	10	0.14
(1,4313)	1:73:A:PRO:HG3	1:96:A:LEU:HD12	20	0.14
(1,4291)	1:89:A:ALA:HB1	1:86:A:ASP:HA	20	0.14
(1,4237)	2:218:B:VAL:HG12	2:198:B:ALA:H	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4150)	2:263:B:LEU:HD22	2:263:B:LEU:H	6	0.14
(1,4105)	2:221:B:ILE:HG22	2:225:B:PHE:H	13	0.14
(1,4079)	2:201:B:LYS:HG2	2:198:B:ALA:H	18	0.14
(1,4030)	2:192:B:SER:HB3	2:188:B:LYS:HG2	9	0.14
(1,4030)	2:192:B:SER:HB3	2:188:B:LYS:HG2	12	0.14
(1,4009)	2:264:B:LEU:HB3	2:268:B:VAL:HG22	19	0.14
(1,3988)	2:263:B:LEU:HD13	2:298:B:LEU:HD11	4	0.14
(1,3965)	2:290:B:TYR:HE2	2:286:B:LEU:HG	12	0.14
(1,3956)	2:282:B:LYS:HE2	2:282:B:LYS:HA	19	0.14
(1,3953)	2:317:B:GLU:HB3	2:317:B:GLU:HG2	8	0.14
(1,3949)	2:302:B:SER:HB3	2:305:B:LEU:HD13	7	0.14
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG23	15	0.14
(1,3910)	2:257:B:VAL:HG23	2:256:B:GLN:HG2	5	0.14
(1,3866)	1:102:A:GLU:HA	2:231:B:THR:HG23	5	0.14
(1,3852)	2:218:B:VAL:HG23	2:202:B:LYS:HE3	11	0.14
(1,3832)	2:217:B:VAL:HG13	2:213:B:ALA:HB2	4	0.14
(1,3795)	2:194:B:LEU:HD22	2:190:B:VAL:HG12	3	0.14
(1,3746)	2:306:B:PHE:HE1	2:298:B:LEU:HD21	8	0.14
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	19	0.14
(1,3689)	2:318:B:TYR:HE1	2:241:B:GLN:HG2	18	0.14
(1,3689)	2:318:B:TYR:HE2	2:241:B:GLN:HG2	18	0.14
(1,3578)	2:249:B:HIS:HD2	2:245:B:ILE:HA	11	0.14
(1,3564)	2:235:B:TYR:HE1	2:235:B:TYR:HA	15	0.14
(1,3564)	2:235:B:TYR:HE2	2:235:B:TYR:HA	15	0.14
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	9	0.14
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	9	0.14
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB3	6	0.14
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	2	0.14
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	2	0.14
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	2	0.14
(1,3280)	1:105:A:PHE:HA	1:106:A:VAL:H	6	0.14
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	2	0.14
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	3	0.14
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	4	0.14
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	9	0.14
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	19	0.14
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	7	0.14
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	15	0.14
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	20	0.14
(1,3172)	1:88:A:GLN:HB2	1:88:A:GLN:HE21	8	0.14
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD11	6	0.14
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD12	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3072)	1:78:A:TRP:HD1	1:81:A:LEU:HD13	6	0.14
(1,2963)	1:110:A:GLU:HA	1:113:A:GLN:HG3	20	0.14
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	11	0.14
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	11	0.14
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	11	0.14
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	11	0.14
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	11	0.14
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	11	0.14
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	19	0.14
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	19	0.14
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	19	0.14
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	19	0.14
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	19	0.14
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	19	0.14
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB1	13	0.14
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB2	13	0.14
(1,2660)	1:92:A:GLU:HG3	1:89:A:ALA:HB3	13	0.14
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	3	0.14
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	3	0.14
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	3	0.14
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	3	0.14
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	3	0.14
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	3	0.14
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	3	0.14
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	3	0.14
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	3	0.14
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	7	0.14
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	7	0.14
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	7	0.14
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	10	0.14
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	10	0.14
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	10	0.14
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	12	0.14
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	12	0.14
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	12	0.14
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	13	0.14
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	13	0.14
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	13	0.14
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	20	0.14
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	20	0.14
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	20	0.14
(1,2501)	1:72:A:VAL:HG11	1:74:A:SER:HA	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2501)	1:72:A:VAL:HG12	1:74:A:SER:HA	19	0.14
(1,2501)	1:72:A:VAL:HG13	1:74:A:SER:HA	19	0.14
(1,2466)	1:72:A:VAL:HG11	1:71:A:GLN:HA	3	0.14
(1,2466)	1:72:A:VAL:HG12	1:71:A:GLN:HA	3	0.14
(1,2466)	1:72:A:VAL:HG13	1:71:A:GLN:HA	3	0.14
(1,2449)	2:183:B:TYR:HD1	2:183:B:TYR:H	7	0.14
(1,2449)	2:183:B:TYR:HD2	2:183:B:TYR:H	7	0.14
(1,2374)	2:312:B:GLU:HG2	2:312:B:GLU:H	7	0.14
(1,2272)	2:300:B:LYS:HB3	2:300:B:LYS:H	12	0.14
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	17	0.14
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	17	0.14
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	17	0.14
(1,2147)	2:280:B:ASP:HB3	2:281:B:GLU:H	6	0.14
(1,1985)	2:251:B:ASP:HB2	2:251:B:ASP:H	11	0.14
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	12	0.14
(1,1465)	2:174:B:LEU:HD11	2:180:B:GLN:HE22	5	0.14
(1,1465)	2:174:B:LEU:HD12	2:180:B:GLN:HE22	5	0.14
(1,1465)	2:174:B:LEU:HD13	2:180:B:GLN:HE22	5	0.14
(1,1299)	2:154:B:ALA:HA	2:155:B:GLU:H	2	0.14
(1,1299)	2:154:B:ALA:HA	2:155:B:GLU:H	4	0.14
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	4	0.14
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	17	0.14
(1,1115)	2:297:B:TYR:HA	2:300:B:LYS:HD3	4	0.14
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD23	19	0.14
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG11	12	0.14
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG12	12	0.14
(1,823)	2:254:B:MET:HE1	2:257:B:VAL:HG13	12	0.14
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG11	12	0.14
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG12	12	0.14
(1,823)	2:254:B:MET:HE2	2:257:B:VAL:HG13	12	0.14
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG11	12	0.14
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG12	12	0.14
(1,823)	2:254:B:MET:HE3	2:257:B:VAL:HG13	12	0.14
(1,682)	2:239:B:ARG:HA	2:239:B:ARG:HG2	5	0.14
(1,622)	2:266:B:LEU:HB3	2:233:B:LEU:HD21	8	0.14
(1,622)	2:266:B:LEU:HB3	2:233:B:LEU:HD22	8	0.14
(1,622)	2:266:B:LEU:HB3	2:233:B:LEU:HD23	8	0.14
(1,437)	2:201:B:LYS:HA	2:204:B:ARG:HG3	8	0.14
(1,386)	2:195:B:GLU:HA	2:195:B:GLU:HG3	2	0.14
(1,45)	2:159:B:LYS:HA	2:159:B:LYS:HD3	17	0.14
(1,40)	2:159:B:LYS:HD3	2:159:B:LYS:HG2	10	0.14
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	15	0.14
(3,13)	1:89:A:ALA:O	1:93:A:SER:H	4	0.13
(3,11)	1:88:A:GLN:O	1:92:A:GLU:H	2	0.13
(3,8)	1:80:A:HIS:O	1:84:A:MET:N	9	0.13
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	11	0.13
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	15	0.13
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	20	0.13
(2,45)	1:85:A:TYR:HD1	1:81:A:LEU:HG	2	0.13
(2,45)	1:85:A:TYR:HD2	1:81:A:LEU:HG	2	0.13
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG21	13	0.13
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG22	13	0.13
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG23	13	0.13
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG21	13	0.13
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG22	13	0.13
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG23	13	0.13
(2,12)	2:288:B:LEU:HD21	2:157:B:LYS:H	10	0.13
(2,12)	2:288:B:LEU:HD22	2:157:B:LYS:H	10	0.13
(2,12)	2:288:B:LEU:HD23	2:157:B:LYS:H	10	0.13
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD21	14	0.13
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD22	14	0.13
(2,2)	2:258:B:TYR:HD1	2:184:B:LEU:HD23	14	0.13
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD21	14	0.13
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD22	14	0.13
(2,2)	2:258:B:TYR:HD2	2:184:B:LEU:HD23	14	0.13
(1,4624)	2:267:B:PHE:HE2	2:298:B:LEU:HD22	13	0.13
(1,4623)	2:306:B:PHE:HE2	2:305:B:LEU:HD12	16	0.13
(1,4603)	2:224:B:TYR:HD1	2:266:B:LEU:HD11	1	0.13
(1,4565)	2:262:B:HIS:HD2	2:234:B:LEU:HG	14	0.13
(1,4565)	2:262:B:HIS:HD2	2:234:B:LEU:HG	19	0.13
(1,4565)	2:183:B:TYR:HE1	2:184:B:LEU:HG	20	0.13
(1,4564)	2:197:B:TYR:HE2	2:198:B:ALA:HB1	7	0.13
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	16	0.13
(1,4518)	2:172:B:TRP:HD1	2:176:B:THR:HG22	15	0.13
(1,4490)	1:116:A:ARG:HG2	1:115:A:VAL:H	9	0.13
(1,4472)	1:93:A:SER:HB2	1:95:A:ILE:H	14	0.13
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	16	0.13
(1,4457)	1:84:A:MET:HA	1:85:A:TYR:H	4	0.13
(1,4435)	1:119:A:LYS:HE2	1:119:A:LYS:HA	18	0.13
(1,4429)	1:75:A:LYS:HB3	1:76:A:VAL:HG11	2	0.13
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	11	0.13
(1,4407)	1:114:A:GLU:HG3	1:111:A:ILE:HG21	11	0.13
(1,4384)	1:106:A:VAL:HG12	1:109:A:GLU:HA	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4376)	1:112:A:ILE:HG13	1:108:A:PRO:HA	8	0.13
(1,4363)	2:235:B:TYR:HD1	1:106:A:VAL:HG22	9	0.13
(1,4344)	1:92:A:GLU:HB3	1:95:A:ILE:HD12	3	0.13
(1,4332)	1:93:A:SER:HA	1:94:A:GLU:HG3	6	0.13
(1,4331)	1:89:A:ALA:HA	1:92:A:GLU:HG3	4	0.13
(1,4326)	1:94:A:GLU:HG2	1:94:A:GLU:HB3	17	0.13
(1,4313)	1:87:A:MET:HE1	1:90:A:LEU:HD13	11	0.13
(1,4304)	1:86:A:ASP:HB2	1:89:A:ALA:HB1	4	0.13
(1,4027)	2:320:B:ARG:HA	2:323:B:VAL:HG23	17	0.13
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG11	8	0.13
(1,3953)	2:281:B:GLU:HB3	2:281:B:GLU:HG2	11	0.13
(1,3942)	2:274:B:LEU:HD23	2:270:B:ILE:HG23	8	0.13
(1,3930)	2:168:B:LEU:HD13	2:268:B:VAL:HG13	2	0.13
(1,3900)	2:185:B:PRO:HB2	2:252:B:ALA:HB1	6	0.13
(1,3894)	2:254:B:MET:HE1	2:245:B:ILE:HG21	13	0.13
(1,3851)	2:211:B:GLU:HA	2:202:B:LYS:HE2	4	0.13
(1,3810)	2:222:B:LYS:HB3	2:194:B:LEU:HD11	3	0.13
(1,3749)	2:160:B:ILE:HG23	2:165:B:LYS:HE3	13	0.13
(1,3740)	2:163:B:GLU:HB3	2:163:B:GLU:HG2	18	0.13
(1,3664)	2:183:B:TYR:HD1	2:312:B:GLU:HG2	15	0.13
(1,3664)	2:183:B:TYR:HD2	2:312:B:GLU:HG2	15	0.13
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	5	0.13
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	5	0.13
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	7	0.13
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	7	0.13
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	7	0.13
(1,3394)	1:117:A:GLU:HB3	1:117:A:GLU:H	14	0.13
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	3	0.13
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	3	0.13
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	3	0.13
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	18	0.13
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	18	0.13
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	18	0.13
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	19	0.13
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	19	0.13
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	19	0.13
(1,3221)	1:93:A:SER:HA	1:95:A:ILE:H	7	0.13
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	6	0.13
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	8	0.13
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	13	0.13
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	16	0.13
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	11	0.13
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	16	0.13
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE1	18	0.13
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE2	18	0.13
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE3	18	0.13
(1,2963)	1:110:A:GLU:HA	1:113:A:GLN:HG3	17	0.13
(1,2943)	1:107:A:LEU:HG	1:112:A:ILE:HG13	3	0.13
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD11	17	0.13
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD12	17	0.13
(1,2731)	2:224:B:TYR:HB2	1:96:A:LEU:HD13	17	0.13
(1,2684)	1:92:A:GLU:HG3	1:92:A:GLU:HA	4	0.13
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	8	0.13
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	8	0.13
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	8	0.13
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	8	0.13
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	8	0.13
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	8	0.13
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	16	0.13
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	16	0.13
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	16	0.13
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	16	0.13
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	16	0.13
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	16	0.13
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	11	0.13
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	11	0.13
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	11	0.13
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	11	0.13
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	11	0.13
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	11	0.13
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	11	0.13
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	11	0.13
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	11	0.13
(1,2581)	1:86:A:ASP:HB3	1:83:A:THR:HA	19	0.13
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG11	11	0.13
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG12	11	0.13
(1,2519)	1:73:A:PRO:HA	1:76:A:VAL:HG13	11	0.13
(1,2471)	1:72:A:VAL:HG21	1:71:A:GLN:HB3	16	0.13
(1,2471)	1:72:A:VAL:HG22	1:71:A:GLN:HB3	16	0.13
(1,2471)	1:72:A:VAL:HG23	1:71:A:GLN:HB3	16	0.13
(1,2261)	2:164:B:LEU:HD11	2:298:B:LEU:H	5	0.13
(1,2261)	2:164:B:LEU:HD12	2:298:B:LEU:H	5	0.13
(1,2261)	2:164:B:LEU:HD13	2:298:B:LEU:H	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2206)	2:286:B:LEU:HD11	2:289:B:ASN:HD22	1	0.13
(1,2206)	2:286:B:LEU:HD12	2:289:B:ASN:HD22	1	0.13
(1,2206)	2:286:B:LEU:HD13	2:289:B:ASN:HD22	1	0.13
(1,2147)	2:280:B:ASP:HB3	2:281:B:GLU:H	12	0.13
(1,2138)	2:279:B:LEU:HB3	2:279:B:LEU:H	1	0.13
(1,1703)	2:211:B:GLU:HG3	2:212:B:TYR:H	11	0.13
(1,1539)	2:188:B:LYS:HD3	2:189:B:ASN:H	18	0.13
(1,1505)	2:184:B:LEU:HD11	2:186:B:ALA:H	5	0.13
(1,1505)	2:184:B:LEU:HD12	2:186:B:ALA:H	5	0.13
(1,1505)	2:184:B:LEU:HD13	2:186:B:ALA:H	5	0.13
(1,1494)	2:183:B:TYR:HB2	2:183:B:TYR:H	14	0.13
(1,1337)	2:162:B:GLU:HB2	2:162:B:GLU:H	13	0.13
(1,1316)	2:157:B:LYS:HB3	2:157:B:LYS:H	7	0.13
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	16	0.13
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	20	0.13
(1,1228)	2:320:B:ARG:HG2	2:320:B:ARG:HA	14	0.13
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD22	7	0.13
(1,1008)	1:81:A:LEU:HD11	2:286:B:LEU:HD11	14	0.13
(1,1008)	1:81:A:LEU:HD11	2:286:B:LEU:HD12	14	0.13
(1,1008)	1:81:A:LEU:HD11	2:286:B:LEU:HD13	14	0.13
(1,1008)	1:81:A:LEU:HD12	2:286:B:LEU:HD11	14	0.13
(1,1008)	1:81:A:LEU:HD12	2:286:B:LEU:HD12	14	0.13
(1,1008)	1:81:A:LEU:HD12	2:286:B:LEU:HD13	14	0.13
(1,1008)	1:81:A:LEU:HD13	2:286:B:LEU:HD11	14	0.13
(1,1008)	1:81:A:LEU:HD13	2:286:B:LEU:HD12	14	0.13
(1,1008)	1:81:A:LEU:HD13	2:286:B:LEU:HD13	14	0.13
(1,1003)	2:288:B:LEU:HD11	2:285:B:ALA:HA	3	0.13
(1,1003)	2:288:B:LEU:HD12	2:285:B:ALA:HA	3	0.13
(1,1003)	2:288:B:LEU:HD13	2:285:B:ALA:HA	3	0.13
(1,923)	2:155:B:GLU:HG3	2:272:B:ALA:HA	3	0.13
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	1	0.13
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	6	0.13
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	12	0.13
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG21	14	0.13
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG22	14	0.13
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG23	14	0.13
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG21	14	0.13
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG22	14	0.13
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG23	14	0.13
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG21	14	0.13
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG22	14	0.13
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG23	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	2:218:B:VAL:HB	2:215:B:ASN:HA	16	0.13
(1,453)	2:211:B:GLU:HG3	2:211:B:GLU:HB2	11	0.13
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	14	0.13
(1,437)	2:201:B:LYS:HA	2:204:B:ARG:HG2	10	0.13
(1,427)	2:204:B:ARG:HG2	2:204:B:ARG:HA	13	0.13
(1,386)	2:195:B:GLU:HA	2:195:B:GLU:HG3	7	0.13
(1,45)	2:159:B:LYS:HA	2:159:B:LYS:HD3	8	0.13
(1,39)	2:159:B:LYS:HB2	2:159:B:LYS:HG3	10	0.13
(1,37)	2:159:B:LYS:HA	2:159:B:LYS:HG3	5	0.13
(1,26)	2:157:B:LYS:HG2	2:157:B:LYS:HD3	18	0.13
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	9	0.13
(3,7)	1:80:A:HIS:O	1:84:A:MET:H	16	0.12
(3,2)	1:77:A:ILE:O	1:81:A:LEU:N	11	0.12
(3,2)	1:77:A:ILE:O	1:81:A:LEU:N	17	0.12
(2,50)	1:85:A:TYR:HE1	1:84:A:MET:HG2	3	0.12
(2,50)	1:85:A:TYR:HE1	1:84:A:MET:HG3	3	0.12
(2,50)	1:85:A:TYR:HE2	1:84:A:MET:HG2	3	0.12
(2,50)	1:85:A:TYR:HE2	1:84:A:MET:HG3	3	0.12
(2,45)	1:85:A:TYR:HD1	1:81:A:LEU:HG	5	0.12
(2,45)	1:85:A:TYR:HD2	1:81:A:LEU:HG	5	0.12
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG21	15	0.12
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG22	15	0.12
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG23	15	0.12
(1,4621)	2:267:B:PHE:HE2	2:221:B:ILE:HG12	1	0.12
(1,4599)	2:292:B:HIS:HD2	2:295:B:LEU:HG	8	0.12
(1,4589)	2:182:B:PHE:HD1	2:261:B:PRO:HD3	13	0.12
(1,4567)	2:306:B:PHE:HD2	2:305:B:LEU:HB2	19	0.12
(1,4560)	2:225:B:PHE:HD1	2:233:B:LEU:HD11	13	0.12
(1,4535)	2:262:B:HIS:HD2	2:238:B:GLU:HB2	6	0.12
(1,4493)	1:90:A:LEU:HD13	1:90:A:LEU:H	11	0.12
(1,4492)	2:212:B:TYR:HE2	1:81:A:LEU:H	6	0.12
(1,4483)	1:110:A:GLU:HB3	1:110:A:GLU:H	8	0.12
(1,4476)	1:92:A:GLU:HG3	1:90:A:LEU:H	13	0.12
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	1	0.12
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	8	0.12
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	9	0.12
(1,4438)	2:166:B:PRO:HA	1:111:A:ILE:HG23	16	0.12
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	7	0.12
(1,4413)	2:169:B:VAL:HG22	1:112:A:ILE:HB	9	0.12
(1,4405)	2:165:B:LYS:HB3	1:111:A:ILE:HG21	10	0.12
(1,4384)	2:169:B:VAL:HG21	1:109:A:GLU:HA	15	0.12
(1,4376)	1:112:A:ILE:HG13	1:108:A:PRO:HA	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD23	12	0.12
(1,4340)	1:92:A:GLU:HG2	1:92:A:GLU:HB2	1	0.12
(1,4340)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	7	0.12
(1,4340)	1:94:A:GLU:HG2	1:94:A:GLU:HB2	8	0.12
(1,4340)	1:94:A:GLU:HG2	1:94:A:GLU:HB2	15	0.12
(1,4340)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	17	0.12
(1,4333)	1:90:A:LEU:HD11	1:93:A:SER:HA	2	0.12
(1,4326)	1:94:A:GLU:HG2	1:94:A:GLU:HB3	12	0.12
(1,4326)	1:94:A:GLU:HG3	1:94:A:GLU:HB3	15	0.12
(1,4324)	1:95:A:ILE:HG22	1:91:A:HIS:HB2	7	0.12
(1,4304)	1:86:A:ASP:HB2	1:89:A:ALA:HB1	5	0.12
(1,4304)	1:86:A:ASP:HB2	1:89:A:ALA:HB3	11	0.12
(1,4303)	1:71:A:GLN:HB3	1:71:A:GLN:HG2	6	0.12
(1,4274)	2:287:B:LEU:HA	1:81:A:LEU:HD11	5	0.12
(1,4208)	2:305:B:LEU:HG	2:305:B:LEU:H	16	0.12
(1,4087)	2:202:B:LYS:HG2	2:202:B:LYS:H	1	0.12
(1,4063)	2:186:B:ALA:HB2	2:188:B:LYS:H	2	0.12
(1,4009)	2:180:B:GLN:HG3	2:313:B:VAL:HG12	12	0.12
(1,4008)	2:180:B:GLN:HB3	2:313:B:VAL:HG12	17	0.12
(1,3990)	2:263:B:LEU:HD12	2:298:B:LEU:HD21	15	0.12
(1,3956)	2:282:B:LYS:HE2	2:282:B:LYS:HA	15	0.12
(1,3953)	2:281:B:GLU:HB3	2:281:B:GLU:HG2	2	0.12
(1,3953)	2:281:B:GLU:HB3	2:281:B:GLU:HG2	5	0.12
(1,3842)	2:214:B:VAL:HG21	2:207:B:THR:HG23	4	0.12
(1,3766)	2:235:B:TYR:HD2	2:175:B:ILE:HD13	5	0.12
(1,3752)	2:160:B:ILE:HG22	2:165:B:LYS:HG3	19	0.12
(1,3732)	2:168:B:LEU:HD12	2:160:B:ILE:HD11	8	0.12
(1,3730)	2:267:B:PHE:HB3	2:158:B:VAL:HG13	20	0.12
(1,3564)	2:235:B:TYR:HE1	2:235:B:TYR:HA	17	0.12
(1,3564)	2:235:B:TYR:HE2	2:235:B:TYR:HA	17	0.12
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	1	0.12
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	1	0.12
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	18	0.12
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	18	0.12
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	20	0.12
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	20	0.12
(1,3455)	2:292:B:HIS:HD2	2:159:B:LYS:HB2	7	0.12
(1,3395)	1:117:A:GLU:HG3	1:117:A:GLU:H	18	0.12
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	6	0.12
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	6	0.12
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	6	0.12
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	8	0.12
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	8	0.12
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	9	0.12
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	9	0.12
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	9	0.12
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	11	0.12
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	11	0.12
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	11	0.12
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	12	0.12
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	12	0.12
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	12	0.12
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	13	0.12
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	13	0.12
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	13	0.12
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	15	0.12
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	15	0.12
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	15	0.12
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	7	0.12
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	14	0.12
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	15	0.12
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	18	0.12
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	20	0.12
(1,3076)	1:116:A:ARG:HG2	1:113:A:GLN:HA	20	0.12
(1,3019)	1:117:A:GLU:HG2	1:117:A:GLU:HA	14	0.12
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG21	20	0.12
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG22	20	0.12
(1,2995)	1:116:A:ARG:HA	1:115:A:VAL:HG23	20	0.12
(1,2900)	1:112:A:ILE:HD11	1:109:A:GLU:HB3	13	0.12
(1,2900)	1:112:A:ILE:HD12	1:109:A:GLU:HB3	13	0.12
(1,2900)	1:112:A:ILE:HD13	1:109:A:GLU:HB3	13	0.12
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	1	0.12
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	1	0.12
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	1	0.12
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	1	0.12
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	1	0.12
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	1	0.12
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	1	0.12
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	1	0.12
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	1	0.12
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB1	15	0.12
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB2	15	0.12
(1,2658)	1:90:A:LEU:HD11	1:89:A:ALA:HB3	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB1	15	0.12
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB2	15	0.12
(1,2658)	1:90:A:LEU:HD12	1:89:A:ALA:HB3	15	0.12
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB1	15	0.12
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB2	15	0.12
(1,2658)	1:90:A:LEU:HD13	1:89:A:ALA:HB3	15	0.12
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE1	2	0.12
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE2	2	0.12
(1,2628)	1:83:A:THR:HG21	1:87:A:MET:HE3	2	0.12
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE1	2	0.12
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE2	2	0.12
(1,2628)	1:83:A:THR:HG22	1:87:A:MET:HE3	2	0.12
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE1	2	0.12
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE2	2	0.12
(1,2628)	1:83:A:THR:HG23	1:87:A:MET:HE3	2	0.12
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	3	0.12
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	3	0.12
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	3	0.12
(1,2246)	2:295:B:LEU:HG	2:295:B:LEU:H	9	0.12
(1,2169)	2:282:B:LYS:HB2	2:283:B:SER:H	9	0.12
(1,2160)	2:282:B:LYS:HB3	2:282:B:LYS:H	3	0.12
(1,1985)	2:251:B:ASP:HB2	2:251:B:ASP:H	8	0.12
(1,1967)	2:248:B:ASP:HB2	2:249:B:HIS:H	16	0.12
(1,1904)	2:241:B:GLN:HG2	2:241:B:GLN:H	14	0.12
(1,1844)	2:232:B:GLN:HG2	2:232:B:GLN:H	14	0.12
(1,1514)	2:257:B:VAL:HG21	2:186:B:ALA:H	12	0.12
(1,1514)	2:257:B:VAL:HG22	2:186:B:ALA:H	12	0.12
(1,1514)	2:257:B:VAL:HG23	2:186:B:ALA:H	12	0.12
(1,1323)	2:158:B:VAL:HG11	2:158:B:VAL:H	10	0.12
(1,1323)	2:158:B:VAL:HG12	2:158:B:VAL:H	10	0.12
(1,1323)	2:158:B:VAL:HG13	2:158:B:VAL:H	10	0.12
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	12	0.12
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	3	0.12
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG2	9	0.12
(1,1234)	2:320:B:ARG:HB3	2:320:B:ARG:HG3	18	0.12
(1,1115)	2:297:B:TYR:HA	2:300:B:LYS:HD3	13	0.12
(1,1038)	2:291:B:LEU:HD21	2:291:B:LEU:HA	9	0.12
(1,1038)	2:291:B:LEU:HD22	2:291:B:LEU:HA	9	0.12
(1,1038)	2:291:B:LEU:HD23	2:291:B:LEU:HA	9	0.12
(1,978)	2:282:B:LYS:HD3	2:282:B:LYS:HB3	9	0.12
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	17	0.12
(1,833)	2:189:B:ASN:HA	2:259:B:GLY:HA2	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG21	6	0.12
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG22	6	0.12
(1,827)	2:185:B:PRO:HB2	2:257:B:VAL:HG23	6	0.12
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD11	15	0.12
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD12	15	0.12
(1,721)	2:184:B:LEU:HD21	2:245:B:ILE:HD13	15	0.12
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD11	15	0.12
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD12	15	0.12
(1,721)	2:184:B:LEU:HD22	2:245:B:ILE:HD13	15	0.12
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD11	15	0.12
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD12	15	0.12
(1,721)	2:184:B:LEU:HD23	2:245:B:ILE:HD13	15	0.12
(1,664)	2:239:B:ARG:HA	2:239:B:ARG:HD3	12	0.12
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG21	14	0.12
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG22	14	0.12
(1,534)	2:190:B:VAL:HG11	2:221:B:ILE:HG23	14	0.12
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG21	14	0.12
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG22	14	0.12
(1,534)	2:190:B:VAL:HG12	2:221:B:ILE:HG23	14	0.12
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG21	14	0.12
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG22	14	0.12
(1,534)	2:190:B:VAL:HG13	2:221:B:ILE:HG23	14	0.12
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	4	0.12
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	5	0.12
(1,427)	2:204:B:ARG:HG3	2:204:B:ARG:HA	10	0.12
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB1	10	0.12
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB2	10	0.12
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB3	10	0.12
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB1	10	0.12
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB2	10	0.12
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB3	10	0.12
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB1	10	0.12
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB2	10	0.12
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB3	10	0.12
(1,338)	2:263:B:LEU:HD21	2:190:B:VAL:HG21	14	0.12
(1,338)	2:263:B:LEU:HD21	2:190:B:VAL:HG22	14	0.12
(1,338)	2:263:B:LEU:HD21	2:190:B:VAL:HG23	14	0.12
(1,338)	2:263:B:LEU:HD22	2:190:B:VAL:HG21	14	0.12
(1,338)	2:263:B:LEU:HD22	2:190:B:VAL:HG22	14	0.12
(1,338)	2:263:B:LEU:HD22	2:190:B:VAL:HG23	14	0.12
(1,338)	2:263:B:LEU:HD23	2:190:B:VAL:HG21	14	0.12
(1,338)	2:263:B:LEU:HD23	2:190:B:VAL:HG22	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	2:263:B:LEU:HD23	2:190:B:VAL:HG23	14	0.12
(1,306)	2:192:B:SER:HB3	2:188:B:LYS:HE3	4	0.12
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD21	1	0.12
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD22	1	0.12
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD23	1	0.12
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	4	0.12
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	20	0.12
(1,39)	2:159:B:LYS:HD2	2:159:B:LYS:HG3	9	0.12
(3,121)	2:296:B:LYS:O	2:300:B:LYS:H	17	0.11
(3,77)	2:223:B:GLU:O	2:227:B:VAL:H	13	0.11
(3,75)	2:222:B:LYS:O	2:226:B:ASN:H	5	0.11
(3,35)	2:171:B:ASP:O	2:175:B:ILE:H	6	0.11
(3,17)	1:110:A:GLU:O	1:114:A:GLU:H	5	0.11
(3,13)	1:89:A:ALA:O	1:93:A:SER:H	11	0.11
(3,13)	1:89:A:ALA:O	1:93:A:SER:H	16	0.11
(3,9)	1:87:A:MET:O	1:91:A:HIS:H	16	0.11
(3,7)	1:80:A:HIS:O	1:84:A:MET:H	5	0.11
(3,7)	1:80:A:HIS:O	1:84:A:MET:H	13	0.11
(3,3)	1:78:A:TRP:O	1:82:A:SER:H	6	0.11
(3,2)	1:77:A:ILE:O	1:81:A:LEU:N	15	0.11
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	1	0.11
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	4	0.11
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	5	0.11
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	8	0.11
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	14	0.11
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	18	0.11
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	13	0.11
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	13	0.11
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	13	0.11
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	13	0.11
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	13	0.11
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	13	0.11
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	13	0.11
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	13	0.11
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	13	0.11
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	13	0.11
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	13	0.11
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	13	0.11
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	16	0.11
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	16	0.11
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	16	0.11
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	16	0.11
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	16	0.11
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	16	0.11
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	16	0.11
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	16	0.11
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	16	0.11
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	16	0.11
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	16	0.11
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	18	0.11
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	18	0.11
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	18	0.11
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	18	0.11
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	18	0.11
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	18	0.11
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	18	0.11
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	18	0.11
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	18	0.11
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	18	0.11
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	18	0.11
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	18	0.11
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG2	20	0.11
(2,258)	2:227:B:VAL:HG11	1:97:A:PRO:HG3	20	0.11
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG2	20	0.11
(2,258)	2:227:B:VAL:HG12	1:97:A:PRO:HG3	20	0.11
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG2	20	0.11
(2,258)	2:227:B:VAL:HG13	1:97:A:PRO:HG3	20	0.11
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG2	20	0.11
(2,258)	2:227:B:VAL:HG21	1:97:A:PRO:HG3	20	0.11
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG2	20	0.11
(2,258)	2:227:B:VAL:HG22	1:97:A:PRO:HG3	20	0.11
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG2	20	0.11
(2,258)	2:227:B:VAL:HG23	1:97:A:PRO:HG3	20	0.11
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD11	12	0.11
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD12	12	0.11
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD13	12	0.11
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD21	12	0.11
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD22	12	0.11
(2,53)	1:85:A:TYR:HE1	1:81:A:LEU:HD23	12	0.11
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD11	12	0.11
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD12	12	0.11
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD13	12	0.11
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD21	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD22	12	0.11
(2,53)	1:85:A:TYR:HE2	1:81:A:LEU:HD23	12	0.11
(2,45)	1:85:A:TYR:HD1	1:81:A:LEU:HG	1	0.11
(2,45)	1:85:A:TYR:HD2	1:81:A:LEU:HG	1	0.11
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG21	18	0.11
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG22	18	0.11
(2,21)	2:224:B:TYR:HE1	1:77:A:ILE:HG23	18	0.11
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG21	18	0.11
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG22	18	0.11
(2,21)	2:224:B:TYR:HE2	1:77:A:ILE:HG23	18	0.11
(1,4644)	2:182:B:PHE:HD2	2:245:B:ILE:HD12	19	0.11
(1,4623)	2:306:B:PHE:HE1	2:298:B:LEU:HD11	19	0.11
(1,4597)	2:267:B:PHE:HE2	2:263:B:LEU:HG	10	0.11
(1,4566)	2:262:B:HIS:HD2	2:234:B:LEU:HD12	19	0.11
(1,4531)	2:182:B:PHE:HE1	2:186:B:ALA:HA	18	0.11
(1,4511)	2:182:B:PHE:HD2	2:181:B:LEU:HG	11	0.11
(1,4499)	2:306:B:PHE:HE2	2:298:B:LEU:HD21	11	0.11
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	15	0.11
(1,4458)	1:85:A:TYR:HA	1:86:A:ASP:H	18	0.11
(1,4451)	1:71:A:GLN:HA	1:72:A:VAL:H	2	0.11
(1,4451)	1:71:A:GLN:HA	1:72:A:VAL:H	17	0.11
(1,4450)	1:71:A:GLN:HB3	1:72:A:VAL:H	19	0.11
(1,4447)	2:232:B:GLN:HG2	1:103:A:ARG:HG2	12	0.11
(1,4424)	1:116:A:ARG:HG2	1:115:A:VAL:HG13	14	0.11
(1,4413)	2:169:B:VAL:HG22	1:112:A:ILE:HB	2	0.11
(1,4413)	2:169:B:VAL:HG23	1:112:A:ILE:HB	4	0.11
(1,4413)	2:169:B:VAL:HG22	1:112:A:ILE:HB	14	0.11
(1,4413)	2:169:B:VAL:HG21	1:112:A:ILE:HB	17	0.11
(1,4364)	1:111:A:ILE:HD11	1:107:A:LEU:HA	11	0.11
(1,4362)	2:223:B:GLU:HG3	1:76:A:VAL:HG22	7	0.11
(1,4340)	1:94:A:GLU:HG2	1:94:A:GLU:HB2	2	0.11
(1,4340)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	5	0.11
(1,4340)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	12	0.11
(1,4340)	1:94:A:GLU:HG2	1:94:A:GLU:HB2	14	0.11
(1,4340)	1:94:A:GLU:HG2	1:94:A:GLU:HB2	19	0.11
(1,4334)	1:95:A:ILE:HG22	1:74:A:SER:HB3	8	0.11
(1,4326)	1:94:A:GLU:HG2	1:94:A:GLU:HB3	1	0.11
(1,4326)	1:94:A:GLU:HG3	1:94:A:GLU:HB3	2	0.11
(1,4310)	1:85:A:TYR:HD2	1:90:A:LEU:HB3	5	0.11
(1,4303)	1:88:A:GLN:HB3	1:88:A:GLN:HG2	4	0.11
(1,4283)	1:82:A:SER:HA	1:84:A:MET:HE2	5	0.11
(1,4279)	1:88:A:GLN:HG3	1:90:A:LEU:HD22	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4198)	2:164:B:LEU:HD21	2:299:B:ALA:H	18	0.11
(1,4175)	2:284:B:LEU:HB3	2:285:B:ALA:H	11	0.11
(1,4175)	2:284:B:LEU:HB3	2:285:B:ALA:H	13	0.11
(1,4173)	2:281:B:GLU:HA	2:285:B:ALA:H	15	0.11
(1,4150)	2:263:B:LEU:HD22	2:263:B:LEU:H	13	0.11
(1,3960)	2:282:B:LYS:HB3	2:282:B:LYS:HD3	12	0.11
(1,3732)	2:168:B:LEU:HD13	2:160:B:ILE:HD12	3	0.11
(1,3564)	2:235:B:TYR:HE1	2:235:B:TYR:HA	12	0.11
(1,3564)	2:235:B:TYR:HE2	2:235:B:TYR:HA	12	0.11
(1,3564)	2:235:B:TYR:HE1	2:235:B:TYR:HA	16	0.11
(1,3564)	2:235:B:TYR:HE2	2:235:B:TYR:HA	16	0.11
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD21	20	0.11
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD22	20	0.11
(1,3563)	2:242:B:TYR:HD1	2:234:B:LEU:HD23	20	0.11
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD21	20	0.11
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD22	20	0.11
(1,3563)	2:242:B:TYR:HD2	2:234:B:LEU:HD23	20	0.11
(1,3517)	2:183:B:TYR:HD1	2:321:B:LYS:HE2	12	0.11
(1,3517)	2:183:B:TYR:HD2	2:321:B:LYS:HE2	12	0.11
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	2	0.11
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	2	0.11
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	3	0.11
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	3	0.11
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	6	0.11
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	6	0.11
(1,3485)	2:319:B:HIS:HE1	2:179:B:LYS:HD2	5	0.11
(1,3402)	1:117:A:GLU:HB3	1:119:A:LYS:H	10	0.11
(1,3380)	1:116:A:ARG:HG3	1:116:A:ARG:H	8	0.11
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	4	0.11
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	4	0.11
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	4	0.11
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	7	0.11
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	7	0.11
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	7	0.11
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	17	0.11
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	17	0.11
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	17	0.11
(1,3220)	1:95:A:ILE:H	1:94:A:GLU:H	4	0.11
(1,3220)	1:95:A:ILE:H	1:94:A:GLU:H	16	0.11
(1,3179)	1:88:A:GLN:HB3	1:88:A:GLN:H	5	0.11
(1,3172)	1:88:A:GLN:HB2	1:88:A:GLN:HE21	9	0.11
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE1	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE2	16	0.11
(1,3094)	1:78:A:TRP:HZ3	1:87:A:MET:HE3	16	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD11	2	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD12	2	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD13	2	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD11	2	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD12	2	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD13	2	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD11	5	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD12	5	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD13	5	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD11	5	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD12	5	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD13	5	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD11	16	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD12	16	0.11
(1,3042)	2:224:B:TYR:HE1	1:77:A:ILE:HD13	16	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD11	16	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD12	16	0.11
(1,3042)	2:224:B:TYR:HE2	1:77:A:ILE:HD13	16	0.11
(1,3025)	2:169:B:VAL:HG21	1:112:A:ILE:HD11	7	0.11
(1,3025)	2:169:B:VAL:HG21	1:112:A:ILE:HD12	7	0.11
(1,3025)	2:169:B:VAL:HG21	1:112:A:ILE:HD13	7	0.11
(1,3025)	2:169:B:VAL:HG22	1:112:A:ILE:HD11	7	0.11
(1,3025)	2:169:B:VAL:HG22	1:112:A:ILE:HD12	7	0.11
(1,3025)	2:169:B:VAL:HG22	1:112:A:ILE:HD13	7	0.11
(1,3025)	2:169:B:VAL:HG23	1:112:A:ILE:HD11	7	0.11
(1,3025)	2:169:B:VAL:HG23	1:112:A:ILE:HD12	7	0.11
(1,3025)	2:169:B:VAL:HG23	1:112:A:ILE:HD13	7	0.11
(1,2965)	1:113:A:GLN:HA	1:113:A:GLN:HG2	9	0.11
(1,2900)	1:112:A:ILE:HD11	1:109:A:GLU:HB3	4	0.11
(1,2900)	1:112:A:ILE:HD12	1:109:A:GLU:HB3	4	0.11
(1,2900)	1:112:A:ILE:HD13	1:109:A:GLU:HB3	4	0.11
(1,2830)	2:172:B:TRP:HD1	1:106:A:VAL:HG11	20	0.11
(1,2830)	2:172:B:TRP:HD1	1:106:A:VAL:HG12	20	0.11
(1,2830)	2:172:B:TRP:HD1	1:106:A:VAL:HG13	20	0.11
(1,2777)	1:98:A:PHE:HD1	1:100:A:ASN:HB2	9	0.11
(1,2777)	1:98:A:PHE:HD2	1:100:A:ASN:HB2	9	0.11
(1,2746)	1:98:A:PHE:HD1	1:97:A:PRO:HB3	5	0.11
(1,2746)	1:98:A:PHE:HD2	1:97:A:PRO:HB3	5	0.11
(1,2746)	1:98:A:PHE:HD1	1:97:A:PRO:HB3	11	0.11
(1,2746)	1:98:A:PHE:HD2	1:97:A:PRO:HB3	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2721)	1:97:A:PRO:HD2	1:96:A:LEU:HA	11	0.11
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD21	5	0.11
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD22	5	0.11
(1,2673)	1:85:A:TYR:HD1	1:90:A:LEU:HD23	5	0.11
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD21	5	0.11
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD22	5	0.11
(1,2673)	1:85:A:TYR:HD2	1:90:A:LEU:HD23	5	0.11
(1,2624)	1:90:A:LEU:HD21	1:87:A:MET:HA	14	0.11
(1,2624)	1:90:A:LEU:HD22	1:87:A:MET:HA	14	0.11
(1,2624)	1:90:A:LEU:HD23	1:87:A:MET:HA	14	0.11
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	6	0.11
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	6	0.11
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	6	0.11
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	11	0.11
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	11	0.11
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	11	0.11
(1,2617)	1:89:A:ALA:HB1	1:86:A:ASP:HB3	15	0.11
(1,2617)	1:89:A:ALA:HB2	1:86:A:ASP:HB3	15	0.11
(1,2617)	1:89:A:ALA:HB3	1:86:A:ASP:HB3	15	0.11
(1,2581)	1:86:A:ASP:HB3	1:83:A:THR:HA	6	0.11
(1,2581)	1:86:A:ASP:HB3	1:83:A:THR:HA	13	0.11
(1,2581)	1:86:A:ASP:HB3	1:83:A:THR:HA	15	0.11
(1,2461)	1:70:A:ARG:HG2	1:70:A:ARG:HB3	14	0.11
(1,2374)	2:312:B:GLU:HG2	2:312:B:GLU:H	2	0.11
(1,2374)	2:312:B:GLU:HG3	2:312:B:GLU:H	12	0.11
(1,2261)	2:164:B:LEU:HD11	2:298:B:LEU:H	20	0.11
(1,2261)	2:164:B:LEU:HD12	2:298:B:LEU:H	20	0.11
(1,2261)	2:164:B:LEU:HD13	2:298:B:LEU:H	20	0.11
(1,2169)	2:282:B:LYS:HB2	2:283:B:SER:H	6	0.11
(1,2155)	2:280:B:ASP:HB3	2:282:B:LYS:H	1	0.11
(1,2155)	2:280:B:ASP:HB3	2:282:B:LYS:H	20	0.11
(1,2138)	2:279:B:LEU:HG	2:279:B:LEU:H	17	0.11
(1,1978)	2:250:B:PRO:HA	2:251:B:ASP:H	2	0.11
(1,1978)	2:250:B:PRO:HA	2:251:B:ASP:H	6	0.11
(1,1626)	2:195:B:GLU:HG2	2:199:B:ASN:HD22	9	0.11
(1,1623)	2:195:B:GLU:HG2	2:199:B:ASN:HD21	20	0.11
(1,1561)	2:190:B:VAL:HB	2:191:B:ASP:H	11	0.11
(1,1505)	2:184:B:LEU:HD11	2:186:B:ALA:H	7	0.11
(1,1505)	2:184:B:LEU:HD12	2:186:B:ALA:H	7	0.11
(1,1505)	2:184:B:LEU:HD13	2:186:B:ALA:H	7	0.11
(1,1251)	2:240:B:PRO:HG3	2:322:B:ALA:HA	15	0.11
(1,1242)	2:321:B:LYS:HG2	2:321:B:LYS:HD3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	12	0.11
(1,1232)	2:320:B:ARG:HB2	2:320:B:ARG:HD2	12	0.11
(1,1072)	2:298:B:LEU:HB2	2:295:B:LEU:HD22	18	0.11
(1,1067)	2:298:B:LEU:HD11	2:295:B:LEU:HA	20	0.11
(1,1067)	2:298:B:LEU:HD12	2:295:B:LEU:HA	20	0.11
(1,1067)	2:298:B:LEU:HD13	2:295:B:LEU:HA	20	0.11
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG21	19	0.11
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG22	19	0.11
(1,727)	2:184:B:LEU:HD21	2:245:B:ILE:HG23	19	0.11
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG21	19	0.11
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG22	19	0.11
(1,727)	2:184:B:LEU:HD22	2:245:B:ILE:HG23	19	0.11
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG21	19	0.11
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG22	19	0.11
(1,727)	2:184:B:LEU:HD23	2:245:B:ILE:HG23	19	0.11
(1,572)	2:233:B:LEU:HB2	2:229:B:LEU:HA	2	0.11
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE1	19	0.11
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE2	19	0.11
(1,566)	2:233:B:LEU:HD11	2:228:B:MET:HE3	19	0.11
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE1	19	0.11
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE2	19	0.11
(1,566)	2:233:B:LEU:HD12	2:228:B:MET:HE3	19	0.11
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE1	19	0.11
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE2	19	0.11
(1,566)	2:233:B:LEU:HD13	2:228:B:MET:HE3	19	0.11
(1,474)	2:201:B:LYS:HG3	2:214:B:VAL:HG21	16	0.11
(1,474)	2:201:B:LYS:HG3	2:214:B:VAL:HG22	16	0.11
(1,474)	2:201:B:LYS:HG3	2:214:B:VAL:HG23	16	0.11
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	3	0.11
(1,453)	2:211:B:GLU:HG2	2:211:B:GLU:HB3	8	0.11
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB1	20	0.11
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB2	20	0.11
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB3	20	0.11
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB1	20	0.11
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB2	20	0.11
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB3	20	0.11
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB1	20	0.11
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB2	20	0.11
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB3	20	0.11
(1,386)	2:195:B:GLU:HA	2:195:B:GLU:HG3	11	0.11
(1,351)	2:188:B:LYS:HG3	2:193:B:ILE:HD11	18	0.11
(1,351)	2:188:B:LYS:HG3	2:193:B:ILE:HD12	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	2:188:B:LYS:HG3	2:193:B:ILE:HD13	18	0.11
(1,301)	2:192:B:SER:HB2	2:188:B:LYS:HD2	19	0.11
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD21	3	0.11
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD22	3	0.11
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD23	3	0.11
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD21	16	0.11
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD22	16	0.11
(1,241)	2:181:B:LEU:HA	2:181:B:LEU:HD23	16	0.11
(1,197)	2:173:B:ASP:HA	2:177:B:ARG:HG2	14	0.11
(1,50)	2:159:B:LYS:HG2	2:159:B:LYS:HE2	2	0.11
(1,40)	2:159:B:LYS:HD3	2:159:B:LYS:HG2	2	0.11
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	7	0.11
(1,33)	2:158:B:VAL:HA	2:158:B:VAL:HG11	10	0.11
(1,33)	2:158:B:VAL:HA	2:158:B:VAL:HG12	10	0.11
(1,33)	2:158:B:VAL:HA	2:158:B:VAL:HG13	10	0.11
(1,24)	2:157:B:LYS:HA	2:157:B:LYS:HD3	7	0.11
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	19	0.11
(3,67)	2:218:B:VAL:O	2:222:B:LYS:H	15	0.1
(3,29)	2:168:B:LEU:O	2:172:B:TRP:H	4	0.1
(3,13)	1:89:A:ALA:O	1:93:A:SER:H	9	0.1
(3,13)	1:89:A:ALA:O	1:93:A:SER:H	18	0.1
(3,7)	1:80:A:HIS:O	1:84:A:MET:H	7	0.1
(3,7)	1:80:A:HIS:O	1:84:A:MET:H	10	0.1
(3,2)	1:77:A:ILE:O	1:81:A:LEU:N	20	0.1
(3,1)	1:77:A:ILE:O	1:81:A:LEU:H	2	0.1
(2,317)	2:274:B:LEU:HG	1:98:A:PHE:HZ	10	0.1
(2,312)	2:286:B:LEU:HD11	1:87:A:MET:HA	20	0.1
(2,312)	2:286:B:LEU:HD12	1:87:A:MET:HA	20	0.1
(2,312)	2:286:B:LEU:HD13	1:87:A:MET:HA	20	0.1
(2,312)	2:286:B:LEU:HD21	1:87:A:MET:HA	20	0.1
(2,312)	2:286:B:LEU:HD22	1:87:A:MET:HA	20	0.1
(2,312)	2:286:B:LEU:HD23	1:87:A:MET:HA	20	0.1
(2,70)	1:98:A:PHE:HD1	1:97:A:PRO:HB2	7	0.1
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG21	3	0.1
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG22	3	0.1
(2,41)	1:78:A:TRP:HD1	1:77:A:ILE:HG23	3	0.1
(1,4623)	2:306:B:PHE:HE2	2:305:B:LEU:HD12	13	0.1
(1,4574)	2:242:B:TYR:HD1	2:234:B:LEU:HD13	12	0.1
(1,4551)	2:197:B:TYR:HE1	2:296:B:LYS:HB3	20	0.1
(1,4515)	2:172:B:TRP:HZ3	2:169:B:VAL:HG12	6	0.1
(1,4497)	2:292:B:HIS:HE1	2:158:B:VAL:HG21	1	0.1
(1,4374)	2:172:B:TRP:HZ3	1:107:A:LEU:HD22	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4345)	1:92:A:GLU:HB2	1:95:A:ILE:HD11	9	0.1
(1,4340)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	16	0.1
(1,4326)	1:94:A:GLU:HG3	1:94:A:GLU:HB3	8	0.1
(1,4326)	1:94:A:GLU:HG3	1:94:A:GLU:HB3	14	0.1
(1,4326)	1:94:A:GLU:HG3	1:94:A:GLU:HB3	19	0.1
(1,4310)	1:85:A:TYR:HD2	1:90:A:LEU:HB3	12	0.1
(1,3956)	2:282:B:LYS:HE2	2:282:B:LYS:HA	16	0.1
(1,3921)	2:221:B:ILE:HG23	2:263:B:LEU:HD22	2	0.1
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG22	8	0.1
(1,3845)	2:202:B:LYS:HE3	2:218:B:VAL:HG23	15	0.1
(1,3719)	2:289:B:ASN:HB3	2:286:B:LEU:HD13	3	0.1
(1,3666)	2:167:B:TRP:HD1	2:164:B:LEU:HA	6	0.1
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD21	11	0.1
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD22	11	0.1
(1,3601)	2:225:B:PHE:HD1	2:266:B:LEU:HD23	11	0.1
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD21	11	0.1
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD22	11	0.1
(1,3601)	2:225:B:PHE:HD2	2:266:B:LEU:HD23	11	0.1
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	4	0.1
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	4	0.1
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	8	0.1
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	8	0.1
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	10	0.1
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	10	0.1
(1,3512)	2:182:B:PHE:HD1	2:184:B:LEU:HG	19	0.1
(1,3512)	2:182:B:PHE:HD2	2:184:B:LEU:HG	19	0.1
(1,3450)	1:81:A:LEU:HD11	1:85:A:TYR:H	3	0.1
(1,3450)	1:81:A:LEU:HD12	1:85:A:TYR:H	3	0.1
(1,3450)	1:81:A:LEU:HD13	1:85:A:TYR:H	3	0.1
(1,3399)	1:117:A:GLU:HB3	1:118:A:GLY:H	8	0.1
(1,3316)	1:111:A:ILE:HD11	1:110:A:GLU:H	5	0.1
(1,3316)	1:111:A:ILE:HD12	1:110:A:GLU:H	5	0.1
(1,3316)	1:111:A:ILE:HD13	1:110:A:GLU:H	5	0.1
(1,3220)	1:95:A:ILE:H	1:94:A:GLU:H	2	0.1
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	1	0.1
(1,3215)	1:93:A:SER:HA	1:94:A:GLU:H	11	0.1
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG21	16	0.1
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG22	16	0.1
(1,2996)	1:116:A:ARG:HD3	1:115:A:VAL:HG23	16	0.1
(1,2965)	1:113:A:GLN:HA	1:113:A:GLN:HG2	14	0.1
(1,2943)	1:107:A:LEU:HG	1:112:A:ILE:HG13	8	0.1
(1,2760)	1:98:A:PHE:HD1	1:98:A:PHE:HA	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2760)	1:98:A:PHE:HD2	1:98:A:PHE:HA	4	0.1
(1,2640)	1:87:A:MET:HB3	1:87:A:MET:HG2	16	0.1
(1,2581)	1:86:A:ASP:HB3	1:83:A:THR:HA	7	0.1
(1,2581)	1:86:A:ASP:HB3	1:83:A:THR:HA	8	0.1
(1,2566)	1:78:A:TRP:HE3	1:81:A:LEU:HD11	6	0.1
(1,2566)	1:78:A:TRP:HE3	1:81:A:LEU:HD12	6	0.1
(1,2566)	1:78:A:TRP:HE3	1:81:A:LEU:HD13	6	0.1
(1,2206)	2:286:B:LEU:HD21	2:289:B:ASN:HD22	9	0.1
(1,2206)	2:286:B:LEU:HD22	2:289:B:ASN:HD22	9	0.1
(1,2206)	2:286:B:LEU:HD23	2:289:B:ASN:HD22	9	0.1
(1,2147)	2:280:B:ASP:HB3	2:281:B:GLU:H	3	0.1
(1,2147)	2:280:B:ASP:HB3	2:281:B:GLU:H	11	0.1
(1,1724)	2:214:B:VAL:HB	2:215:B:ASN:H	12	0.1
(1,1539)	2:188:B:LYS:HD3	2:189:B:ASN:H	4	0.1
(1,1494)	2:183:B:TYR:HB2	2:183:B:TYR:H	5	0.1
(1,1465)	2:174:B:LEU:HD11	2:180:B:GLN:HE22	4	0.1
(1,1465)	2:174:B:LEU:HD12	2:180:B:GLN:HE22	4	0.1
(1,1465)	2:174:B:LEU:HD13	2:180:B:GLN:HE22	4	0.1
(1,1433)	2:174:B:LEU:HD11	2:178:B:GLN:HE21	7	0.1
(1,1433)	2:174:B:LEU:HD12	2:178:B:GLN:HE21	7	0.1
(1,1433)	2:174:B:LEU:HD13	2:178:B:GLN:HE21	7	0.1
(1,1337)	2:162:B:GLU:HB2	2:162:B:GLU:H	10	0.1
(1,1238)	2:321:B:LYS:HE2	2:321:B:LYS:HA	14	0.1
(1,1235)	2:320:B:ARG:HB2	2:320:B:ARG:HG3	6	0.1
(1,1232)	2:320:B:ARG:HB2	2:320:B:ARG:HD2	14	0.1
(1,1130)	2:305:B:LEU:HD11	2:305:B:LEU:HA	8	0.1
(1,1130)	2:305:B:LEU:HD12	2:305:B:LEU:HA	8	0.1
(1,1130)	2:305:B:LEU:HD13	2:305:B:LEU:HA	8	0.1
(1,1130)	2:305:B:LEU:HD11	2:305:B:LEU:HA	11	0.1
(1,1130)	2:305:B:LEU:HD12	2:305:B:LEU:HA	11	0.1
(1,1130)	2:305:B:LEU:HD13	2:305:B:LEU:HA	11	0.1
(1,978)	2:282:B:LYS:HD3	2:282:B:LYS:HB3	13	0.1
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE1	6	0.1
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE2	6	0.1
(1,938)	1:98:A:PHE:HB3	2:273:B:MET:HE3	6	0.1
(1,664)	2:239:B:ARG:HA	2:239:B:ARG:HD3	2	0.1
(1,654)	2:236:B:LYS:HG2	2:236:B:LYS:HE3	5	0.1
(1,613)	2:229:B:LEU:HA	2:233:B:LEU:HD11	19	0.1
(1,613)	2:229:B:LEU:HA	2:233:B:LEU:HD12	19	0.1
(1,613)	2:229:B:LEU:HA	2:233:B:LEU:HD13	19	0.1
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG21	12	0.1
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG22	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	2:263:B:LEU:HD21	2:221:B:ILE:HG23	12	0.1
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG21	12	0.1
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG22	12	0.1
(1,538)	2:263:B:LEU:HD22	2:221:B:ILE:HG23	12	0.1
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG21	12	0.1
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG22	12	0.1
(1,538)	2:263:B:LEU:HD23	2:221:B:ILE:HG23	12	0.1
(1,478)	2:218:B:VAL:HB	2:215:B:ASN:HA	5	0.1
(1,454)	2:202:B:LYS:HD3	2:211:B:GLU:HG3	10	0.1
(1,437)	2:201:B:LYS:HA	2:204:B:ARG:HG2	14	0.1
(1,432)	2:204:B:ARG:HA	2:204:B:ARG:HD3	8	0.1
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB1	3	0.1
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB2	3	0.1
(1,406)	2:218:B:VAL:HG21	2:198:B:ALA:HB3	3	0.1
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB1	3	0.1
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB2	3	0.1
(1,406)	2:218:B:VAL:HG22	2:198:B:ALA:HB3	3	0.1
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB1	3	0.1
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB2	3	0.1
(1,406)	2:218:B:VAL:HG23	2:198:B:ALA:HB3	3	0.1
(1,282)	2:183:B:TYR:HE1	2:321:B:LYS:HE3	4	0.1
(1,282)	2:183:B:TYR:HE2	2:321:B:LYS:HE3	4	0.1
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD21	16	0.1
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD22	16	0.1
(1,259)	2:184:B:LEU:HB2	2:184:B:LEU:HD23	16	0.1
(1,40)	2:159:B:LYS:HD3	2:159:B:LYS:HG2	8	0.1
(1,40)	2:159:B:LYS:HB3	2:159:B:LYS:HG2	15	0.1
(1,16)	2:155:B:GLU:HG2	2:155:B:GLU:HB3	2	0.1
(1,16)	2:155:B:GLU:HG3	2:155:B:GLU:HB2	17	0.1

10 Dihedral-angle violation analysis

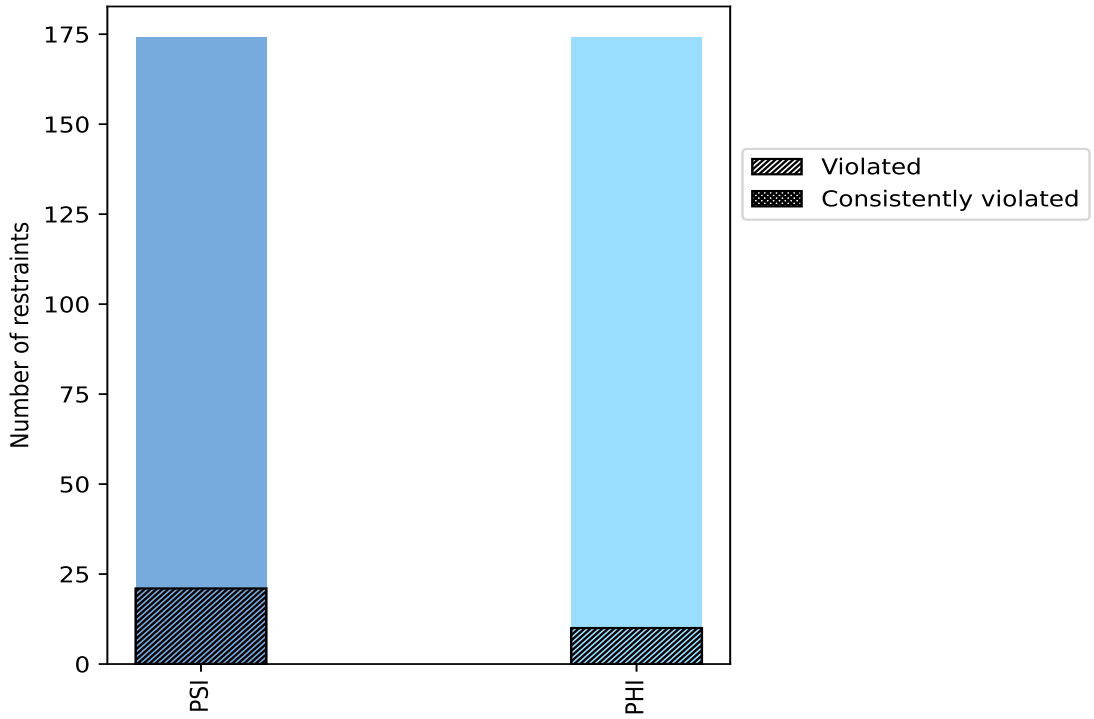
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	174	50.0	21	12.1	6.0	0	0.0	0.0
PHI	174	50.0	10	5.7	2.9	0	0.0	0.0
Total	348	100.0	31	8.9	8.9	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



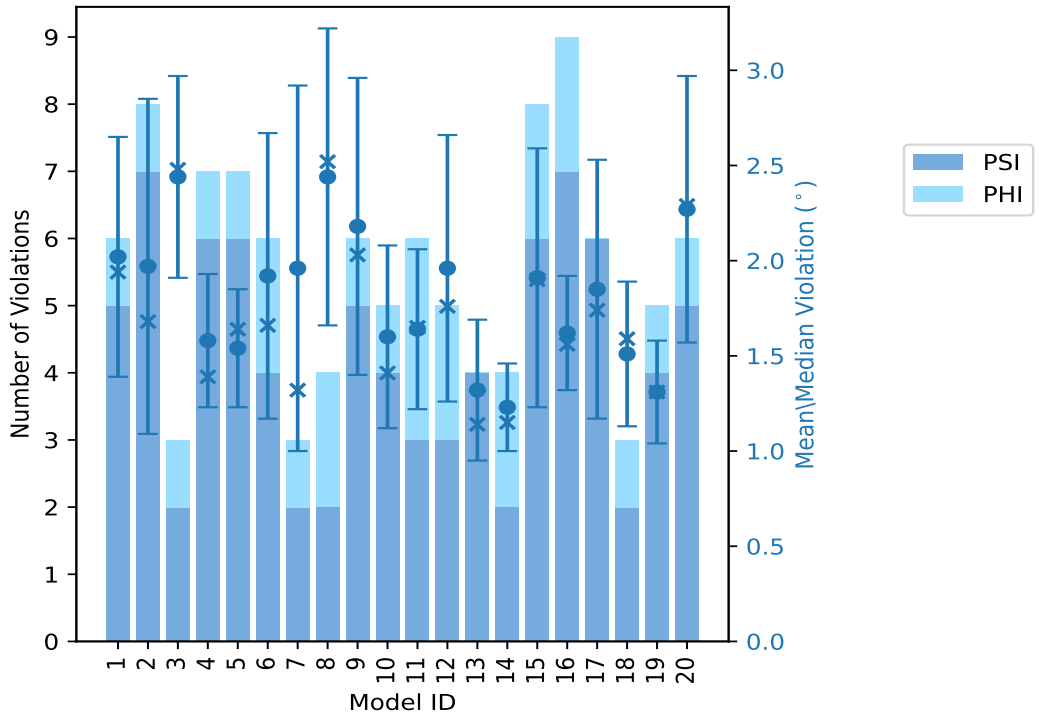
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	5	1	6	2.02	3.15	0.63	1.94
2	7	1	8	1.97	3.5	0.88	1.68
3	2	1	3	2.44	3.07	0.53	2.48
4	6	1	7	1.58	2.19	0.35	1.39
5	6	1	7	1.54	1.93	0.31	1.64
6	4	2	6	1.92	3.08	0.75	1.66
7	2	1	3	1.96	3.32	0.96	1.32
8	2	2	4	2.44	3.45	0.78	2.52
9	5	1	6	2.18	3.6	0.78	2.03
10	4	1	5	1.6	2.19	0.48	1.41
11	3	3	6	1.64	2.17	0.42	1.65
12	3	2	5	1.96	3.29	0.7	1.76
13	4	0	4	1.32	1.95	0.37	1.14
14	2	2	4	1.23	1.62	0.23	1.15
15	6	2	8	1.91	2.98	0.68	1.9
16	7	2	9	1.62	2.2	0.3	1.56
17	6	0	6	1.85	2.81	0.68	1.74
18	2	1	3	1.51	1.93	0.38	1.59
19	4	1	5	1.31	1.7	0.27	1.31
20	5	1	6	2.27	3.39	0.7	2.29

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

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

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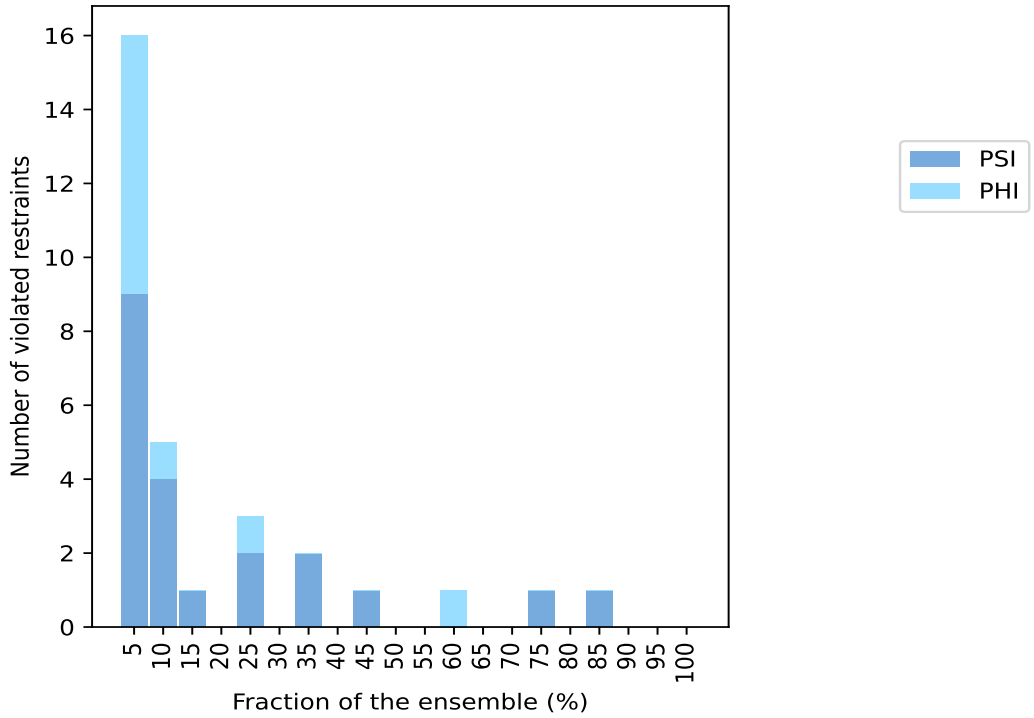
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	1	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

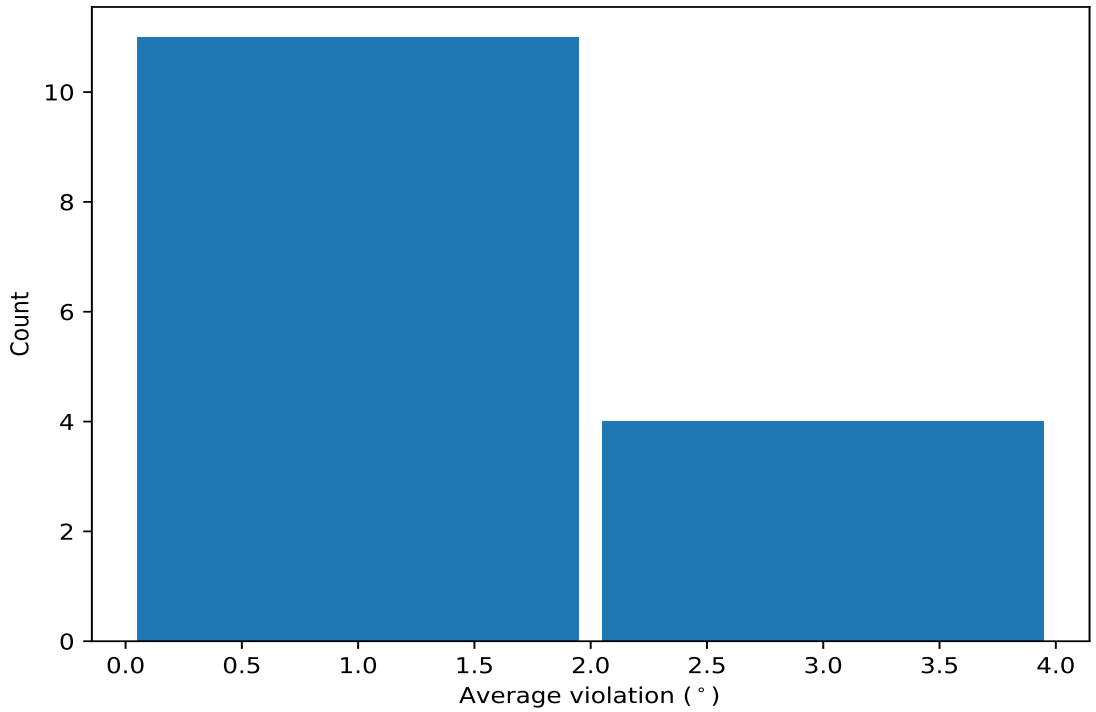


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

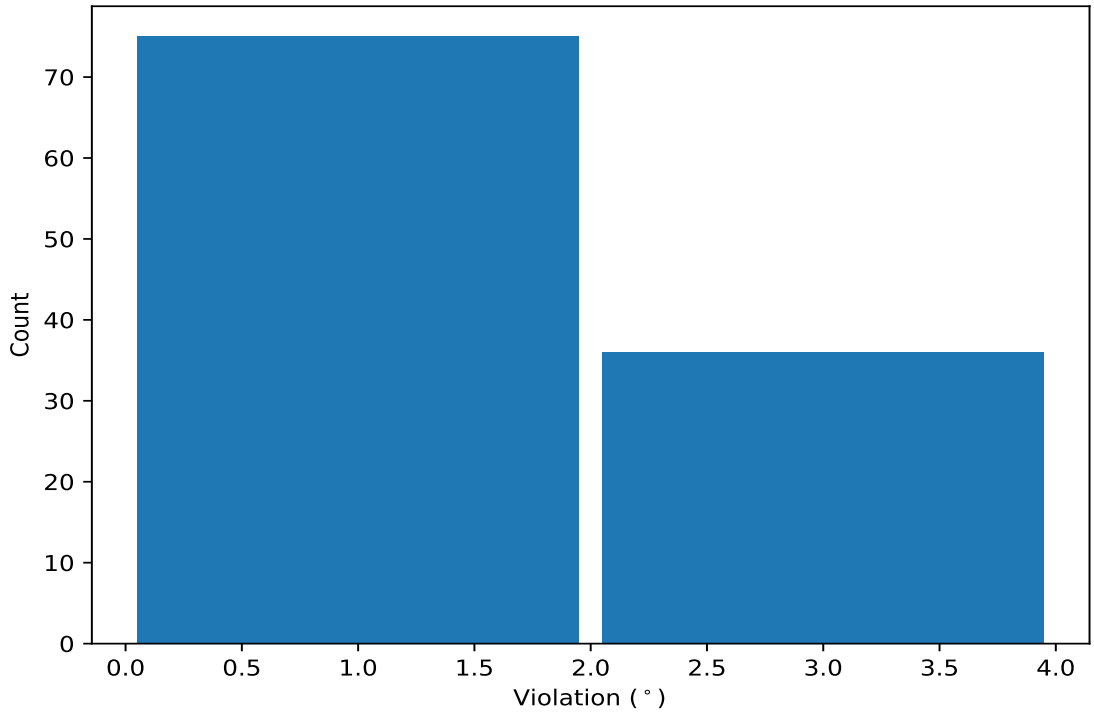
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	17	2.24	0.64	2.18
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	15	2.02	0.86	1.93
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	12	1.62	0.47	1.56
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	9	2.16	0.9	2.04
(1,221)	2:182:B:PHE:N	2:182:B:PHE:CA	2:182:B:PHE:C	2:183:B:TYR:N	7	2.18	0.68	1.98
(1,264)	2:229:B:LEU:N	2:229:B:LEU:CA	2:229:B:LEU:C	2:230:B:GLY:N	7	1.45	0.51	1.32
(1,266)	2:231:B:THR:N	2:231:B:THR:CA	2:231:B:THR:C	2:232:B:GLN:N	5	1.94	0.57	2.16
(1,142)	2:261:B:PRO:C	2:262:B:HIS:N	2:262:B:HIS:CA	2:262:B:HIS:C	5	1.77	0.31	1.58
(1,224)	2:185:B:PRO:N	2:185:B:PRO:CA	2:185:B:PRO:C	2:186:B:ALA:N	5	1.58	0.13	1.64
(1,295)	2:264:B:LEU:N	2:264:B:LEU:CA	2:264:B:LEU:C	2:265:B:ARG:N	3	1.56	0.47	1.5
(1,265)	2:230:B:GLY:N	2:230:B:GLY:CA	2:230:B:GLY:C	2:231:B:THR:N	2	1.82	0.01	1.82
(1,245)	2:210:B:LYS:N	2:210:B:LYS:CA	2:210:B:LYS:C	2:211:B:GLU:N	2	1.44	0.05	1.44
(1,140)	2:259:B:GLY:C	2:260:B:ALA:N	2:260:B:ALA:CA	2:260:B:ALA:C	2	1.43	0.21	1.43
(1,226)	2:187:B:LYS:N	2:187:B:LYS:CA	2:187:B:LYS:C	2:188:B:LYS:N	2	1.14	0.06	1.14
(1,296)	2:265:B:ARG:N	2:265:B:ARG:CA	2:265:B:ARG:C	2:266:B:LEU:N	2	1.02	0.01	1.02

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	9	3.6
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	2	3.5
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	8	3.45
(1,221)	2:182:B:PHE:N	2:182:B:PHE:CA	2:182:B:PHE:C	2:183:B:TYR:N	20	3.39
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	7	3.32
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	12	3.29
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	2	3.19
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	1	3.15
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	6	3.08
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	3	3.07
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	15	2.98
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	17	2.81
(1,221)	2:182:B:PHE:N	2:182:B:PHE:CA	2:182:B:PHE:C	2:183:B:TYR:N	6	2.76
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	20	2.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,264)	2:229:B:LEU:N	2:229:B:LEU:CA	2:229:B:LEU:C	2:230:B:GLY:N	9	2.66
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	8	2.65
(1,266)	2:231:B:THR:N	2:231:B:THR:CA	2:231:B:THR:C	2:232:B:GLN:N	15	2.55
(1,221)	2:182:B:PHE:N	2:182:B:PHE:CA	2:182:B:PHE:C	2:183:B:TYR:N	17	2.54
(1,266)	2:231:B:THR:N	2:231:B:THR:CA	2:231:B:THR:C	2:232:B:GLN:N	3	2.48
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	20	2.48
(1,116)	2:231:B:THR:C	2:232:B:GLN:N	2:232:B:GLN:CA	2:232:B:GLN:C	15	2.45
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	8	2.39
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	1	2.38
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	9	2.22
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	16	2.2
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	10	2.19
(1,142)	2:261:B:PRO:C	2:262:B:HIS:N	2:262:B:HIS:CA	2:262:B:HIS:C	4	2.19
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	2	2.18
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	11	2.17
(1,295)	2:264:B:LEU:N	2:264:B:LEU:CA	2:264:B:LEU:C	2:265:B:ARG:N	17	2.16
(1,266)	2:231:B:THR:N	2:231:B:THR:CA	2:231:B:THR:C	2:232:B:GLN:N	10	2.16
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	15	2.16
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	1	2.15
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	11	2.14
(1,142)	2:261:B:PRO:C	2:262:B:HIS:N	2:262:B:HIS:CA	2:262:B:HIS:C	20	2.1
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	4	2.04
(1,221)	2:182:B:PHE:N	2:182:B:PHE:CA	2:182:B:PHE:C	2:183:B:TYR:N	2	1.98
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	13	1.95
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	18	1.93
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	5	1.93
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	6	1.88
(1,93)	2:208:B:ASP:C	2:209:B:ASN:N	2:209:B:ASN:CA	2:209:B:ASN:C	12	1.86
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	16	1.83
(1,265)	2:230:B:GLY:N	2:230:B:GLY:CA	2:230:B:GLY:C	2:231:B:THR:N	16	1.83
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	9	1.83
(1,265)	2:230:B:GLY:N	2:230:B:GLY:CA	2:230:B:GLY:C	2:231:B:THR:N	20	1.81
(1,94)	2:209:B:ASN:C	2:210:B:LYS:N	2:210:B:LYS:CA	2:210:B:LYS:C	3	1.77
(1,304)	2:274:B:LEU:N	2:274:B:LEU:CA	2:274:B:LEU:C	2:275:B:ALA:N	12	1.76
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	5	1.76
(1,293)	2:262:B:HIS:N	2:262:B:HIS:CA	2:262:B:HIS:C	2:263:B:LEU:N	5	1.73
(1,221)	2:182:B:PHE:N	2:182:B:PHE:CA	2:182:B:PHE:C	2:183:B:TYR:N	1	1.73
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	11	1.72
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	19	1.7
(1,224)	2:185:B:PRO:N	2:185:B:PRO:CA	2:185:B:PRO:C	2:186:B:ALA:N	16	1.67
(1,224)	2:185:B:PRO:N	2:185:B:PRO:CA	2:185:B:PRO:C	2:186:B:ALA:N	5	1.64
(1,224)	2:185:B:PRO:N	2:185:B:PRO:CA	2:185:B:PRO:C	2:186:B:ALA:N	15	1.64
(1,140)	2:259:B:GLY:C	2:260:B:ALA:N	2:260:B:ALA:CA	2:260:B:ALA:C	12	1.64
(1,224)	2:185:B:PRO:N	2:185:B:PRO:CA	2:185:B:PRO:C	2:186:B:ALA:N	14	1.62
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	18	1.59
(1,142)	2:261:B:PRO:C	2:262:B:HIS:N	2:262:B:HIS:CA	2:262:B:HIS:C	11	1.58
(1,142)	2:261:B:PRO:C	2:262:B:HIS:N	2:262:B:HIS:CA	2:262:B:HIS:C	16	1.56
(1,257)	2:222:B:LYS:N	2:222:B:LYS:CA	2:222:B:LYS:C	2:223:B:GLU:N	5	1.53
(1,301)	2:271:B:GLY:N	2:271:B:GLY:CA	2:271:B:GLY:C	2:272:B:ALA:N	4	1.52
(1,295)	2:264:B:LEU:N	2:264:B:LEU:CA	2:264:B:LEU:C	2:265:B:ARG:N	16	1.5
(1,264)	2:229:B:LEU:N	2:229:B:LEU:CA	2:229:B:LEU:C	2:230:B:GLY:N	16	1.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,245)	2:210:B:LYS:N	2:210:B:LYS:CA	2:210:B:LYS:C	2:211:B:GLU:N	19	1.49
(1,221)	2:182:B:PHE:N	2:182:B:PHE:CA	2:182:B:PHE:C	2:183:B:TYR:N	16	1.46
(1,142)	2:261:B:PRO:C	2:262:B:HIS:N	2:262:B:HIS:CA	2:262:B:HIS:C	6	1.44
(1,203)	2:162:B:GLU:N	2:162:B:GLU:CA	2:162:B:GLU:C	2:163:B:GLU:N	1	1.43
(1,221)	2:182:B:PHE:N	2:182:B:PHE:CA	2:182:B:PHE:C	2:183:B:TYR:N	10	1.41
(1,31)	1:84:A:MET:N	1:84:A:MET:CA	1:84:A:MET:C	1:85:A:TYR:N	9	1.4
(1,245)	2:210:B:LYS:N	2:210:B:LYS:CA	2:210:B:LYS:C	2:211:B:GLU:N	4	1.39
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	2	1.39
(1,266)	2:231:B:THR:N	2:231:B:THR:CA	2:231:B:THR:C	2:232:B:GLN:N	4	1.37
(1,264)	2:229:B:LEU:N	2:229:B:LEU:CA	2:229:B:LEU:C	2:230:B:GLY:N	6	1.37
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	9	1.36
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	4	1.35
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	15	1.34
(1,224)	2:185:B:PRO:N	2:185:B:PRO:CA	2:185:B:PRO:C	2:186:B:ALA:N	17	1.33
(1,264)	2:229:B:LEU:N	2:229:B:LEU:CA	2:229:B:LEU:C	2:230:B:GLY:N	7	1.32
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	19	1.31
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	1	1.3
(1,72)	2:183:B:TYR:C	2:184:B:LEU:N	2:184:B:LEU:CA	2:184:B:LEU:C	8	1.27
(1,222)	2:183:B:TYR:N	2:183:B:TYR:CA	2:183:B:TYR:C	2:184:B:LEU:N	17	1.25
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	12	1.25
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	7	1.24
(1,140)	2:259:B:GLY:C	2:260:B:ALA:N	2:260:B:ALA:CA	2:260:B:ALA:C	14	1.22
(1,335)	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	2:309:B:SER:N	13	1.21
(1,226)	2:187:B:LYS:N	2:187:B:LYS:CA	2:187:B:LYS:C	2:188:B:LYS:N	2	1.2
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	4	1.19
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	10	1.19
(1,264)	2:229:B:LEU:N	2:229:B:LEU:CA	2:229:B:LEU:C	2:230:B:GLY:N	2	1.18
(1,266)	2:231:B:THR:N	2:231:B:THR:CA	2:231:B:THR:C	2:232:B:GLN:N	20	1.16
(1,115)	2:230:B:GLY:C	2:231:B:THR:N	2:231:B:THR:CA	2:231:B:THR:C	11	1.16
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	5	1.12
(1,264)	2:229:B:LEU:N	2:229:B:LEU:CA	2:229:B:LEU:C	2:230:B:GLY:N	15	1.12
(1,345)	2:318:B:TYR:N	2:318:B:TYR:CA	2:318:B:TYR:C	2:319:B:HIS:N	2	1.11
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	11	1.09
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	14	1.08
(1,226)	2:187:B:LYS:N	2:187:B:LYS:CA	2:187:B:LYS:C	2:188:B:LYS:N	13	1.07
(1,278)	2:244:B:GLU:N	2:244:B:GLU:CA	2:244:B:GLU:C	2:245:B:ILE:N	15	1.05
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	5	1.05
(1,48)	2:157:B:LYS:C	2:158:B:VAL:N	2:158:B:VAL:CA	2:158:B:VAL:C	10	1.05
(1,346)	2:319:B:HIS:N	2:319:B:HIS:CA	2:319:B:HIS:C	2:320:B:ARG:N	17	1.04
(1,296)	2:265:B:ARG:N	2:265:B:ARG:CA	2:265:B:ARG:C	2:266:B:LEU:N	13	1.03
(1,184)	2:307:B:SER:C	2:308:B:ALA:N	2:308:B:ALA:CA	2:308:B:ALA:C	16	1.03
(1,296)	2:265:B:ARG:N	2:265:B:ARG:CA	2:265:B:ARG:C	2:266:B:LEU:N	14	1.02
(1,264)	2:229:B:LEU:N	2:229:B:LEU:CA	2:229:B:LEU:C	2:230:B:GLY:N	18	1.02
(1,32)	1:87:A:MET:N	1:87:A:MET:CA	1:87:A:MET:C	1:88:A:GLN:N	19	1.02
(1,295)	2:264:B:LEU:N	2:264:B:LEU:CA	2:264:B:LEU:C	2:265:B:ARG:N	6	1.01
(1,181)	2:303:B:ALA:C	2:304:B:THR:N	2:304:B:THR:CA	2:304:B:THR:C	19	1.01