



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 10:29 PM UTC

PDB ID : 8JRA / pdb_00008jra
BMRB ID : 36577
Title : N-terminal domain of Hsp90a mutant
Authors : Wan, C.J.
Deposited on : 2023-06-16

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

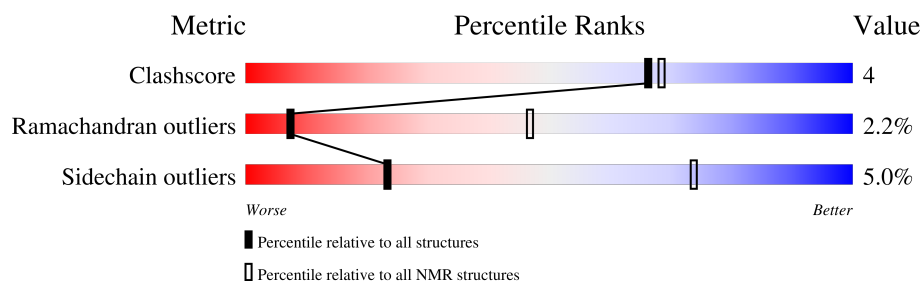
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 40%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	237	 84% 14%

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:16-A:135, A:141-A:223 (203)	2.55	1

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3718 atoms, of which 1840 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms						Trace
1	A	237	Total	C	H	N	O	S	0
			3718	1177	1840	306	388	7	

There is a discrepancy between the modelled and reference sequences:

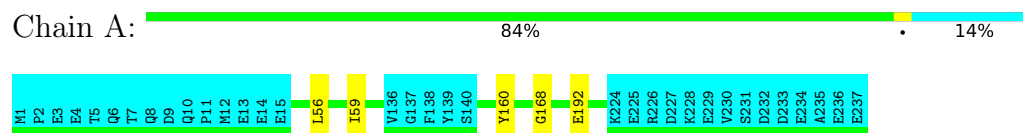
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	GLU	THR	engineered mutation	UNP P07900

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Heat shock protein HSP 90-alpha

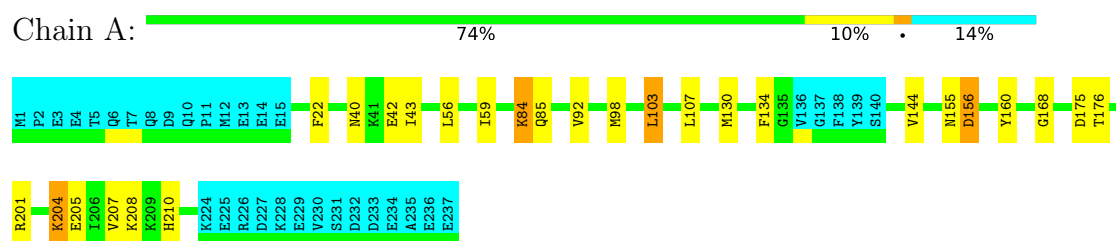


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

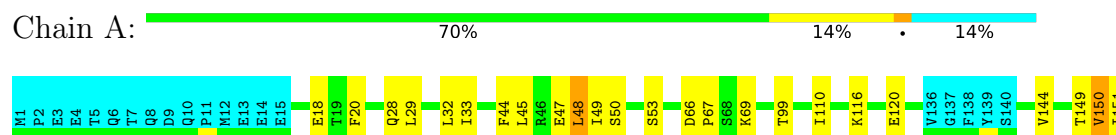
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Heat shock protein HSP 90-alpha



4.2.2 Score per residue for model 2

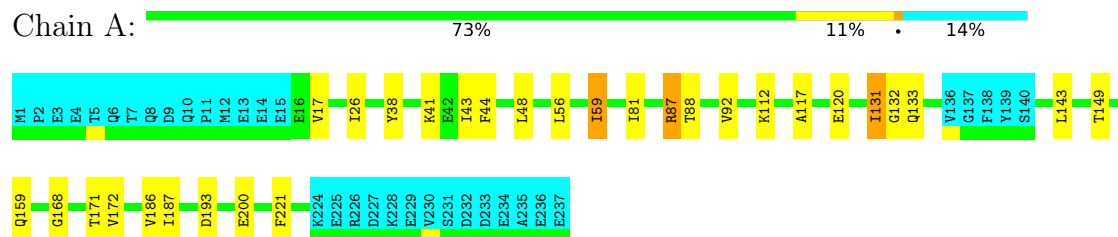
- Molecule 1: Heat shock protein HSP 90-alpha





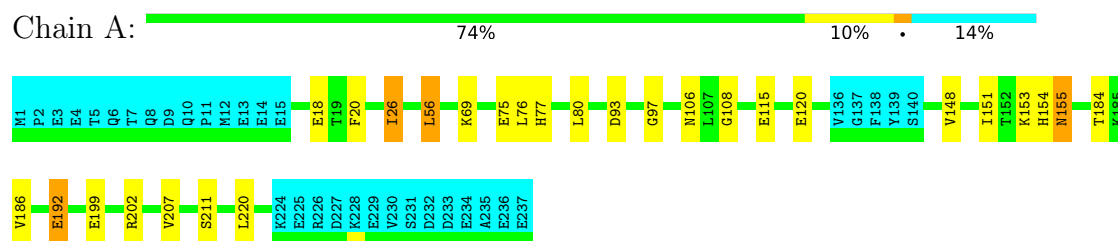
4.2.3 Score per residue for model 3

- Molecule 1: Heat shock protein HSP 90-alpha



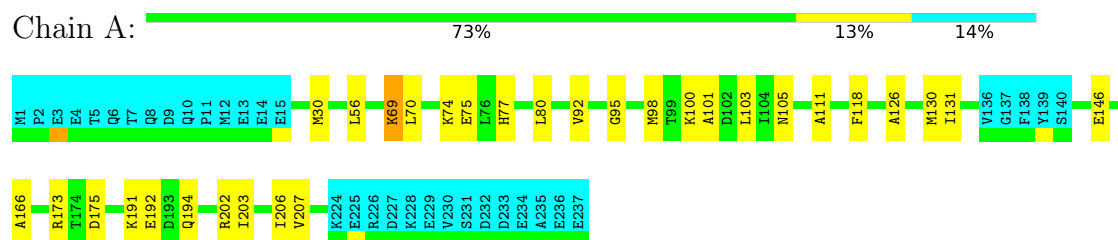
4.2.4 Score per residue for model 4

- Molecule 1: Heat shock protein HSP 90-alpha



4.2.5 Score per residue for model 5

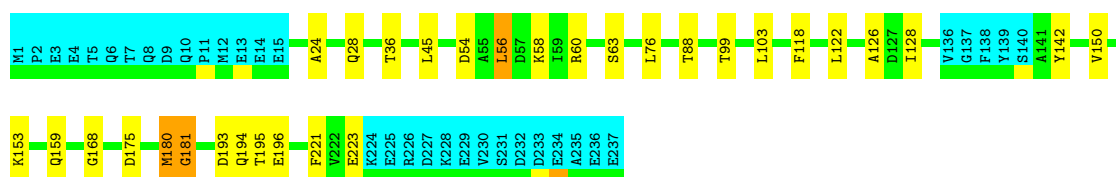
- Molecule 1: Heat shock protein HSP 90-alpha



4.2.6 Score per residue for model 6

- Molecule 1: Heat shock protein HSP 90-alpha

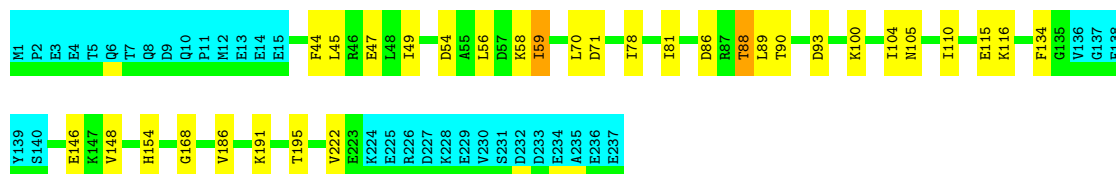




4.2.7 Score per residue for model 7

- Molecule 1: Heat shock protein HSP 90-alpha

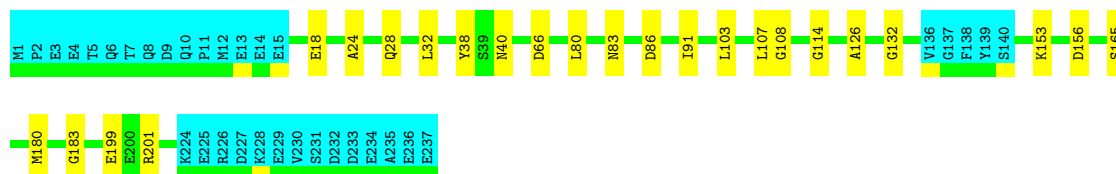
Chain A: 72% 13% 14%



4.2.8 Score per residue for model 8

- Molecule 1: Heat shock protein HSP 90-alpha

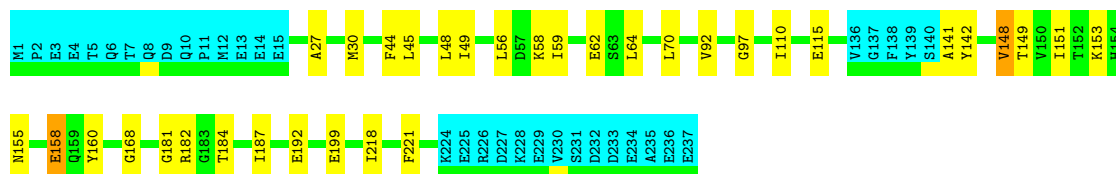
Chain A: 76% 10% 14%



4.2.9 Score per residue for model 9

- Molecule 1: Heat shock protein HSP 90-alpha

Chain A: 71% 14% 14%



4.2.10 Score per residue for model 10

- Molecule 1: Heat shock protein HSP 90-alpha

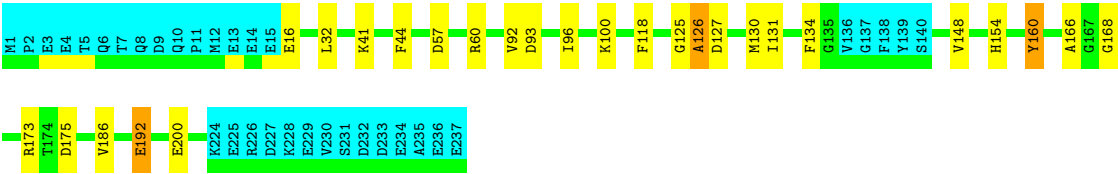
Chain A:

74%

10%

•

14%



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1228
Number of shifts mapped to atoms	1228
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1597	1599	1599	12±2
All	All	15970	15990	15990	125

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ILE:HA	1:A:134:PHE:CE2	0.70	2.22	10	1
1:A:99:THR:O	1:A:103:LEU:HG	0.65	1.91	6	1
1:A:153:LYS:HA	1:A:159:GLN:NE2	0.65	2.06	6	1
1:A:98:MET:SD	1:A:103:LEU:HG	0.61	2.34	1	1
1:A:44:PHE:O	1:A:48:LEU:HB2	0.58	1.98	3	3
1:A:38:TYR:CE2	1:A:40:ASN:HB3	0.57	2.34	8	1
1:A:75:GLU:HB3	1:A:77:HIS:CD2	0.57	2.35	5	2
1:A:118:PHE:CD1	1:A:131:ILE:HB	0.57	2.35	5	1
1:A:78:ILE:HA	1:A:93:ASP:OD1	0.56	2.01	7	1
1:A:96:ILE:O	1:A:154:HIS:HA	0.56	2.00	10	1
1:A:159:GLN:NE2	1:A:159:GLN:HA	0.56	2.16	6	1
1:A:130:MET:O	1:A:134:PHE:HB3	0.56	2.01	1	1
1:A:103:LEU:O	1:A:107:LEU:HB2	0.54	2.02	1	1
1:A:88:THR:CG2	1:A:187:ILE:HG23	0.54	2.33	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LEU:HD12	1:A:76:LEU:HD23	0.52	1.81	4	2
1:A:29:LEU:O	1:A:33:ILE:HG12	0.52	2.04	2	1
1:A:153:LYS:HD2	1:A:180:MET:SD	0.52	2.45	8	1
1:A:56:LEU:O	1:A:59:ILE:HG22	0.51	2.05	3	2
1:A:88:THR:HG23	1:A:187:ILE:HG23	0.51	1.81	3	1
1:A:54:ASP:O	1:A:58:LYS:HG3	0.51	2.04	7	2
1:A:18:GLU:HG3	1:A:20:PHE:CE1	0.51	2.41	4	1
1:A:202:ARG:O	1:A:206:ILE:HG12	0.50	2.06	5	1
1:A:44:PHE:HA	1:A:47:GLU:CG	0.50	2.37	7	1
1:A:69:LYS:HG3	1:A:70:LEU:H	0.50	1.67	5	1
1:A:118:PHE:CE1	1:A:131:ILE:HB	0.49	2.41	5	1
1:A:149:THR:HA	1:A:162:TRP:O	0.49	2.07	2	1
1:A:16:GLU:O	1:A:173:ARG:HG3	0.49	2.07	10	1
1:A:153:LYS:HG3	1:A:158:GLU:O	0.49	2.08	9	1
1:A:201:ARG:O	1:A:205:GLU:HG2	0.49	2.07	1	1
1:A:56:LEU:O	1:A:60:ARG:HG2	0.49	2.08	6	1
1:A:45:LEU:O	1:A:49:ILE:HB	0.49	2.07	9	2
1:A:199:GLU:HB2	1:A:202:ARG:CG	0.48	2.39	4	1
1:A:22:PHE:CD1	1:A:168:GLY:HA2	0.48	2.44	1	1
1:A:38:TYR:CD2	1:A:143:LEU:HG	0.47	2.44	3	1
1:A:97:GLY:HA2	1:A:184:THR:OG1	0.47	2.10	9	2
1:A:146:GLU:OE2	1:A:191:LYS:HA	0.47	2.10	7	1
1:A:127:ASP:O	1:A:130:MET:HG2	0.47	2.08	10	1
1:A:32:LEU:HD21	1:A:126:ALA:O	0.47	2.10	8	1
1:A:58:LYS:O	1:A:62:GLU:HG2	0.47	2.09	9	1
1:A:199:GLU:OE1	1:A:201:ARG:HG2	0.46	2.10	8	1
1:A:42:GLU:HB3	1:A:210:HIS:CE1	0.46	2.46	1	1
1:A:150:VAL:HA	1:A:185:LYS:O	0.46	2.11	2	1
1:A:26:ILE:O	1:A:26:ILE:HD13	0.46	2.11	4	1
1:A:81:ILE:CG2	1:A:90:THR:HB	0.46	2.40	7	1
1:A:116:LYS:O	1:A:120:GLU:HG2	0.46	2.10	2	1
1:A:80:LEU:O	1:A:220:LEU:HA	0.46	2.11	4	1
1:A:84:LYS:HG2	1:A:85:GLN:OE1	0.46	2.10	1	1
1:A:66:ASP:OD1	1:A:69:LYS:HB2	0.45	2.11	2	1
1:A:17:VAL:HG22	1:A:171:THR:OG1	0.45	2.11	3	1
1:A:60:ARG:HG3	1:A:76:LEU:HD21	0.45	1.88	6	1
1:A:118:PHE:O	1:A:122:LEU:HG	0.45	2.11	6	1
1:A:18:GLU:HB3	1:A:20:PHE:CE1	0.45	2.46	2	1
1:A:81:ILE:CG2	1:A:221:PHE:HB3	0.45	2.42	3	1
1:A:87:ARG:HD2	1:A:193:ASP:OD1	0.45	2.12	3	1
1:A:199:GLU:HB2	1:A:202:ARG:HG2	0.45	1.89	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ALA:CB	1:A:131:ILE:HA	0.45	2.42	5	1
1:A:116:LYS:NZ	1:A:116:LYS:HB2	0.44	2.27	2	1
1:A:38:TYR:OH	1:A:43:ILE:HB	0.44	2.12	3	1
1:A:45:LEU:O	1:A:49:ILE:HG12	0.44	2.12	2	1
1:A:84:LYS:H	1:A:84:LYS:HD3	0.44	1.70	1	1
1:A:132:GLY:O	1:A:133:GLN:HG3	0.44	2.12	3	1
1:A:118:PHE:CE1	1:A:131:ILE:HD13	0.44	2.47	5	1
1:A:28:GLN:O	1:A:32:LEU:HD23	0.44	2.13	2	1
1:A:117:ALA:HB1	1:A:120:GLU:HB2	0.44	1.90	3	1
1:A:193:ASP:C	1:A:195:THR:H	0.43	2.21	6	1
1:A:151:ILE:CG2	1:A:153:LYS:HE3	0.43	2.44	4	1
1:A:24:ALA:O	1:A:28:GLN:HG3	0.43	2.14	8	1
1:A:203:ILE:O	1:A:207:VAL:HB	0.43	2.13	5	1
1:A:80:LEU:CD1	1:A:91:ILE:HG12	0.43	2.43	8	1
1:A:118:PHE:CD1	1:A:134:PHE:CE2	0.43	3.06	10	1
1:A:202:ARG:O	1:A:206:ILE:HG22	0.43	2.13	2	1
1:A:141:ALA:HB3	1:A:148:VAL:HG21	0.43	1.90	9	1
1:A:22:PHE:CE1	1:A:168:GLY:HA2	0.43	2.47	1	1
1:A:50:SER:HA	1:A:53:SER:OG	0.43	2.13	2	1
1:A:60:ARG:HA	1:A:63:SER:OG	0.43	2.14	6	1
1:A:181:GLY:O	1:A:182:ARG:HB2	0.43	2.14	9	1
1:A:204:LYS:O	1:A:208:LYS:HB2	0.43	2.14	1	1
1:A:126:ALA:HB3	1:A:130:MET:SD	0.43	2.53	10	1
1:A:101:ALA:O	1:A:105:ASN:HB2	0.42	2.13	5	1
1:A:149:THR:HB	1:A:187:ILE:HB	0.42	1.91	9	1
1:A:153:LYS:HG3	1:A:180:MET:SD	0.42	2.54	6	1
1:A:115:GLU:O	1:A:116:LYS:HB2	0.42	2.14	7	1
1:A:151:ILE:HA	1:A:160:TYR:O	0.42	2.14	9	2
1:A:130:MET:HG3	1:A:130:MET:O	0.42	2.14	5	1
1:A:100:LYS:HG3	1:A:160:TYR:OH	0.42	2.14	10	1
1:A:153:LYS:HB3	1:A:153:LYS:NZ	0.42	2.29	2	1
1:A:24:ALA:O	1:A:28:GLN:HG2	0.42	2.14	6	1
1:A:107:LEU:HD13	1:A:108:GLY:N	0.42	2.29	8	1
1:A:103:LEU:CD2	1:A:107:LEU:HG	0.42	2.44	8	1
1:A:56:LEU:HA	1:A:95:GLY:HA2	0.42	1.92	5	1
1:A:146:GLU:OE1	1:A:191:LYS:HG2	0.42	2.15	5	1
1:A:83:ASN:ND2	1:A:86:ASP:HB2	0.41	2.30	8	1
1:A:98:MET:HB3	1:A:103:LEU:HD21	0.41	1.91	5	1
1:A:81:ILE:HG23	1:A:90:THR:HB	0.41	1.92	7	1
1:A:80:LEU:HB2	1:A:220:LEU:HD23	0.41	1.92	4	1
1:A:100:LYS:O	1:A:104:ILE:HG12	0.41	2.16	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ASP:O	1:A:60:ARG:HB3	0.41	2.15	10	1
1:A:180:MET:SD	1:A:185:LYS:HE3	0.41	2.56	2	1
1:A:180:MET:O	1:A:181:GLY:C	0.41	2.63	6	1
1:A:192:GLU:H	1:A:192:GLU:CD	0.41	2.23	4	1
1:A:30:MET:SD	1:A:166:ALA:HB1	0.41	2.56	5	1
1:A:45:LEU:HA	1:A:49:ILE:CG1	0.41	2.46	9	1
1:A:207:VAL:O	1:A:211:SER:HB3	0.41	2.16	4	1
1:A:41:LYS:O	1:A:44:PHE:HD1	0.41	1.98	3	2
1:A:118:PHE:CE1	1:A:122:LEU:HD11	0.41	2.51	6	1
1:A:153:LYS:CD	1:A:180:MET:HB3	0.41	2.46	8	1
1:A:40:ASN:OD1	1:A:43:ILE:HG13	0.41	2.16	1	1
1:A:198:LEU:HG	1:A:198:LEU:O	0.41	2.15	2	1
1:A:132:GLY:C	1:A:133:GLN:HG3	0.41	2.41	3	1
1:A:180:MET:SD	1:A:183:GLY:HA3	0.41	2.55	8	1
1:A:27:ALA:O	1:A:30:MET:HB2	0.40	2.16	9	1
1:A:66:ASP:N	1:A:67:PRO:HD3	0.40	2.31	2	1
1:A:69:LYS:HD2	1:A:69:LYS:N	0.40	2.31	4	1
1:A:155:ASN:O	1:A:156:ASP:HB2	0.40	2.15	1	1
1:A:86:ASP:HB3	1:A:88:THR:OG1	0.40	2.16	7	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	203/237 (86%)	176±7 (87±4%)	22±7 (11±3%)	4±1 (2±1%)	7	47
All	All	2030/2370 (86%)	1763 (87%)	222 (11%)	45 (2%)	7	47

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

Mol	Chain	Res	Type	Models (Total)
1	A	168	GLY	6
1	A	175	ASP	4
1	A	192	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	144	VAL	2
1	A	156	ASP	2
1	A	158	GLU	2
1	A	115	GLU	2
1	A	155	ASN	2
1	A	126	ALA	2
1	A	177	GLY	1
1	A	191	LYS	1
1	A	222	VAL	1
1	A	112	LYS	1
1	A	131	ILE	1
1	A	106	ASN	1
1	A	108	GLY	1
1	A	69	LYS	1
1	A	74	LYS	1
1	A	111	ALA	1
1	A	181	GLY	1
1	A	194	GLN	1
1	A	105	ASN	1
1	A	110	ILE	1
1	A	195	THR	1
1	A	66	ASP	1
1	A	114	GLY	1
1	A	165	SER	1
1	A	125	GLY	1
1	A	166	ALA	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/207 (85%)	150±50 (86±29%)	8±3 (4±2%)	26	77
All	All	1575/2070 (76%)	1497 (95%)	78 (5%)	23	74

All 50 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	92	VAL	5
1	A	56	LEU	4
1	A	59	ILE	4
1	A	186	VAL	4
1	A	148	VAL	4
1	A	160	TYR	3
1	A	110	ILE	2
1	A	150	VAL	2
1	A	26	ILE	2
1	A	200	GLU	2
1	A	93	ASP	2
1	A	154	HIS	2
1	A	192	GLU	2
1	A	88	THR	2
1	A	221	PHE	2
1	A	70	LEU	2
1	A	84	LYS	1
1	A	103	LEU	1
1	A	176	THR	1
1	A	204	LYS	1
1	A	207	VAL	1
1	A	47	GLU	1
1	A	48	LEU	1
1	A	99	THR	1
1	A	184	THR	1
1	A	202	ARG	1
1	A	87	ARG	1
1	A	131	ILE	1
1	A	149	THR	1
1	A	159	GLN	1
1	A	172	VAL	1
1	A	120	GLU	1
1	A	155	ASN	1
1	A	80	LEU	1
1	A	100	LYS	1
1	A	194	GLN	1
1	A	36	THR	1
1	A	45	LEU	1
1	A	128	ILE	1
1	A	180	MET	1
1	A	196	GLU	1
1	A	223	GLU	1
1	A	71	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	89	LEU	1
1	A	134	PHE	1
1	A	222	VAL	1
1	A	64	LEU	1
1	A	199	GLU	1
1	A	218	ILE	1
1	A	32	LEU	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 40% for the well-defined parts and 38% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	1228
Number of shifts mapped to atoms	1228
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	207	2.02 ± 0.16	Should be checked
$^{13}\text{C}_\beta$	184	3.06 ± 0.13	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	192	0.56 ± 0.40	None needed (imprecise)

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 40%, i.e. 1114 atoms were assigned a chemical shift out of a possible 2767. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	529/1021 (52%)	173/416 (42%)	183/406 (45%)	173/199 (87%)
Sidechain	585/1562 (37%)	327/1015 (32%)	258/495 (52%)	0/52 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/184 (0%)	0/91 (0%)	0/88 (0%)	0/5 (0%)
Overall	1114/2767 (40%)	500/1522 (33%)	441/989 (45%)	173/256 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 1228 atoms were assigned a chemical shift out of a possible 3199. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	591/1188 (50%)	192/483 (40%)	207/474 (44%)	192/231 (83%)
Sidechain	637/1808 (35%)	351/1167 (30%)	286/581 (49%)	0/60 (0%)
Aromatic	0/203 (0%)	0/100 (0%)	0/98 (0%)	0/5 (0%)
Overall	1228/3199 (38%)	543/1750 (31%)	493/1153 (43%)	192/296 (65%)

7.1.4 Statistically unusual chemical shifts [i](#)

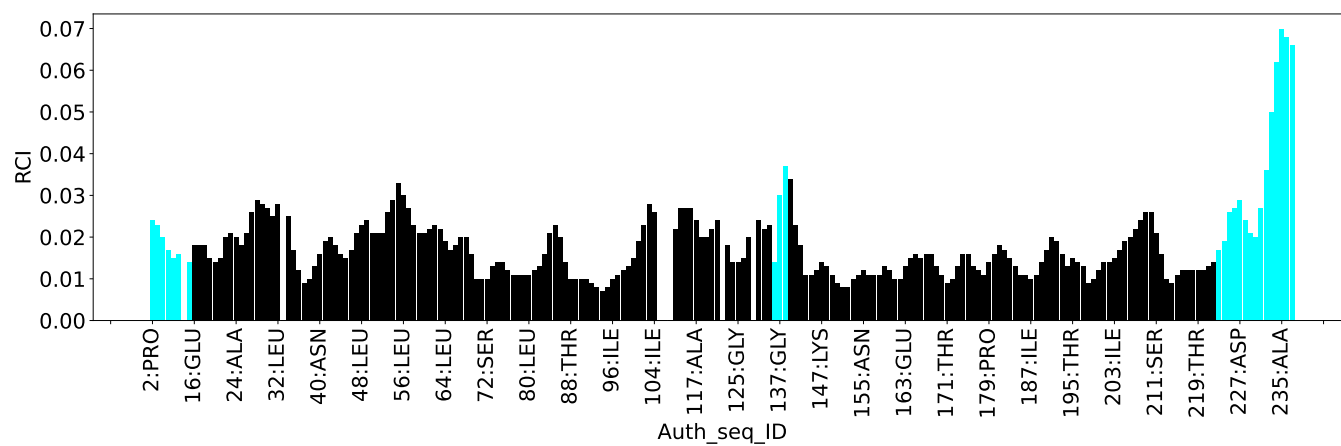
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	144	VAL	CG1	12.75	14.71 – 28.29	-6.4
1	A	37	PHE	CB	27.52	29.72 – 50.07	-6.1
1	A	107	LEU	HD11	-0.90	-0.61 – 2.12	-6.1
1	A	107	LEU	HD12	-0.90	-0.61 – 2.12	-6.1
1	A	107	LEU	HD13	-0.90	-0.61 – 2.12	-6.1
1	A	144	VAL	HG11	-0.70	-0.48 – 2.12	-5.9
1	A	144	VAL	HG12	-0.70	-0.48 – 2.12	-5.9
1	A	144	VAL	HG13	-0.70	-0.48 – 2.12	-5.9
1	A	107	LEU	HD21	-0.67	-0.65 – 2.13	-5.1
1	A	107	LEU	HD22	-0.67	-0.65 – 2.13	-5.1
1	A	107	LEU	HD23	-0.67	-0.65 – 2.13	-5.1

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1126
Intra-residue ($ i-j =0$)	78
Sequential ($ i-j =1$)	254
Medium range ($ i-j >1$ and $ i-j <5$)	237
Long range ($ i-j \geq 5$)	407
Inter-chain	0
Hydrogen bond restraints	150
Disulfide bond restraints	0
Total dihedral-angle restraints	235
Number of unmapped restraints	0
Number of restraints per residue	5.7
Number of long range restraints per residue ¹	2.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	66.0	0.2
0.2-0.5 (Medium)	33.9	0.5
>0.5 (Large)	1.0	0.89

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)	11.3	5.35
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

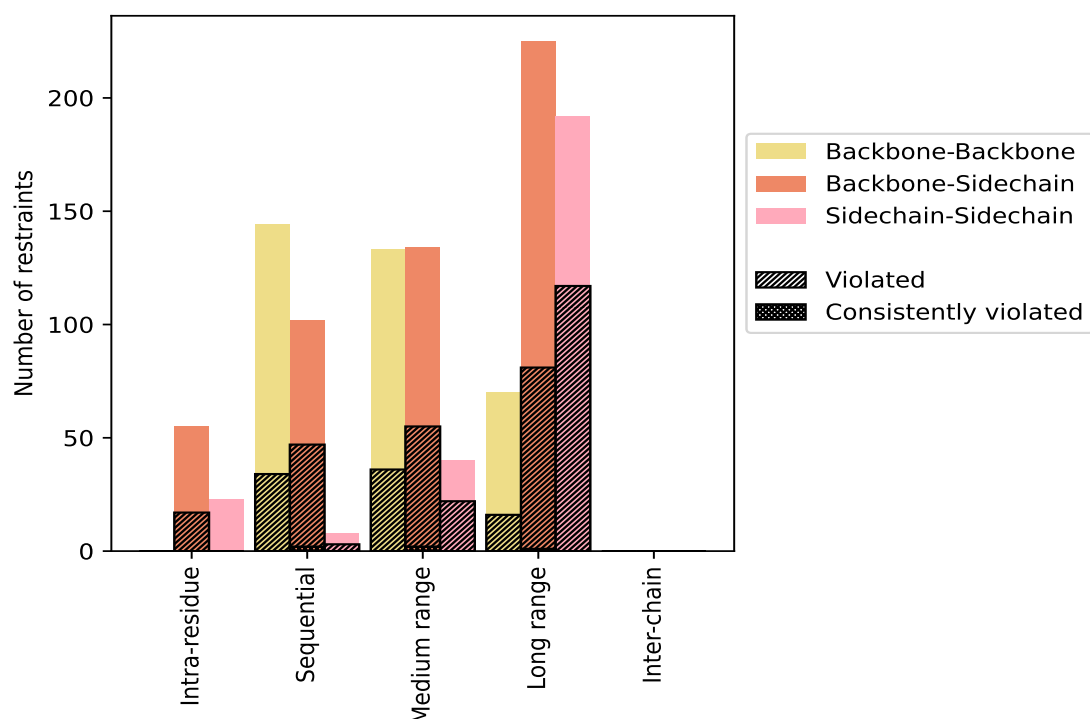
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	78	6.9	17	21.8	1.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	55	4.9	17	30.9	1.5	0	0.0	0.0
Sidechain-Sidechain	23	2.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	254	22.6	84	33.1	7.5	2	0.8	0.2
Backbone-Backbone	144	12.8	34	23.6	3.0	0	0.0	0.0
Backbone-Sidechain	102	9.1	47	46.1	4.2	2	2.0	0.2
Sidechain-Sidechain	8	0.7	3	37.5	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	237	21.0	99	41.8	8.8	2	0.8	0.2
Backbone-Backbone	133	11.8	36	27.1	3.2	0	0.0	0.0
Backbone-Sidechain	64	5.7	41	64.1	3.6	2	3.1	0.2
Sidechain-Sidechain	40	3.6	22	55.0	2.0	0	0.0	0.0
Long range ($i-j \geq 5$)	407	36.1	205	50.4	18.2	1	0.2	0.1
Backbone-Backbone	70	6.2	16	22.9	1.4	0	0.0	0.0
Backbone-Sidechain	145	12.9	72	49.7	6.4	1	0.7	0.1
Sidechain-Sidechain	192	17.1	117	60.9	10.4	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	150	13.3	23	15.3	2.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1126	100.0	428	38.0	38.0	5	0.4	0.4
Backbone-Backbone	347	30.8	86	24.8	7.6	0	0.0	0.0
Backbone-Sidechain	516	45.8	200	38.8	17.8	5	1.0	0.4
Sidechain-Sidechain	263	23.4	142	54.0	12.6	0	0.0	0.0

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

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



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

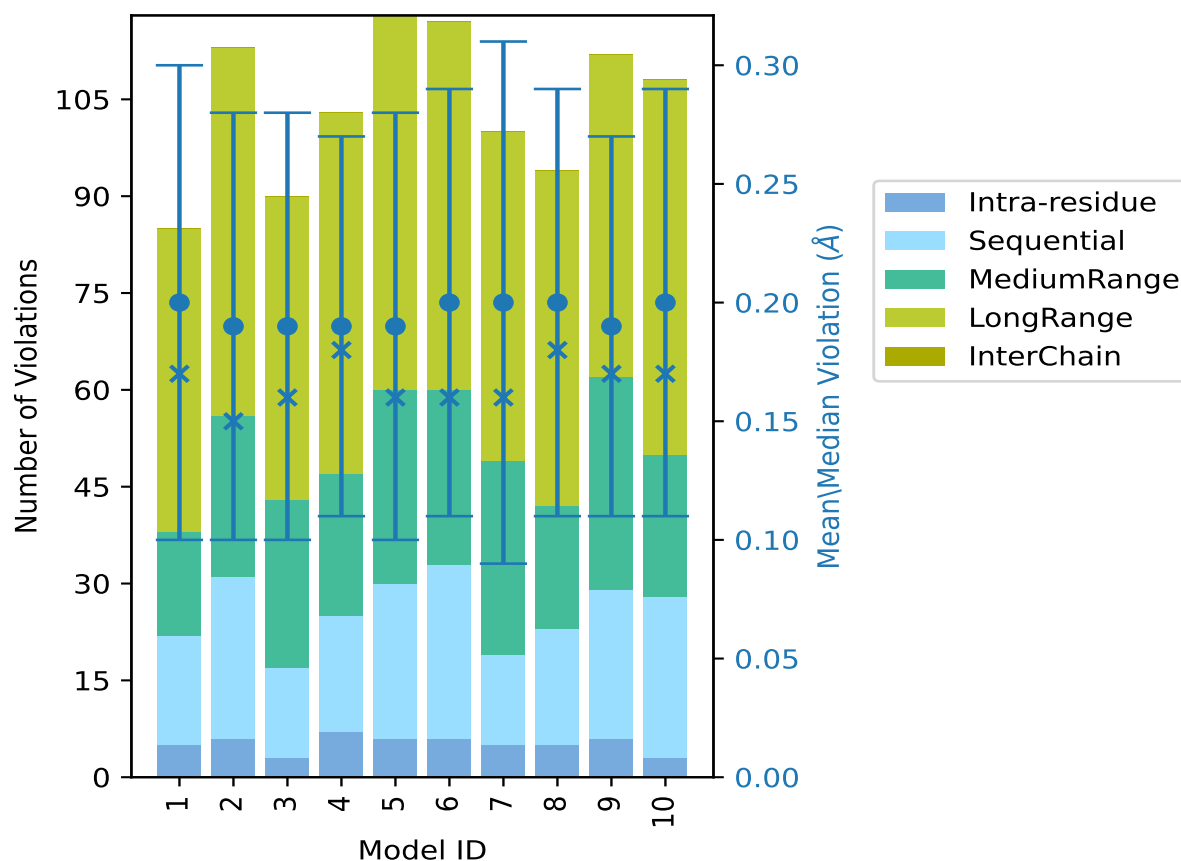
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	5	17	16	47	0	85	0.2	0.61	0.1	0.17
2	6	25	25	57	0	113	0.19	0.6	0.09	0.15
3	3	14	26	47	0	90	0.19	0.5	0.09	0.16
4	7	18	22	56	0	103	0.19	0.51	0.08	0.18
5	6	24	30	58	0	118	0.19	0.51	0.09	0.16
6	6	27	27	57	0	117	0.2	0.56	0.09	0.16
7	5	14	30	51	0	100	0.2	0.89	0.11	0.16
8	5	18	19	52	0	94	0.2	0.57	0.09	0.18
9	6	23	33	50	0	112	0.19	0.51	0.08	0.17
10	3	25	22	58	0	108	0.2	0.59	0.09	0.17

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 571(IR:61, SQ:170, MR:138, LR:202, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	41	41	82	0	169	1	10.0
3	15	27	55	0	100	2	20.0
3	12	17	21	0	53	3	30.0

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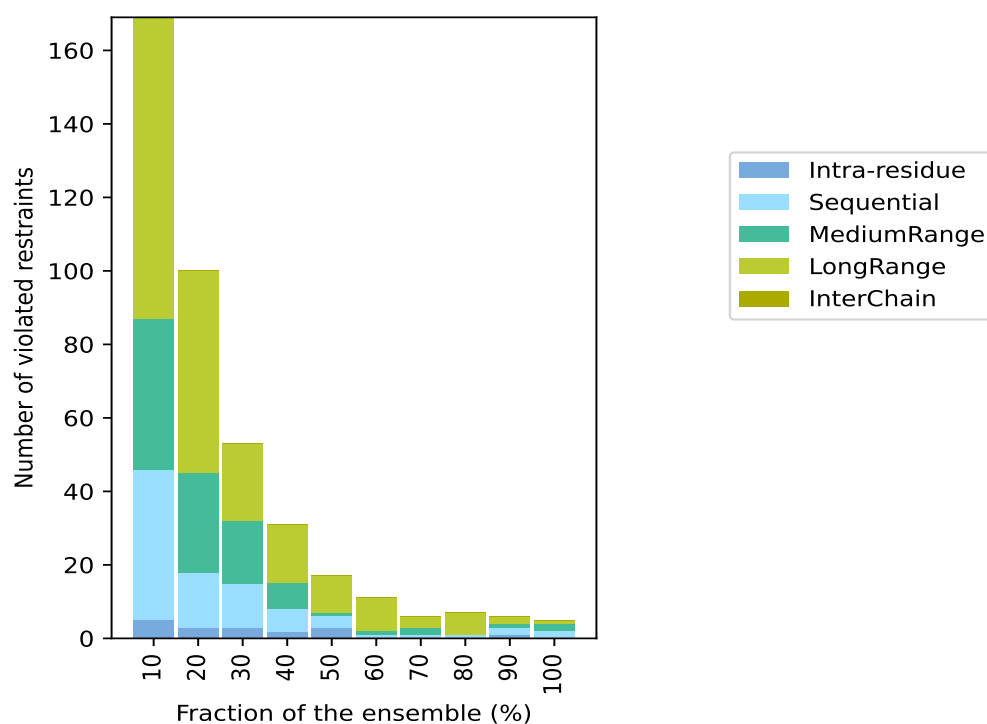
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	6	7	16	0	31	4	40.0
3	3	1	10	0	17	5	50.0
0	1	1	9	0	11	6	60.0
0	1	2	3	0	6	7	70.0
0	1	0	6	0	7	8	80.0
1	2	1	2	0	6	9	90.0
0	2	2	1	0	5	10	100.0

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

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

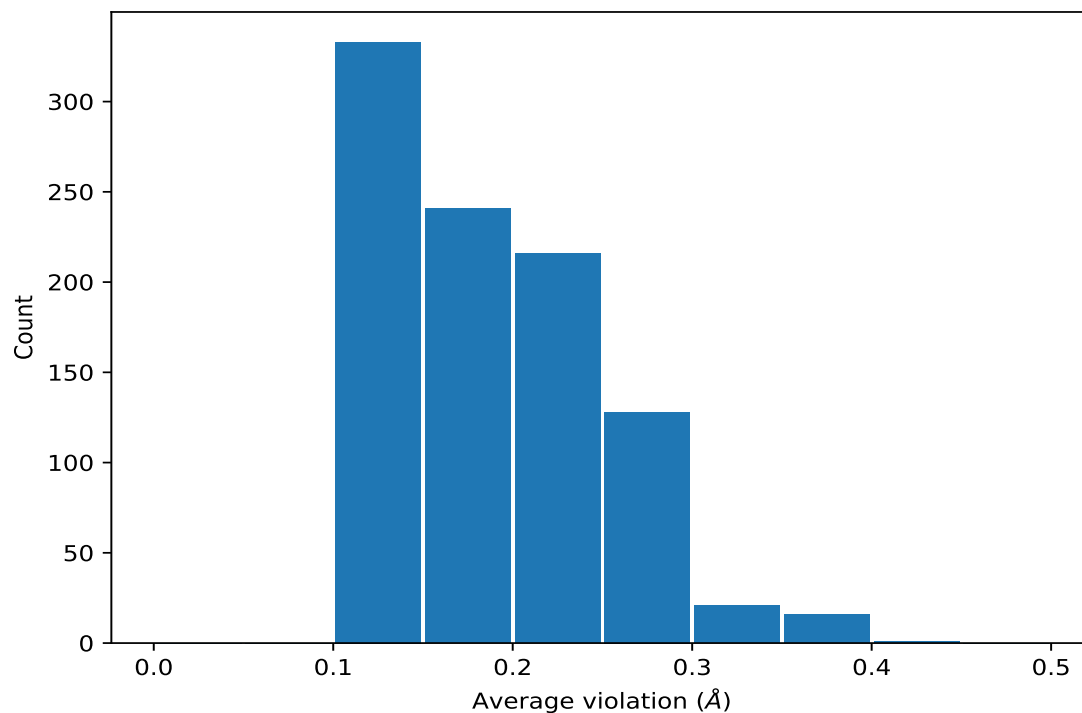


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	10	0.28	0.05	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	10	0.28	0.05	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	10	0.28	0.05	0.26
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	10	0.27	0.07	0.26
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	10	0.27	0.07	0.26
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	10	0.27	0.07	0.26
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	10	0.26	0.07	0.24
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	10	0.26	0.07	0.24
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	10	0.26	0.07	0.24
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	10	0.19	0.06	0.18
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	10	0.19	0.06	0.18
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	10	0.19	0.06	0.18
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	10	0.17	0.04	0.16
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	10	0.17	0.04	0.16
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	10	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	9	0.29	0.1	0.34
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	9	0.29	0.1	0.34
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	9	0.29	0.1	0.34
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	9	0.25	0.08	0.24
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	9	0.25	0.08	0.24
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	9	0.25	0.08	0.24
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	9	0.25	0.08	0.24
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	9	0.25	0.08	0.24
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	9	0.25	0.08	0.24
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	9	0.25	0.08	0.24
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	9	0.25	0.08	0.24
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	9	0.25	0.08	0.24
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	9	0.21	0.06	0.21
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	9	0.21	0.06	0.21
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	9	0.21	0.06	0.21
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	9	0.21	0.05	0.2
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	9	0.21	0.05	0.2
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	9	0.16	0.04	0.15
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	9	0.16	0.04	0.15
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	9	0.16	0.04	0.15
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	9	0.14	0.01	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	9	0.14	0.01	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	9	0.14	0.01	0.14
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	8	0.29	0.14	0.26
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	8	0.29	0.14	0.26
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	8	0.29	0.14	0.26
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	8	0.29	0.14	0.26
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	8	0.29	0.14	0.26
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	8	0.29	0.14	0.26
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	8	0.28	0.09	0.28
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	8	0.28	0.09	0.28
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	8	0.28	0.09	0.28
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	8	0.28	0.09	0.28
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	8	0.28	0.09	0.28
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	8	0.28	0.09	0.28
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	8	0.28	0.09	0.28
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	8	0.28	0.09	0.28
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	8	0.28	0.09	0.28
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	8	0.28	0.13	0.23
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	8	0.28	0.13	0.23
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	8	0.28	0.13	0.23
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	8	0.26	0.12	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	8	0.26	0.12	0.2
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	8	0.26	0.12	0.2
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	8	0.18	0.07	0.16
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	8	0.18	0.07	0.16
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	8	0.18	0.07	0.16
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	8	0.18	0.06	0.19
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	8	0.18	0.06	0.19
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	8	0.18	0.06	0.19
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	8	0.18	0.06	0.19
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	8	0.18	0.06	0.19
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	8	0.18	0.06	0.19
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	8	0.18	0.06	0.19
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	8	0.18	0.06	0.19
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	8	0.18	0.06	0.19
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	8	0.18	0.05	0.18
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	7	0.31	0.06	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	7	0.31	0.06	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	7	0.31	0.06	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	7	0.31	0.06	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	7	0.31	0.06	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	7	0.31	0.06	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	7	0.31	0.06	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	7	0.31	0.06	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	7	0.31	0.06	0.31
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG21	7	0.22	0.08	0.18
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG22	7	0.22	0.08	0.18
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG23	7	0.22	0.08	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG21	7	0.22	0.08	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG22	7	0.22	0.08	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG23	7	0.22	0.08	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG21	7	0.22	0.08	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG22	7	0.22	0.08	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG23	7	0.22	0.08	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG21	7	0.2	0.06	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG22	7	0.2	0.06	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG23	7	0.2	0.06	0.18
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	7	0.19	0.07	0.15
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	7	0.19	0.07	0.15
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	7	0.19	0.07	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	7	0.19	0.07	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	7	0.19	0.07	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	7	0.19	0.07	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	7	0.19	0.07	0.15
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	7	0.19	0.07	0.15
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	7	0.19	0.07	0.15
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG11	7	0.18	0.04	0.17
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG12	7	0.18	0.04	0.17
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG13	7	0.18	0.04	0.17
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG11	7	0.18	0.04	0.17
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG12	7	0.18	0.04	0.17
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG13	7	0.18	0.04	0.17
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG11	7	0.18	0.04	0.17
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG12	7	0.18	0.04	0.17
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG13	7	0.18	0.04	0.17
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG11	7	0.17	0.06	0.14
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG12	7	0.17	0.06	0.14
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG13	7	0.17	0.06	0.14
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD21	6	0.29	0.09	0.32
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD22	6	0.29	0.09	0.32
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD23	6	0.29	0.09	0.32
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG11	6	0.28	0.07	0.29
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG12	6	0.28	0.07	0.29
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG13	6	0.28	0.07	0.29
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG21	6	0.25	0.04	0.24
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG22	6	0.25	0.04	0.24
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG23	6	0.25	0.04	0.24
(1,671)	1:73:A:GLY:H	1:74:A:LYS:H	6	0.24	0.08	0.24
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD11	6	0.22	0.06	0.24
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD12	6	0.22	0.06	0.24
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD13	6	0.22	0.06	0.24
(1,85)	1:152:A:THR:HG21	1:160:A:TYR:HE2	6	0.21	0.04	0.23
(1,85)	1:152:A:THR:HG22	1:160:A:TYR:HE2	6	0.21	0.04	0.23
(1,85)	1:152:A:THR:HG23	1:160:A:TYR:HE2	6	0.21	0.04	0.23
(1,98)	1:172:A:VAL:HG21	1:170:A:PHE:HE1	6	0.2	0.1	0.17
(1,98)	1:172:A:VAL:HG22	1:170:A:PHE:HE1	6	0.2	0.1	0.17
(1,98)	1:172:A:VAL:HG23	1:170:A:PHE:HE1	6	0.2	0.1	0.17
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	6	0.19	0.05	0.18
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	6	0.19	0.05	0.18
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	6	0.19	0.05	0.18
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	6	0.19	0.05	0.18
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	6	0.19	0.05	0.18
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	6	0.19	0.05	0.18
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	6	0.19	0.05	0.18
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	6	0.19	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	6	0.19	0.05	0.18
(1,81)	1:148:A:VAL:HG11	1:142:A:TYR:HE2	6	0.18	0.05	0.2
(1,81)	1:148:A:VAL:HG12	1:142:A:TYR:HE2	6	0.18	0.05	0.2
(1,81)	1:148:A:VAL:HG13	1:142:A:TYR:HE2	6	0.18	0.05	0.2
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB1	6	0.16	0.03	0.16
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB2	6	0.16	0.03	0.16
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB3	6	0.16	0.03	0.16
(1,77)	1:144:A:VAL:HG11	1:197:A:TYR:HD2	6	0.14	0.03	0.14
(1,77)	1:144:A:VAL:HG12	1:197:A:TYR:HD2	6	0.14	0.03	0.14
(1,77)	1:144:A:VAL:HG13	1:197:A:TYR:HD2	6	0.14	0.03	0.14
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG11	5	0.31	0.02	0.31
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG12	5	0.31	0.02	0.31
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG13	5	0.31	0.02	0.31
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD21	5	0.27	0.16	0.17
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD22	5	0.27	0.16	0.17
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD23	5	0.27	0.16	0.17
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG21	5	0.24	0.06	0.23
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG22	5	0.24	0.06	0.23
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG23	5	0.24	0.06	0.23
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG21	5	0.23	0.09	0.25
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG22	5	0.23	0.09	0.25
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG23	5	0.23	0.09	0.25
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD21	5	0.21	0.09	0.2
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD22	5	0.21	0.09	0.2
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD23	5	0.21	0.09	0.2
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG11	5	0.2	0.09	0.15
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG12	5	0.2	0.09	0.15
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG13	5	0.2	0.09	0.15
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD11	5	0.19	0.07	0.15
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD12	5	0.19	0.07	0.15
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD13	5	0.19	0.07	0.15
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	5	0.19	0.1	0.14
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	5	0.19	0.1	0.14
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	5	0.19	0.1	0.14
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	5	0.19	0.1	0.14
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	5	0.19	0.1	0.14
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	5	0.19	0.1	0.14
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	5	0.19	0.1	0.14
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	5	0.19	0.1	0.14
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	5	0.19	0.1	0.14
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	5	0.18	0.03	0.18
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	5	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	5	0.18	0.03	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	5	0.18	0.03	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	5	0.18	0.03	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	5	0.18	0.03	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	5	0.18	0.03	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	5	0.18	0.03	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	5	0.18	0.03	0.18
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD11	5	0.17	0.04	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD12	5	0.17	0.04	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD13	5	0.17	0.04	0.2
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG21	5	0.16	0.04	0.16
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG22	5	0.16	0.04	0.16
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG23	5	0.16	0.04	0.16
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE1	5	0.16	0.03	0.16
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE2	5	0.16	0.03	0.16
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE3	5	0.16	0.03	0.16
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD11	5	0.16	0.02	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD12	5	0.16	0.02	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD13	5	0.16	0.02	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD11	5	0.16	0.02	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD12	5	0.16	0.02	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD13	5	0.16	0.02	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD11	5	0.16	0.02	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD12	5	0.16	0.02	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD13	5	0.16	0.02	0.15
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG21	5	0.15	0.02	0.14
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG22	5	0.15	0.02	0.14
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG23	5	0.15	0.02	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG21	5	0.14	0.02	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG22	5	0.14	0.02	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG23	5	0.14	0.02	0.14
(2,126)	1:59:A:ILE:H	1:55:A:ALA:O	5	0.14	0.02	0.13
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG21	5	0.13	0.02	0.12
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG22	5	0.13	0.02	0.12
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG23	5	0.13	0.02	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG21	5	0.13	0.02	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG22	5	0.13	0.02	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG23	5	0.13	0.02	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG21	5	0.13	0.02	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG22	5	0.13	0.02	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG23	5	0.13	0.02	0.12
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB1	5	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB2	5	0.13	0.01	0.13
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB3	5	0.13	0.01	0.13
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG11	4	0.39	0.16	0.47
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG12	4	0.39	0.16	0.47
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG13	4	0.39	0.16	0.47
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE1	4	0.38	0.31	0.25
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE2	4	0.38	0.31	0.25
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE1	4	0.38	0.31	0.25
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE2	4	0.38	0.31	0.25
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE1	4	0.38	0.31	0.25
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE2	4	0.38	0.31	0.25
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG21	4	0.36	0.01	0.36
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG22	4	0.36	0.01	0.36
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG23	4	0.36	0.01	0.36
(1,16)	1:30:A:MET:HE1	1:139:A:TYR:HD1	4	0.29	0.09	0.29
(1,16)	1:30:A:MET:HE2	1:139:A:TYR:HD1	4	0.29	0.09	0.29
(1,16)	1:30:A:MET:HE3	1:139:A:TYR:HD1	4	0.29	0.09	0.29
(1,102)	1:188:A:LEU:HD11	1:44:A:PHE:HD2	4	0.25	0.02	0.25
(1,102)	1:188:A:LEU:HD12	1:44:A:PHE:HD2	4	0.25	0.02	0.25
(1,102)	1:188:A:LEU:HD13	1:44:A:PHE:HD2	4	0.25	0.02	0.25
(1,744)	1:192:A:GLU:H	1:193:A:ASP:H	4	0.25	0.15	0.16
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD21	4	0.23	0.18	0.13
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD22	4	0.23	0.18	0.13
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD23	4	0.23	0.18	0.13
(1,831)	1:192:A:GLU:H	1:194:A:GLN:H	4	0.22	0.09	0.2
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG11	4	0.22	0.03	0.22
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG12	4	0.22	0.03	0.22
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG13	4	0.22	0.03	0.22
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG21	4	0.21	0.04	0.2
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG22	4	0.21	0.04	0.2
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG23	4	0.21	0.04	0.2
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD11	4	0.21	0.08	0.2
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD12	4	0.21	0.08	0.2
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD13	4	0.21	0.08	0.2
(1,703)	1:137:A:GLY:H	1:138:A:PHE:H	4	0.21	0.09	0.2
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG21	4	0.21	0.04	0.2
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG22	4	0.21	0.04	0.2
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG23	4	0.21	0.04	0.2
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG21	4	0.21	0.04	0.2
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG22	4	0.21	0.04	0.2
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG23	4	0.21	0.04	0.2
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG21	4	0.21	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG22	4	0.21	0.04	0.2
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG23	4	0.21	0.04	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD21	4	0.2	0.07	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD22	4	0.2	0.07	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD23	4	0.2	0.07	0.2
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD11	4	0.2	0.07	0.17
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD12	4	0.2	0.07	0.17
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD13	4	0.2	0.07	0.17
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	4	0.2	0.03	0.2
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	4	0.2	0.03	0.2
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	4	0.2	0.03	0.2
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	4	0.2	0.03	0.2
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	4	0.2	0.03	0.2
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	4	0.2	0.03	0.2
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	4	0.2	0.03	0.2
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	4	0.2	0.03	0.2
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	4	0.2	0.03	0.2
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE1	4	0.2	0.09	0.18
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE2	4	0.2	0.09	0.18
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE3	4	0.2	0.09	0.18
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE1	4	0.2	0.09	0.18
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE2	4	0.2	0.09	0.18
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE3	4	0.2	0.09	0.18
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE1	4	0.2	0.09	0.18
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE2	4	0.2	0.09	0.18
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE3	4	0.2	0.09	0.18
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE1	4	0.19	0.07	0.16
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE2	4	0.19	0.07	0.16
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE3	4	0.19	0.07	0.16
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD21	4	0.19	0.07	0.17
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD22	4	0.19	0.07	0.17
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD23	4	0.19	0.07	0.17
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG21	4	0.18	0.11	0.14
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG22	4	0.18	0.11	0.14
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG23	4	0.18	0.11	0.14
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG21	4	0.18	0.11	0.14
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG22	4	0.18	0.11	0.14
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG23	4	0.18	0.11	0.14
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG21	4	0.18	0.11	0.14
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG22	4	0.18	0.11	0.14
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG23	4	0.18	0.11	0.14
(1,816)	1:117:A:ALA:H	1:119:A:MET:H	4	0.18	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	4	0.18	0.05	0.18
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	4	0.18	0.05	0.18
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	4	0.18	0.05	0.18
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	4	0.18	0.05	0.18
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	4	0.18	0.05	0.18
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	4	0.18	0.05	0.18
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	4	0.18	0.05	0.18
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	4	0.18	0.05	0.18
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	4	0.18	0.05	0.18
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG11	4	0.17	0.04	0.17
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG12	4	0.17	0.04	0.17
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG13	4	0.17	0.04	0.17
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG11	4	0.17	0.04	0.17
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG12	4	0.17	0.04	0.17
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG13	4	0.17	0.04	0.17
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG11	4	0.17	0.04	0.17
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG12	4	0.17	0.04	0.17
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG13	4	0.17	0.04	0.17
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD21	4	0.17	0.08	0.13
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD22	4	0.17	0.08	0.13
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD23	4	0.17	0.08	0.13
(1,773)	1:224:A:LYS:H	1:223:A:GLU:H	4	0.16	0.05	0.16
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG21	4	0.15	0.03	0.15
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG22	4	0.15	0.03	0.15
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG23	4	0.15	0.03	0.15
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG21	4	0.15	0.03	0.15
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG22	4	0.15	0.03	0.15
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG23	4	0.15	0.03	0.15
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG21	4	0.15	0.03	0.15
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG22	4	0.15	0.03	0.15
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG23	4	0.15	0.03	0.15
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD11	4	0.15	0.04	0.12
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD12	4	0.15	0.04	0.12
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD13	4	0.15	0.04	0.12
(1,829)	1:180:A:MET:H	1:182:A:ARG:H	4	0.15	0.04	0.13
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	4	0.15	0.04	0.14
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD11	4	0.14	0.03	0.14
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD12	4	0.14	0.03	0.14
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD13	4	0.14	0.03	0.14
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB1	4	0.14	0.02	0.14
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB2	4	0.14	0.02	0.14
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB3	4	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,875)	1:68:A:SER:H	1:71:A:ASP:H	4	0.12	0.02	0.12
(1,885)	1:121:A:ALA:H	1:124:A:ALA:H	3	0.41	0.19	0.5
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD21	3	0.39	0.2	0.44
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD22	3	0.39	0.2	0.44
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD23	3	0.39	0.2	0.44
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD11	3	0.29	0.05	0.3
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD12	3	0.29	0.05	0.3
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD13	3	0.29	0.05	0.3
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD21	3	0.28	0.04	0.29
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD22	3	0.28	0.04	0.29
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD23	3	0.28	0.04	0.29
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD21	3	0.28	0.04	0.29
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD22	3	0.28	0.04	0.29
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD23	3	0.28	0.04	0.29
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD21	3	0.28	0.04	0.29
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD22	3	0.28	0.04	0.29
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD23	3	0.28	0.04	0.29
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD21	3	0.26	0.11	0.27
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD22	3	0.26	0.11	0.27
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD23	3	0.26	0.11	0.27
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG21	3	0.26	0.01	0.26
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG22	3	0.26	0.01	0.26
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG23	3	0.26	0.01	0.26
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG21	3	0.26	0.01	0.26
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG22	3	0.26	0.01	0.26
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG23	3	0.26	0.01	0.26
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG21	3	0.26	0.01	0.26
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG22	3	0.26	0.01	0.26
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG23	3	0.26	0.01	0.26
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE1	3	0.25	0.11	0.26
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE2	3	0.25	0.11	0.26
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE3	3	0.25	0.11	0.26
(1,222)	1:134:A:PHE:HD1	1:121:A:ALA:H	3	0.25	0.06	0.22
(1,222)	1:134:A:PHE:HD2	1:121:A:ALA:H	3	0.25	0.06	0.22
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG11	3	0.25	0.05	0.26
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG12	3	0.25	0.05	0.26
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG13	3	0.25	0.05	0.26
(1,745)	1:193:A:ASP:H	1:194:A:GLN:H	3	0.25	0.09	0.3
(1,43)	1:103:A:LEU:HD21	1:160:A:TYR:HE1	3	0.23	0.13	0.16
(1,43)	1:103:A:LEU:HD21	1:160:A:TYR:HE2	3	0.23	0.13	0.16
(1,43)	1:103:A:LEU:HD22	1:160:A:TYR:HE1	3	0.23	0.13	0.16
(1,43)	1:103:A:LEU:HD22	1:160:A:TYR:HE2	3	0.23	0.13	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,43)	1:103:A:LEU:HD23	1:160:A:TYR:HE1	3	0.23	0.13	0.16
(1,43)	1:103:A:LEU:HD23	1:160:A:TYR:HE2	3	0.23	0.13	0.16
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG21	3	0.23	0.05	0.25
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG22	3	0.23	0.05	0.25
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG23	3	0.23	0.05	0.25
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD11	3	0.23	0.07	0.2
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD12	3	0.23	0.07	0.2
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD13	3	0.23	0.07	0.2
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG21	3	0.22	0.03	0.24
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG22	3	0.22	0.03	0.24
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG23	3	0.22	0.03	0.24
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG21	3	0.22	0.09	0.19
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG22	3	0.22	0.09	0.19
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG23	3	0.22	0.09	0.19
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG21	3	0.22	0.09	0.19
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG22	3	0.22	0.09	0.19
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG23	3	0.22	0.09	0.19
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG21	3	0.22	0.09	0.19
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG22	3	0.22	0.09	0.19
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG23	3	0.22	0.09	0.19
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB1	3	0.22	0.11	0.15
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB2	3	0.22	0.11	0.15
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB3	3	0.22	0.11	0.15
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB1	3	0.22	0.11	0.15
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB2	3	0.22	0.11	0.15
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB3	3	0.22	0.11	0.15
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB1	3	0.22	0.11	0.15
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB2	3	0.22	0.11	0.15
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB3	3	0.22	0.11	0.15
(1,97)	1:172:A:VAL:HG21	1:160:A:TYR:HE1	3	0.22	0.06	0.25
(1,97)	1:172:A:VAL:HG22	1:160:A:TYR:HE1	3	0.22	0.06	0.25
(1,97)	1:172:A:VAL:HG23	1:160:A:TYR:HE1	3	0.22	0.06	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG21	3	0.22	0.05	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG22	3	0.22	0.05	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG23	3	0.22	0.05	0.25
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD11	3	0.21	0.03	0.23
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD12	3	0.21	0.03	0.23
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD13	3	0.21	0.03	0.23
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB1	3	0.21	0.05	0.23
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB2	3	0.21	0.05	0.23
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB3	3	0.21	0.05	0.23
(1,68)	1:130:A:MET:HE1	1:134:A:PHE:HD2	3	0.21	0.07	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,68)	1:130:A:MET:HE2	1:134:A:PHE:HD2	3	0.21	0.07	0.19
(1,68)	1:130:A:MET:HE3	1:134:A:PHE:HD2	3	0.21	0.07	0.19
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG21	3	0.21	0.12	0.13
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG22	3	0.21	0.12	0.13
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG23	3	0.21	0.12	0.13
(1,106)	1:206:A:ILE:HD11	1:44:A:PHE:HE1	3	0.21	0.09	0.15
(1,106)	1:206:A:ILE:HD11	1:44:A:PHE:HE2	3	0.21	0.09	0.15
(1,106)	1:206:A:ILE:HD12	1:44:A:PHE:HE1	3	0.21	0.09	0.15
(1,106)	1:206:A:ILE:HD12	1:44:A:PHE:HE2	3	0.21	0.09	0.15
(1,106)	1:206:A:ILE:HD13	1:44:A:PHE:HE1	3	0.21	0.09	0.15
(1,106)	1:206:A:ILE:HD13	1:44:A:PHE:HE2	3	0.21	0.09	0.15
(1,70)	1:141:A:ALA:HB1	1:138:A:PHE:HD1	3	0.21	0.02	0.2
(1,70)	1:141:A:ALA:HB1	1:138:A:PHE:HD2	3	0.21	0.02	0.2
(1,70)	1:141:A:ALA:HB2	1:138:A:PHE:HD1	3	0.21	0.02	0.2
(1,70)	1:141:A:ALA:HB2	1:138:A:PHE:HD2	3	0.21	0.02	0.2
(1,70)	1:141:A:ALA:HB3	1:138:A:PHE:HD1	3	0.21	0.02	0.2
(1,70)	1:141:A:ALA:HB3	1:138:A:PHE:HD2	3	0.21	0.02	0.2
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD21	3	0.2	0.06	0.23
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD22	3	0.2	0.06	0.23
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD23	3	0.2	0.06	0.23
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD21	3	0.2	0.06	0.23
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD22	3	0.2	0.06	0.23
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD23	3	0.2	0.06	0.23
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD21	3	0.2	0.06	0.23
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD22	3	0.2	0.06	0.23
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD23	3	0.2	0.06	0.23
(1,667)	1:69:A:LYS:H	1:70:A:LEU:H	3	0.2	0.11	0.13
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG21	3	0.2	0.05	0.16
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG22	3	0.2	0.05	0.16
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG23	3	0.2	0.05	0.16
(1,730)	1:176:A:THR:H	1:177:A:GLY:H	3	0.19	0.04	0.2
(1,743)	1:191:A:LYS:H	1:192:A:GLU:H	3	0.19	0.09	0.13
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD11	3	0.19	0.05	0.22
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD12	3	0.19	0.05	0.22
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD13	3	0.19	0.05	0.22
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD11	3	0.19	0.04	0.16
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD12	3	0.19	0.04	0.16
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD13	3	0.19	0.04	0.16
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB1	3	0.19	0.04	0.19
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB2	3	0.19	0.04	0.19
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB3	3	0.19	0.04	0.19
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB1	3	0.19	0.04	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB2	3	0.19	0.04	0.19
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB3	3	0.19	0.04	0.19
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB1	3	0.19	0.04	0.19
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB2	3	0.19	0.04	0.19
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB3	3	0.19	0.04	0.19
(1,167)	1:184:A:THR:H	1:180:A:MET:HE1	3	0.18	0.07	0.15
(1,167)	1:184:A:THR:H	1:180:A:MET:HE2	3	0.18	0.07	0.15
(1,167)	1:184:A:THR:H	1:180:A:MET:HE3	3	0.18	0.07	0.15
(1,99)	1:174:A:THR:HG21	1:160:A:TYR:HE1	3	0.18	0.09	0.12
(1,99)	1:174:A:THR:HG22	1:160:A:TYR:HE1	3	0.18	0.09	0.12
(1,99)	1:174:A:THR:HG23	1:160:A:TYR:HE1	3	0.18	0.09	0.12
(1,823)	1:141:A:ALA:H	1:143:A:LEU:H	3	0.18	0.04	0.16
(1,187)	1:160:A:TYR:HD1	1:159:A:GLN:H	3	0.17	0.02	0.18
(1,187)	1:160:A:TYR:HD2	1:159:A:GLN:H	3	0.17	0.02	0.18
(1,192)	1:216:A:TYR:HE1	1:57:A:ASP:H	3	0.17	0.05	0.16
(1,192)	1:216:A:TYR:HE2	1:57:A:ASP:H	3	0.17	0.05	0.16
(1,14)	1:32:A:LEU:HD21	1:118:A:PHE:HE2	3	0.16	0.04	0.17
(1,14)	1:32:A:LEU:HD22	1:118:A:PHE:HE2	3	0.16	0.04	0.17
(1,14)	1:32:A:LEU:HD23	1:118:A:PHE:HE2	3	0.16	0.04	0.17
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB1	3	0.16	0.04	0.16
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB2	3	0.16	0.04	0.16
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB3	3	0.16	0.04	0.16
(1,230)	1:134:A:PHE:HD1	1:131:A:ILE:H	3	0.15	0.04	0.13
(1,230)	1:134:A:PHE:HD2	1:131:A:ILE:H	3	0.15	0.04	0.13
(1,722)	1:167:A:GLY:H	1:168:A:GLY:H	3	0.15	0.03	0.16
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD11	3	0.15	0.04	0.13
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD12	3	0.15	0.04	0.13
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD13	3	0.15	0.04	0.13
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD21	3	0.15	0.05	0.11
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD22	3	0.15	0.05	0.11
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD23	3	0.15	0.05	0.11
(1,966)	1:154:A:HIS:H	1:183:A:GLY:H	3	0.14	0.03	0.13
(1,110)	1:219:A:THR:HG21	1:221:A:PHE:HE1	3	0.14	0.03	0.13
(1,110)	1:219:A:THR:HG22	1:221:A:PHE:HE1	3	0.14	0.03	0.13
(1,110)	1:219:A:THR:HG23	1:221:A:PHE:HE1	3	0.14	0.03	0.13
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	3	0.14	0.04	0.12
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	3	0.14	0.04	0.12
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	3	0.14	0.04	0.12
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	3	0.14	0.04	0.12
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	3	0.14	0.04	0.12
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	3	0.14	0.04	0.12
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	3	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	3	0.14	0.04	0.12
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	3	0.14	0.04	0.12
(2,108)	1:50:A:SER:H	1:46:A:ARG:O	3	0.14	0.02	0.15
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG21	3	0.13	0.01	0.13
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG22	3	0.13	0.01	0.13
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG23	3	0.13	0.01	0.13
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG21	3	0.13	0.01	0.13
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG22	3	0.13	0.01	0.13
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG23	3	0.13	0.01	0.13
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG21	3	0.13	0.01	0.13
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG22	3	0.13	0.01	0.13
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG23	3	0.13	0.01	0.13
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD11	3	0.13	0.01	0.12
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD12	3	0.13	0.01	0.12
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD13	3	0.13	0.01	0.12
(1,721)	1:168:A:GLY:H	1:169:A:SER:H	3	0.13	0.02	0.12
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD11	3	0.12	0.01	0.13
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD12	3	0.12	0.01	0.13
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD13	3	0.12	0.01	0.13
(1,828)	1:167:A:GLY:H	1:169:A:SER:H	3	0.12	0.02	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB1	3	0.12	0.01	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB2	3	0.12	0.01	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB3	3	0.12	0.01	0.11
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD21	3	0.11	0.01	0.1
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD22	3	0.11	0.01	0.1
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD23	3	0.11	0.01	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD21	3	0.11	0.01	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD22	3	0.11	0.01	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD23	3	0.11	0.01	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD21	3	0.11	0.01	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD22	3	0.11	0.01	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD23	3	0.11	0.01	0.1
(1,830)	1:191:A:LYS:H	1:193:A:ASP:H	2	0.38	0.06	0.38
(1,733)	1:181:A:GLY:H	1:182:A:ARG:H	2	0.33	0.02	0.33
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG21	2	0.32	0.01	0.32
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG22	2	0.32	0.01	0.32
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG23	2	0.32	0.01	0.32
(1,221)	1:134:A:PHE:HE1	1:121:A:ALA:H	2	0.32	0.04	0.32
(1,221)	1:134:A:PHE:HE2	1:121:A:ALA:H	2	0.32	0.04	0.32
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD11	2	0.31	0.02	0.31
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD12	2	0.31	0.02	0.31
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD13	2	0.31	0.02	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB1	2	0.28	0.1	0.28
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB2	2	0.28	0.1	0.28
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB3	2	0.28	0.1	0.28
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB1	2	0.28	0.1	0.28
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB2	2	0.28	0.1	0.28
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB3	2	0.28	0.1	0.28
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB1	2	0.28	0.1	0.28
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB2	2	0.28	0.1	0.28
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB3	2	0.28	0.1	0.28
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD21	2	0.27	0.01	0.27
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD22	2	0.27	0.01	0.27
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD23	2	0.27	0.01	0.27
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE1	2	0.26	0.12	0.26
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE2	2	0.26	0.12	0.26
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE3	2	0.26	0.12	0.26
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD11	2	0.26	0.04	0.26
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD12	2	0.26	0.04	0.26
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD13	2	0.26	0.04	0.26
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD21	2	0.26	0.02	0.26
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD22	2	0.26	0.02	0.26
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD23	2	0.26	0.02	0.26
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD21	2	0.26	0.02	0.26
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD22	2	0.26	0.02	0.26
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD23	2	0.26	0.02	0.26
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD21	2	0.26	0.02	0.26
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD22	2	0.26	0.02	0.26
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD23	2	0.26	0.02	0.26
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG11	2	0.26	0.03	0.26
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG12	2	0.26	0.03	0.26
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG13	2	0.26	0.03	0.26
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB1	2	0.26	0.01	0.26
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB2	2	0.26	0.01	0.26
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB3	2	0.26	0.01	0.26
(1,772)	1:223:A:GLU:H	1:222:A:VAL:H	2	0.25	0.06	0.25
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD11	2	0.24	0.05	0.24
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD12	2	0.24	0.05	0.24
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD13	2	0.24	0.05	0.24
(1,226)	1:134:A:PHE:HD1	1:130:A:MET:H	2	0.24	0.01	0.24
(1,226)	1:134:A:PHE:HD2	1:130:A:MET:H	2	0.24	0.01	0.24
(1,889)	1:191:A:LYS:H	1:194:A:GLN:H	2	0.24	0.13	0.24
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB1	2	0.24	0.12	0.24
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB2	2	0.24	0.12	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB3	2	0.24	0.12	0.24
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD11	2	0.24	0.03	0.24
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD12	2	0.24	0.03	0.24
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD13	2	0.24	0.03	0.24
(1,223)	1:118:A:PHE:HE1	1:127:A:ASP:H	2	0.23	0.12	0.23
(1,223)	1:118:A:PHE:HE2	1:127:A:ASP:H	2	0.23	0.12	0.23
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG21	2	0.23	0.08	0.23
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG22	2	0.23	0.08	0.23
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG23	2	0.23	0.08	0.23
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG21	2	0.23	0.08	0.23
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG22	2	0.23	0.08	0.23
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG23	2	0.23	0.08	0.23
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG21	2	0.23	0.08	0.23
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG22	2	0.23	0.08	0.23
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG23	2	0.23	0.08	0.23
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD11	2	0.22	0.08	0.22
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD12	2	0.22	0.08	0.22
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD13	2	0.22	0.08	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD11	2	0.22	0.0	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD12	2	0.22	0.0	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD13	2	0.22	0.0	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD11	2	0.22	0.0	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD12	2	0.22	0.0	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD13	2	0.22	0.0	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD11	2	0.22	0.0	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD12	2	0.22	0.0	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD13	2	0.22	0.0	0.22
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD21	2	0.21	0.02	0.21
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD22	2	0.21	0.02	0.21
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD23	2	0.21	0.02	0.21
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD11	2	0.21	0.09	0.21
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD12	2	0.21	0.09	0.21
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD13	2	0.21	0.09	0.21
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD11	2	0.2	0.06	0.2
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD12	2	0.2	0.06	0.2
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD13	2	0.2	0.06	0.2
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD11	2	0.2	0.06	0.2
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD12	2	0.2	0.06	0.2
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD13	2	0.2	0.06	0.2
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD11	2	0.2	0.06	0.2
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD12	2	0.2	0.06	0.2
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD13	2	0.2	0.06	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,948)	1:146:A:GLU:H	1:191:A:LYS:H	2	0.2	0.03	0.2
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG11	2	0.2	0.02	0.2
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG12	2	0.2	0.02	0.2
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG13	2	0.2	0.02	0.2
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB1	2	0.19	0.03	0.19
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB2	2	0.19	0.03	0.19
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB3	2	0.19	0.03	0.19
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE1	2	0.19	0.02	0.19
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE2	2	0.19	0.02	0.19
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE3	2	0.19	0.02	0.19
(1,705)	1:143:A:LEU:H	1:142:A:TYR:H	2	0.19	0.08	0.19
(1,890)	1:198:A:LEU:H	1:195:A:THR:H	2	0.19	0.02	0.19
(1,189)	1:197:A:TYR:HD1	1:195:A:THR:H	2	0.18	0.01	0.18
(1,189)	1:197:A:TYR:HD2	1:195:A:THR:H	2	0.18	0.01	0.18
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG21	2	0.18	0.08	0.18
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG22	2	0.18	0.08	0.18
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG23	2	0.18	0.08	0.18
(1,874)	1:66:A:ASP:H	1:69:A:LYS:H	2	0.18	0.01	0.18
(1,52)	1:109:A:THR:HG21	1:139:A:TYR:HD2	2	0.18	0.0	0.18
(1,52)	1:109:A:THR:HG22	1:139:A:TYR:HD2	2	0.18	0.0	0.18
(1,52)	1:109:A:THR:HG23	1:139:A:TYR:HD2	2	0.18	0.0	0.18
(1,63)	1:126:A:ALA:HB1	1:118:A:PHE:HD1	2	0.18	0.02	0.18
(1,63)	1:126:A:ALA:HB2	1:118:A:PHE:HD1	2	0.18	0.02	0.18
(1,63)	1:126:A:ALA:HB3	1:118:A:PHE:HD1	2	0.18	0.02	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE1	2	0.18	0.0	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE2	2	0.18	0.0	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE3	2	0.18	0.0	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE1	2	0.18	0.0	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE2	2	0.18	0.0	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE3	2	0.18	0.0	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE1	2	0.18	0.0	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE2	2	0.18	0.0	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE3	2	0.18	0.0	0.18
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD11	2	0.18	0.04	0.18
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD12	2	0.18	0.04	0.18
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD13	2	0.18	0.04	0.18
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD11	2	0.18	0.04	0.18
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD12	2	0.18	0.04	0.18
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD13	2	0.18	0.04	0.18
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD11	2	0.18	0.04	0.18
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD12	2	0.18	0.04	0.18
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD13	2	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,964)	1:183:A:GLY:H	1:153:A:LYS:H	2	0.18	0.06	0.18
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG21	2	0.17	0.0	0.17
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG22	2	0.17	0.0	0.17
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG23	2	0.17	0.0	0.17
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	2	0.17	0.0	0.17
(1,48)	1:107:A:LEU:HD11	1:139:A:TYR:HE1	2	0.17	0.01	0.17
(1,48)	1:107:A:LEU:HD11	1:139:A:TYR:HE2	2	0.17	0.01	0.17
(1,48)	1:107:A:LEU:HD12	1:139:A:TYR:HE1	2	0.17	0.01	0.17
(1,48)	1:107:A:LEU:HD12	1:139:A:TYR:HE2	2	0.17	0.01	0.17
(1,48)	1:107:A:LEU:HD13	1:139:A:TYR:HE1	2	0.17	0.01	0.17
(1,48)	1:107:A:LEU:HD13	1:139:A:TYR:HE2	2	0.17	0.01	0.17
(1,851)	1:214:A:ILE:H	1:216:A:TYR:H	2	0.17	0.07	0.17
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG21	2	0.16	0.02	0.16
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG22	2	0.16	0.02	0.16
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG23	2	0.16	0.02	0.16
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG21	2	0.16	0.01	0.16
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG22	2	0.16	0.01	0.16
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG23	2	0.16	0.01	0.16
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG21	2	0.16	0.01	0.16
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG22	2	0.16	0.01	0.16
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG23	2	0.16	0.01	0.16
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG21	2	0.16	0.01	0.16
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG22	2	0.16	0.01	0.16
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG23	2	0.16	0.01	0.16
(1,212)	1:170:A:PHE:HE1	1:22:A:PHE:H	2	0.16	0.04	0.16
(1,212)	1:170:A:PHE:HE2	1:22:A:PHE:H	2	0.16	0.04	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG21	2	0.16	0.0	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG22	2	0.16	0.0	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG23	2	0.16	0.0	0.16
(1,827)	1:164:A:SER:H	1:166:A:ALA:H	2	0.16	0.04	0.16
(1,942)	1:97:A:GLY:H	1:183:A:GLY:H	2	0.16	0.04	0.16
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD11	2	0.16	0.02	0.16
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD12	2	0.16	0.02	0.16
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD13	2	0.16	0.02	0.16
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB1	2	0.15	0.01	0.15
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB2	2	0.15	0.01	0.15
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB3	2	0.15	0.01	0.15
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG11	2	0.15	0.02	0.15
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG12	2	0.15	0.02	0.15
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG13	2	0.15	0.02	0.15
(1,79)	1:144:A:VAL:HG21	1:44:A:PHE:HE1	2	0.15	0.04	0.15
(1,79)	1:144:A:VAL:HG21	1:44:A:PHE:HE2	2	0.15	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,79)	1:144:A:VAL:HG22	1:44:A:PHE:HE1	2	0.15	0.04	0.15
(1,79)	1:144:A:VAL:HG22	1:44:A:PHE:HE2	2	0.15	0.04	0.15
(1,79)	1:144:A:VAL:HG23	1:44:A:PHE:HE1	2	0.15	0.04	0.15
(1,79)	1:144:A:VAL:HG23	1:44:A:PHE:HE2	2	0.15	0.04	0.15
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD11	2	0.15	0.04	0.15
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD12	2	0.15	0.04	0.15
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD13	2	0.15	0.04	0.15
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG21	2	0.15	0.03	0.15
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG22	2	0.15	0.03	0.15
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG23	2	0.15	0.03	0.15
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	2	0.15	0.04	0.15
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	2	0.15	0.04	0.15
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	2	0.15	0.04	0.15
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	2	0.15	0.04	0.15
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	2	0.15	0.04	0.15
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	2	0.15	0.04	0.15
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	2	0.15	0.04	0.15
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	2	0.15	0.04	0.15
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	2	0.15	0.04	0.15
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG11	2	0.15	0.03	0.15
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG12	2	0.15	0.03	0.15
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG13	2	0.15	0.03	0.15
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG11	2	0.15	0.03	0.15
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG12	2	0.15	0.03	0.15
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG13	2	0.15	0.03	0.15
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG11	2	0.15	0.03	0.15
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG12	2	0.15	0.03	0.15
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG13	2	0.15	0.03	0.15
(1,767)	1:215:A:GLY:H	1:216:A:TYR:H	2	0.15	0.0	0.15
(1,7)	1:29:A:LEU:HD11	1:139:A:TYR:HD2	2	0.15	0.02	0.15
(1,7)	1:29:A:LEU:HD12	1:139:A:TYR:HD2	2	0.15	0.02	0.15
(1,7)	1:29:A:LEU:HD13	1:139:A:TYR:HD2	2	0.15	0.02	0.15
(1,65)	1:126:A:ALA:HB1	1:134:A:PHE:HE1	2	0.15	0.03	0.15
(1,65)	1:126:A:ALA:HB1	1:134:A:PHE:HE2	2	0.15	0.03	0.15
(1,65)	1:126:A:ALA:HB2	1:134:A:PHE:HE1	2	0.15	0.03	0.15
(1,65)	1:126:A:ALA:HB2	1:134:A:PHE:HE2	2	0.15	0.03	0.15
(1,65)	1:126:A:ALA:HB3	1:134:A:PHE:HE1	2	0.15	0.03	0.15
(1,65)	1:126:A:ALA:HB3	1:134:A:PHE:HE2	2	0.15	0.03	0.15
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	2	0.15	0.0	0.15
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	2	0.15	0.0	0.15
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	2	0.15	0.0	0.15
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	2	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	2	0.15	0.0	0.15
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	2	0.15	0.0	0.15
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	2	0.15	0.0	0.15
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	2	0.15	0.0	0.15
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD11	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD12	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD13	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD11	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD12	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD13	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD11	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD12	2	0.15	0.0	0.15
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD13	2	0.15	0.0	0.15
(2,132)	1:62:A:GLU:H	1:58:A:LYS:O	2	0.15	0.0	0.15
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD11	2	0.14	0.03	0.14
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD12	2	0.14	0.03	0.14
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD13	2	0.14	0.03	0.14
(1,950)	1:147:A:LYS:H	1:191:A:LYS:H	2	0.14	0.03	0.14
(1,13)	1:32:A:LEU:HD21	1:118:A:PHE:HD2	2	0.14	0.01	0.14
(1,13)	1:32:A:LEU:HD22	1:118:A:PHE:HD2	2	0.14	0.01	0.14
(1,13)	1:32:A:LEU:HD23	1:118:A:PHE:HD2	2	0.14	0.01	0.14
(1,32)	1:81:A:ILE:HD11	1:221:A:PHE:HD1	2	0.14	0.03	0.14
(1,32)	1:81:A:ILE:HD11	1:221:A:PHE:HD2	2	0.14	0.03	0.14
(1,32)	1:81:A:ILE:HD12	1:221:A:PHE:HD1	2	0.14	0.03	0.14
(1,32)	1:81:A:ILE:HD12	1:221:A:PHE:HD2	2	0.14	0.03	0.14
(1,32)	1:81:A:ILE:HD13	1:221:A:PHE:HD1	2	0.14	0.03	0.14
(1,32)	1:81:A:ILE:HD13	1:221:A:PHE:HD2	2	0.14	0.03	0.14
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD11	2	0.14	0.02	0.14
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD12	2	0.14	0.02	0.14
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD13	2	0.14	0.02	0.14
(1,204)	1:22:A:PHE:HD1	1:26:A:ILE:H	2	0.14	0.01	0.14
(1,204)	1:22:A:PHE:HD2	1:26:A:ILE:H	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD11	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD12	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD13	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD11	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD12	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD13	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD11	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD12	2	0.14	0.01	0.14
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD13	2	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD11	2	0.14	0.03	0.14
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD12	2	0.14	0.03	0.14
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD13	2	0.14	0.03	0.14
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD11	2	0.14	0.03	0.14
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD12	2	0.14	0.03	0.14
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD13	2	0.14	0.03	0.14
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD11	2	0.14	0.03	0.14
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD12	2	0.14	0.03	0.14
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD13	2	0.14	0.03	0.14
(1,883)	1:117:A:ALA:H	1:120:A:GLU:H	2	0.14	0.03	0.14
(1,11)	1:32:A:LEU:HD11	1:118:A:PHE:HD2	2	0.14	0.02	0.14
(1,11)	1:32:A:LEU:HD12	1:118:A:PHE:HD2	2	0.14	0.02	0.14
(1,11)	1:32:A:LEU:HD13	1:118:A:PHE:HD2	2	0.14	0.02	0.14
(1,15)	1:30:A:MET:HE1	1:22:A:PHE:HE1	2	0.14	0.02	0.14
(1,15)	1:30:A:MET:HE1	1:22:A:PHE:HE2	2	0.14	0.02	0.14
(1,15)	1:30:A:MET:HE2	1:22:A:PHE:HE1	2	0.14	0.02	0.14
(1,15)	1:30:A:MET:HE2	1:22:A:PHE:HE2	2	0.14	0.02	0.14
(1,15)	1:30:A:MET:HE3	1:22:A:PHE:HE1	2	0.14	0.02	0.14
(1,15)	1:30:A:MET:HE3	1:22:A:PHE:HE2	2	0.14	0.02	0.14
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB1	2	0.14	0.01	0.14
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB2	2	0.14	0.01	0.14
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB3	2	0.14	0.01	0.14
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD21	2	0.14	0.01	0.14
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD22	2	0.14	0.01	0.14
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD23	2	0.14	0.01	0.14
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	2	0.14	0.02	0.14
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	2	0.14	0.02	0.14
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	2	0.14	0.02	0.14
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	2	0.14	0.02	0.14
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	2	0.14	0.02	0.14
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	2	0.14	0.02	0.14
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	2	0.14	0.02	0.14
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	2	0.14	0.02	0.14
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	2	0.14	0.02	0.14
(1,49)	1:107:A:LEU:HD11	1:142:A:TYR:HE2	2	0.13	0.02	0.13
(1,49)	1:107:A:LEU:HD12	1:142:A:TYR:HE2	2	0.13	0.02	0.13
(1,49)	1:107:A:LEU:HD13	1:142:A:TYR:HE2	2	0.13	0.02	0.13
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB1	2	0.13	0.01	0.13
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB2	2	0.13	0.01	0.13
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB3	2	0.13	0.01	0.13
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE1	2	0.13	0.02	0.13
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE2	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)
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE3	2	0.13	0.02	0.13
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE1	2	0.13	0.02	0.13
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE2	2	0.13	0.02	0.13
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE3	2	0.13	0.02	0.13
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE1	2	0.13	0.02	0.13
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE2	2	0.13	0.02	0.13
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE3	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE1	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE2	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE3	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE1	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE2	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE3	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE1	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE2	2	0.13	0.02	0.13
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE3	2	0.13	0.02	0.13
(1,967)	1:159:A:GLN:H	1:175:A:ASP:H	2	0.13	0.01	0.13
(1,104)	1:188:A:LEU:HD21	1:44:A:PHE:HE2	2	0.12	0.01	0.12
(1,104)	1:188:A:LEU:HD22	1:44:A:PHE:HE2	2	0.12	0.01	0.12
(1,104)	1:188:A:LEU:HD23	1:44:A:PHE:HE2	2	0.12	0.01	0.12
(1,229)	1:118:A:PHE:HD1	1:131:A:ILE:H	2	0.12	0.01	0.12
(1,229)	1:118:A:PHE:HD2	1:131:A:ILE:H	2	0.12	0.01	0.12
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD11	2	0.12	0.01	0.12
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD12	2	0.12	0.01	0.12
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD13	2	0.12	0.01	0.12
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD11	2	0.12	0.01	0.12
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD12	2	0.12	0.01	0.12
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD13	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD11	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD12	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD13	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD11	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD12	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD13	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD11	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD12	2	0.12	0.01	0.12
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD13	2	0.12	0.01	0.12
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	2	0.12	0.02	0.12
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	2	0.12	0.02	0.12
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	2	0.12	0.02	0.12
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	2	0.12	0.02	0.12
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	2	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	2	0.12	0.02	0.12
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	2	0.12	0.02	0.12
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	2	0.12	0.02	0.12
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	2	0.12	0.02	0.12
(1,672)	1:74:A:LYS:H	1:75:A:GLU:H	2	0.12	0.01	0.12
(1,939)	1:93:A:ASP:H	1:186:A:VAL:H	2	0.12	0.01	0.12
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD11	2	0.12	0.02	0.12
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD12	2	0.12	0.02	0.12
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD13	2	0.12	0.02	0.12
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD11	2	0.12	0.02	0.12
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD12	2	0.12	0.02	0.12
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD13	2	0.12	0.02	0.12
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD11	2	0.12	0.02	0.12
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD12	2	0.12	0.02	0.12
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD13	2	0.12	0.02	0.12
(1,86)	1:166:A:ALA:HB1	1:22:A:PHE:HE2	2	0.12	0.0	0.12
(1,86)	1:166:A:ALA:HB2	1:22:A:PHE:HE2	2	0.12	0.0	0.12
(1,86)	1:166:A:ALA:HB3	1:22:A:PHE:HE2	2	0.12	0.0	0.12
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD11	2	0.12	0.01	0.12
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD12	2	0.12	0.01	0.12
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD13	2	0.12	0.01	0.12
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG21	2	0.12	0.01	0.12
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG22	2	0.12	0.01	0.12
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG23	2	0.12	0.01	0.12
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG11	2	0.12	0.01	0.12
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG12	2	0.12	0.01	0.12
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG13	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	2	0.12	0.01	0.12
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	2	0.12	0.01	0.12
(1,194)	1:77:A:HIS:HE1	1:76:A:LEU:H	2	0.12	0.02	0.12
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG21	2	0.12	0.02	0.12
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG22	2	0.12	0.02	0.12
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG23	2	0.12	0.02	0.12
(2,125)	1:59:A:ILE:N	1:55:A:ALA:O	2	0.12	0.0	0.12
(1,783)	1:44:A:PHE:H	1:46:A:ARG:H	2	0.11	0.0	0.11

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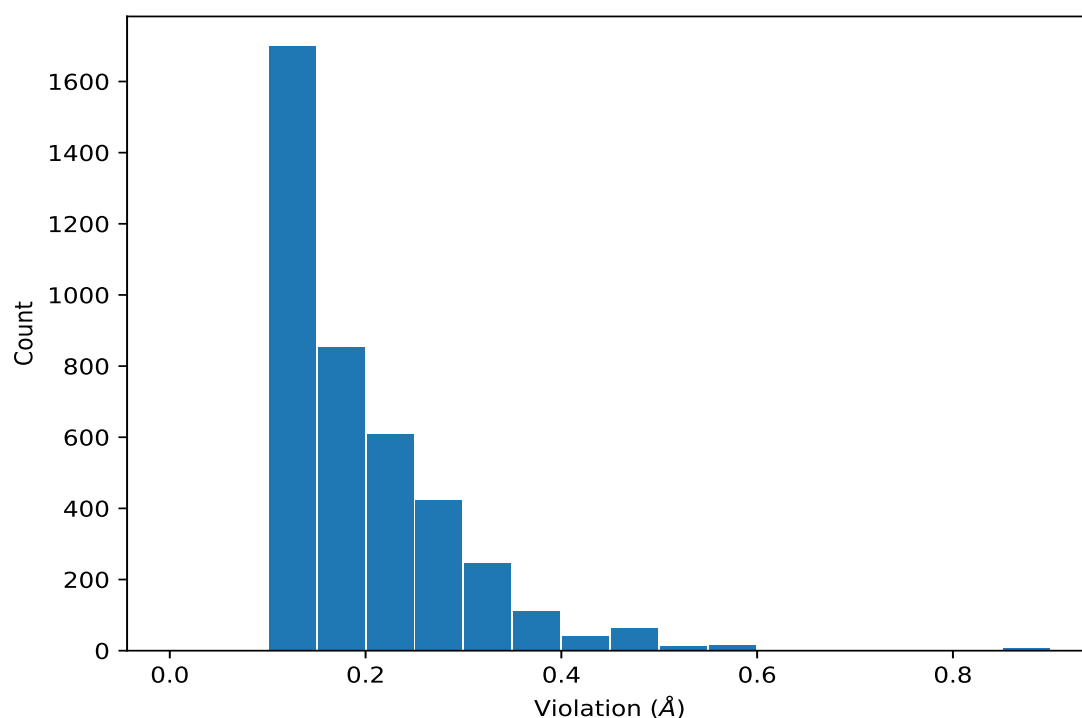
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,44)	1:104:A:ILE:HD11	1:20:A:PHE:HD1	2	0.11	0.0	0.11
(1,44)	1:104:A:ILE:HD11	1:20:A:PHE:HD2	2	0.11	0.0	0.11
(1,44)	1:104:A:ILE:HD12	1:20:A:PHE:HD1	2	0.11	0.0	0.11
(1,44)	1:104:A:ILE:HD12	1:20:A:PHE:HD2	2	0.11	0.0	0.11
(1,44)	1:104:A:ILE:HD13	1:20:A:PHE:HD1	2	0.11	0.0	0.11
(1,44)	1:104:A:ILE:HD13	1:20:A:PHE:HD2	2	0.11	0.0	0.11
(1,218)	1:221:A:PHE:HE1	1:222:A:VAL:H	2	0.11	0.0	0.11
(1,218)	1:221:A:PHE:HE2	1:222:A:VAL:H	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD11	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD12	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD13	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD11	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD12	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD13	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD11	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD12	2	0.11	0.0	0.11
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD13	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE1	7	0.89
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE2	7	0.89
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE1	7	0.89
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE2	7	0.89
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE1	7	0.89
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE2	7	0.89
(1,206)	1:22:A:PHE:HE1	1:169:A:SER:H	1	0.61
(1,206)	1:22:A:PHE:HE2	1:169:A:SER:H	1	0.61
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD21	2	0.6
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD22	2	0.6
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD23	2	0.6
(1,885)	1:121:A:ALA:H	1:124:A:ALA:H	10	0.59
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD21	8	0.57
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD22	8	0.57
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD23	8	0.57
(1,572)	1:92:A:VAL:HG11	1:180:A:MET:HE1	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:92:A:VAL:HG11	1:180:A:MET:HE2	6	0.56
(1,572)	1:92:A:VAL:HG11	1:180:A:MET:HE3	6	0.56
(1,572)	1:92:A:VAL:HG12	1:180:A:MET:HE1	6	0.56
(1,572)	1:92:A:VAL:HG12	1:180:A:MET:HE2	6	0.56
(1,572)	1:92:A:VAL:HG12	1:180:A:MET:HE3	6	0.56
(1,572)	1:92:A:VAL:HG13	1:180:A:MET:HE1	6	0.56
(1,572)	1:92:A:VAL:HG13	1:180:A:MET:HE2	6	0.56
(1,572)	1:92:A:VAL:HG13	1:180:A:MET:HE3	6	0.56
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD21	7	0.54
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD22	7	0.54
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD23	7	0.54
(1,744)	1:192:A:GLU:H	1:193:A:ASP:H	5	0.51
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG11	4	0.51
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG12	4	0.51
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG13	4	0.51
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	9	0.51
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	9	0.51
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	9	0.51
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	9	0.51
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	9	0.51
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	9	0.51
(1,885)	1:121:A:ALA:H	1:124:A:ALA:H	3	0.5
(1,71)	1:141:A:ALA:HB1	1:142:A:TYR:HE1	7	0.49
(1,71)	1:141:A:ALA:HB1	1:142:A:TYR:HE2	7	0.49
(1,71)	1:141:A:ALA:HB2	1:142:A:TYR:HE1	7	0.49
(1,71)	1:141:A:ALA:HB2	1:142:A:TYR:HE2	7	0.49
(1,71)	1:141:A:ALA:HB3	1:142:A:TYR:HE1	7	0.49
(1,71)	1:141:A:ALA:HB3	1:142:A:TYR:HE2	7	0.49
(1,624)	1:207:A:VAL:HG21	1:218:A:ILE:HD11	5	0.48
(1,624)	1:207:A:VAL:HG21	1:218:A:ILE:HD12	5	0.48
(1,624)	1:207:A:VAL:HG21	1:218:A:ILE:HD13	5	0.48
(1,624)	1:207:A:VAL:HG22	1:218:A:ILE:HD11	5	0.48
(1,624)	1:207:A:VAL:HG22	1:218:A:ILE:HD12	5	0.48
(1,624)	1:207:A:VAL:HG22	1:218:A:ILE:HD13	5	0.48
(1,624)	1:207:A:VAL:HG23	1:218:A:ILE:HD11	5	0.48
(1,624)	1:207:A:VAL:HG23	1:218:A:ILE:HD12	5	0.48
(1,624)	1:207:A:VAL:HG23	1:218:A:ILE:HD13	5	0.48
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG11	10	0.48
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG12	10	0.48
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG13	10	0.48
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	3	0.48
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	3	0.48
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	10	0.46
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	10	0.46
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	10	0.46
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	10	0.46
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	10	0.46
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	10	0.46
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	10	0.46
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	10	0.46
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	10	0.46
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	2	0.46
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	2	0.46
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	2	0.46
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	2	0.46
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	2	0.46
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	2	0.46
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	2	0.46
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	2	0.46
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	2	0.46
(1,477)	1:223:A:GLU:H	1:222:A:VAL:HG21	6	0.46
(1,477)	1:223:A:GLU:H	1:222:A:VAL:HG22	6	0.46
(1,477)	1:223:A:GLU:H	1:222:A:VAL:HG23	6	0.46
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG11	6	0.46
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG12	6	0.46
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG13	6	0.46
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	10	0.46
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	10	0.46
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	10	0.46
(1,830)	1:191:A:LYS:H	1:193:A:ASP:H	3	0.45
(1,803)	1:66:A:ASP:H	1:68:A:SER:H	8	0.45
(1,361)	1:93:A:ASP:H	1:92:A:VAL:HG11	6	0.45
(1,361)	1:93:A:ASP:H	1:92:A:VAL:HG12	6	0.45
(1,361)	1:93:A:ASP:H	1:92:A:VAL:HG13	6	0.45
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	9	0.45
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	9	0.45
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	9	0.45
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	1	0.45
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	1	0.45
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	1	0.45
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	1	0.45
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	1	0.45
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD21	5	0.44
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD22	5	0.44
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD23	5	0.44
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	2	0.44
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	2	0.44
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	2	0.44
(1,471)	1:221:A:PHE:H	1:220:A:LEU:HD11	4	0.42
(1,471)	1:221:A:PHE:H	1:220:A:LEU:HD12	4	0.42
(1,471)	1:221:A:PHE:H	1:220:A:LEU:HD13	4	0.42
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	6	0.42
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	6	0.42
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	6	0.42
(1,98)	1:172:A:VAL:HG21	1:170:A:PHE:HE1	1	0.42
(1,98)	1:172:A:VAL:HG22	1:170:A:PHE:HE1	1	0.42
(1,98)	1:172:A:VAL:HG23	1:170:A:PHE:HE1	1	0.42
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	3	0.41
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	3	0.41
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	3	0.41
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	3	0.41
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	3	0.41
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	3	0.41
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	3	0.41
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	3	0.41
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	3	0.41
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	6	0.41
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	6	0.41
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	6	0.41
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	6	0.41
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	6	0.41
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	6	0.41
(1,43)	1:103:A:LEU:HD21	1:160:A:TYR:HE1	8	0.41
(1,43)	1:103:A:LEU:HD21	1:160:A:TYR:HE2	8	0.41
(1,43)	1:103:A:LEU:HD22	1:160:A:TYR:HE1	8	0.41
(1,43)	1:103:A:LEU:HD22	1:160:A:TYR:HE2	8	0.41
(1,43)	1:103:A:LEU:HD23	1:160:A:TYR:HE1	8	0.41
(1,43)	1:103:A:LEU:HD23	1:160:A:TYR:HE2	8	0.41
(1,669)	1:72:A:SER:H	1:71:A:ASP:H	1	0.4
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	10	0.4
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	10	0.4
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	10	0.4
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	5	0.39
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	5	0.39
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	5	0.39
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	5	0.39
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	5	0.39
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE1	5	0.39
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE2	5	0.39
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE3	5	0.39
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE1	10	0.39
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE2	10	0.39
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE3	10	0.39
(1,764)	1:213:A:PHE:H	1:212:A:GLN:H	9	0.38
(1,671)	1:73:A:GLY:H	1:74:A:LYS:H	4	0.38
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	5	0.38
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	5	0.38
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	5	0.38
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	5	0.38
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	5	0.38
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	5	0.38
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	5	0.38
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	5	0.38
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	5	0.38
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG21	6	0.38
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG22	6	0.38
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG23	6	0.38
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD21	2	0.38
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD22	2	0.38
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD23	2	0.38
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	7	0.38
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	7	0.38
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	7	0.38
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG21	7	0.38
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG22	7	0.38
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG23	7	0.38
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD21	8	0.38
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD22	8	0.38
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD23	8	0.38
(1,16)	1:30:A:MET:HE1	1:139:A:TYR:HD1	8	0.38
(1,16)	1:30:A:MET:HE2	1:139:A:TYR:HD1	8	0.38
(1,16)	1:30:A:MET:HE3	1:139:A:TYR:HD1	8	0.38
(1,889)	1:191:A:LYS:H	1:194:A:GLN:H	3	0.37
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG21	6	0.37
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG22	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG23	6	0.37
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG21	6	0.37
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG22	6	0.37
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG23	6	0.37
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG21	6	0.37
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG22	6	0.37
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG23	6	0.37
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB1	7	0.37
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB2	7	0.37
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB3	7	0.37
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB1	7	0.37
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB2	7	0.37
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB3	7	0.37
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB1	7	0.37
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB2	7	0.37
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB3	7	0.37
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB1	7	0.37
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB2	7	0.37
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB3	7	0.37
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB1	7	0.37
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB2	7	0.37
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB3	7	0.37
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB1	7	0.37
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB2	7	0.37
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB3	7	0.37
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG21	8	0.37
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG22	8	0.37
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG23	8	0.37
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	1	0.37
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	1	0.37
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	1	0.37
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD21	2	0.37
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD22	2	0.37
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD23	2	0.37
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG21	1	0.37
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG22	1	0.37
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG23	1	0.37
(1,16)	1:30:A:MET:HE1	1:139:A:TYR:HD1	9	0.37
(1,16)	1:30:A:MET:HE2	1:139:A:TYR:HD1	9	0.37
(1,16)	1:30:A:MET:HE3	1:139:A:TYR:HD1	9	0.37
(1,831)	1:192:A:GLU:H	1:194:A:GLN:H	9	0.36
(1,700)	1:126:A:ALA:H	1:127:A:ASP:H	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:69:A:LYS:H	1:70:A:LEU:H	9	0.36
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG21	10	0.36
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG22	10	0.36
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG23	10	0.36
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG21	10	0.36
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG22	10	0.36
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG23	10	0.36
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG21	10	0.36
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG22	10	0.36
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG23	10	0.36
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG11	5	0.36
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG12	5	0.36
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG13	5	0.36
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	4	0.36
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	4	0.36
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	4	0.36
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG21	5	0.36
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG22	5	0.36
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG23	5	0.36
(1,221)	1:134:A:PHE:HE1	1:121:A:ALA:H	8	0.36
(1,221)	1:134:A:PHE:HE2	1:121:A:ALA:H	8	0.36
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD21	6	0.36
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD22	6	0.36
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD23	6	0.36
(1,805)	1:71:A:ASP:H	1:69:A:LYS:H	5	0.35
(1,733)	1:181:A:GLY:H	1:182:A:ARG:H	6	0.35
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG21	8	0.35
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG22	8	0.35
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG23	8	0.35
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG21	8	0.35
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG22	8	0.35
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG23	8	0.35
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG21	8	0.35
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG22	8	0.35
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG23	8	0.35
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	10	0.35
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	10	0.35
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	10	0.35
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG11	3	0.35
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG12	3	0.35
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG13	3	0.35
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	7	0.35
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	7	0.35
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	10	0.35
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	10	0.35
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	10	0.35
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	1	0.35
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	1	0.35
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	1	0.35
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG21	2	0.35
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG22	2	0.35
(1,234)	1:17:A:VAL:H	1:17:A:VAL:HG23	2	0.35
(1,224)	1:134:A:PHE:HE1	1:127:A:ASP:H	10	0.35
(1,224)	1:134:A:PHE:HE2	1:127:A:ASP:H	10	0.35
(1,223)	1:118:A:PHE:HE1	1:127:A:ASP:H	5	0.35
(1,223)	1:118:A:PHE:HE2	1:127:A:ASP:H	5	0.35
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB1	1	0.35
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB2	1	0.35
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB3	1	0.35
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	1	0.35
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	1	0.35
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	1	0.35
(1,67)	1:130:A:MET:HE1	1:118:A:PHE:HD1	10	0.35
(1,67)	1:130:A:MET:HE2	1:118:A:PHE:HD1	10	0.35
(1,67)	1:130:A:MET:HE3	1:118:A:PHE:HD1	10	0.35
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE1	2	0.35
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE2	2	0.35
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE1	2	0.35
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE2	2	0.35
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE1	2	0.35
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE2	2	0.35
(1,703)	1:137:A:GLY:H	1:138:A:PHE:H	6	0.34
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	4	0.34
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	4	0.34
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	4	0.34
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD11	2	0.34
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD12	2	0.34
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD13	2	0.34
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG21	6	0.34
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG22	6	0.34
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG23	6	0.34
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG11	9	0.34
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG12	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG13	9	0.34
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD11	3	0.34
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD12	3	0.34
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD13	3	0.34
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD21	2	0.34
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD22	2	0.34
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD23	2	0.34
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	8	0.34
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	8	0.34
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	8	0.34
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	8	0.34
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	8	0.34
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	8	0.34
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	5	0.33
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	5	0.33
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	5	0.33
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	5	0.33
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	5	0.33
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	5	0.33
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	5	0.33
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	5	0.33
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	5	0.33
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG21	4	0.33
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG22	4	0.33
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG23	4	0.33
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG21	4	0.33
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG22	4	0.33
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG23	4	0.33
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG21	4	0.33
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG22	4	0.33
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG23	4	0.33
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	7	0.33
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	7	0.33
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	7	0.33
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	7	0.33
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	7	0.33
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	7	0.33
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	7	0.33
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	7	0.33
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	7	0.33
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	6	0.33
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	6	0.33
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	6	0.33
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	6	0.33
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	6	0.33
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	6	0.33
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	6	0.33
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	6	0.33
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	4	0.33
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	4	0.33
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	4	0.33
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD11	2	0.33
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD12	2	0.33
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD13	2	0.33
(1,222)	1:134:A:PHE:HD1	1:121:A:ALA:H	5	0.33
(1,222)	1:134:A:PHE:HD2	1:121:A:ALA:H	5	0.33
(1,106)	1:206:A:ILE:HD11	1:44:A:PHE:HE1	8	0.33
(1,106)	1:206:A:ILE:HD11	1:44:A:PHE:HE2	8	0.33
(1,106)	1:206:A:ILE:HD12	1:44:A:PHE:HE1	8	0.33
(1,106)	1:206:A:ILE:HD12	1:44:A:PHE:HE2	8	0.33
(1,106)	1:206:A:ILE:HD13	1:44:A:PHE:HE1	8	0.33
(1,106)	1:206:A:ILE:HD13	1:44:A:PHE:HE2	8	0.33
(1,830)	1:191:A:LYS:H	1:193:A:ASP:H	5	0.32
(1,745)	1:193:A:ASP:H	1:194:A:GLN:H	6	0.32
(1,743)	1:191:A:LYS:H	1:192:A:GLU:H	9	0.32
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	7	0.32
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	7	0.32
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	7	0.32
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	7	0.32
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	7	0.32
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	7	0.32
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	7	0.32
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	7	0.32
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	7	0.32
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD21	4	0.32
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD22	4	0.32
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD23	4	0.32
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD21	4	0.32
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD22	4	0.32
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD23	4	0.32
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD21	4	0.32
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD22	4	0.32
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD23	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE1	7	0.32
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE2	7	0.32
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE3	7	0.32
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE1	7	0.32
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE2	7	0.32
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE3	7	0.32
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE1	7	0.32
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE2	7	0.32
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE3	7	0.32
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD11	5	0.32
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD12	5	0.32
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD13	5	0.32
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG11	7	0.32
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG12	7	0.32
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG13	7	0.32
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	9	0.32
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	9	0.32
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	9	0.32
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	5	0.32
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	5	0.32
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	5	0.32
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD11	9	0.32
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD12	9	0.32
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD13	9	0.32
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG21	4	0.32
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG22	4	0.32
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG23	4	0.32
(1,772)	1:223:A:GLU:H	1:222:A:VAL:H	2	0.31
(1,733)	1:181:A:GLY:H	1:182:A:ARG:H	9	0.31
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG21	3	0.31
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG22	3	0.31
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG23	3	0.31
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG21	3	0.31
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG22	3	0.31
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG23	3	0.31
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG21	3	0.31
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG22	3	0.31
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG23	3	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	1	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	1	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	1	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	1	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	1	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	1	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	1	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	1	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	4	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	4	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	4	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	4	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	4	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	4	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	4	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	4	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	4	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	10	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	10	0.31
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	10	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	10	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	10	0.31
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	10	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	10	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	10	0.31
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	10	0.31
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG11	10	0.31
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG12	10	0.31
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG13	10	0.31
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD11	2	0.31
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD12	2	0.31
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD13	2	0.31
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG21	8	0.31
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG22	8	0.31
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG23	8	0.31
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE1	10	0.31
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE2	10	0.31
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE3	10	0.31
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	2	0.31
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	2	0.31
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	2	0.31
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	2	0.31
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	2	0.31
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	2	0.31
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG11	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG12	8	0.31
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG13	8	0.31
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG11	10	0.31
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG12	10	0.31
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG13	10	0.31
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG11	4	0.31
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG12	4	0.31
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG13	4	0.31
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG21	1	0.31
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG22	1	0.31
(1,173)	1:198:A:LEU:H	1:195:A:THR:HG23	1	0.31
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG21	3	0.31
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG22	3	0.31
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG23	3	0.31
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD21	7	0.31
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD22	7	0.31
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD23	7	0.31
(1,745)	1:193:A:ASP:H	1:194:A:GLN:H	5	0.3
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	2	0.3
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	2	0.3
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	2	0.3
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	2	0.3
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	2	0.3
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	2	0.3
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	2	0.3
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	2	0.3
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	2	0.3
(1,593)	1:122:A:LEU:HD21	1:128:A:ILE:HD11	10	0.3
(1,593)	1:122:A:LEU:HD21	1:128:A:ILE:HD12	10	0.3
(1,593)	1:122:A:LEU:HD21	1:128:A:ILE:HD13	10	0.3
(1,593)	1:122:A:LEU:HD22	1:128:A:ILE:HD11	10	0.3
(1,593)	1:122:A:LEU:HD22	1:128:A:ILE:HD12	10	0.3
(1,593)	1:122:A:LEU:HD22	1:128:A:ILE:HD13	10	0.3
(1,593)	1:122:A:LEU:HD23	1:128:A:ILE:HD11	10	0.3
(1,593)	1:122:A:LEU:HD23	1:128:A:ILE:HD12	10	0.3
(1,593)	1:122:A:LEU:HD23	1:128:A:ILE:HD13	10	0.3
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	6	0.3
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	6	0.3
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	6	0.3
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	6	0.3
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	6	0.3
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	6	0.3
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	6	0.3
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	6	0.3
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG11	1	0.3
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG12	1	0.3
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG13	1	0.3
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD21	3	0.3
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD22	3	0.3
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD23	3	0.3
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD11	9	0.3
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD12	9	0.3
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD13	9	0.3
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD11	4	0.3
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD12	4	0.3
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD13	4	0.3
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD11	7	0.3
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD12	7	0.3
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD13	7	0.3
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD21	2	0.3
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD22	2	0.3
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD23	2	0.3
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	10	0.3
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	10	0.3
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	10	0.3
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG11	4	0.3
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG12	4	0.3
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG13	4	0.3
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD11	7	0.3
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD12	7	0.3
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD13	7	0.3
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD11	9	0.3
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD12	9	0.3
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD13	9	0.3
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG11	9	0.3
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG12	9	0.3
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG13	9	0.3
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	3	0.3
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	3	0.3
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD21	1	0.3
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD22	1	0.3
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD23	1	0.3
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD11	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD12	6	0.3
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD13	6	0.3
(1,99)	1:174:A:THR:HG21	1:160:A:TYR:HE1	1	0.3
(1,99)	1:174:A:THR:HG22	1:160:A:TYR:HE1	1	0.3
(1,99)	1:174:A:THR:HG23	1:160:A:TYR:HE1	1	0.3
(1,68)	1:130:A:MET:HE1	1:134:A:PHE:HD2	10	0.3
(1,68)	1:130:A:MET:HE2	1:134:A:PHE:HD2	10	0.3
(1,68)	1:130:A:MET:HE3	1:134:A:PHE:HD2	10	0.3
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	8	0.3
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	8	0.3
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	8	0.3
(1,668)	1:71:A:ASP:H	1:70:A:LEU:H	9	0.29
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD21	10	0.29
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD22	10	0.29
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD23	10	0.29
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD21	10	0.29
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD22	10	0.29
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD23	10	0.29
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD21	10	0.29
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD22	10	0.29
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD23	10	0.29
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG21	1	0.29
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG22	1	0.29
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG23	1	0.29
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG21	6	0.29
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG22	6	0.29
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG23	6	0.29
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG11	6	0.29
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG12	6	0.29
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG13	6	0.29
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD21	8	0.29
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD22	8	0.29
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD23	8	0.29
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	7	0.29
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	7	0.29
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	7	0.29
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	6	0.28
(1,670)	1:72:A:SER:H	1:73:A:GLY:H	1	0.28
(1,589)	1:103:A:LEU:HD21	1:172:A:VAL:HG21	4	0.28
(1,589)	1:103:A:LEU:HD21	1:172:A:VAL:HG22	4	0.28
(1,589)	1:103:A:LEU:HD21	1:172:A:VAL:HG23	4	0.28
(1,589)	1:103:A:LEU:HD22	1:172:A:VAL:HG21	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,589)	1:103:A:LEU:HD22	1:172:A:VAL:HG22	4	0.28
(1,589)	1:103:A:LEU:HD22	1:172:A:VAL:HG23	4	0.28
(1,589)	1:103:A:LEU:HD23	1:172:A:VAL:HG21	4	0.28
(1,589)	1:103:A:LEU:HD23	1:172:A:VAL:HG22	4	0.28
(1,589)	1:103:A:LEU:HD23	1:172:A:VAL:HG23	4	0.28
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	8	0.28
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	8	0.28
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	8	0.28
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	8	0.28
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	8	0.28
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	8	0.28
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	8	0.28
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	8	0.28
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	8	0.28
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD21	8	0.28
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD22	8	0.28
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD23	8	0.28
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD21	8	0.28
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD22	8	0.28
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD23	8	0.28
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD21	8	0.28
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD22	8	0.28
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD23	8	0.28
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD11	5	0.28
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD12	5	0.28
(1,351)	1:87:A:ARG:H	1:198:A:LEU:HD13	5	0.28
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD21	5	0.28
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD22	5	0.28
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD23	5	0.28
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG21	10	0.28
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG22	10	0.28
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG23	10	0.28
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG11	6	0.28
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG12	6	0.28
(1,269)	1:186:A:VAL:H	1:186:A:VAL:HG13	6	0.28
(1,228)	1:134:A:PHE:HE1	1:130:A:MET:H	1	0.28
(1,228)	1:134:A:PHE:HE2	1:130:A:MET:H	1	0.28
(1,167)	1:184:A:THR:H	1:180:A:MET:HE1	6	0.28
(1,167)	1:184:A:THR:H	1:180:A:MET:HE2	6	0.28
(1,167)	1:184:A:THR:H	1:180:A:MET:HE3	6	0.28
(1,946)	1:99:A:THR:H	1:103:A:LEU:H	2	0.27
(1,705)	1:143:A:LEU:H	1:142:A:TYR:H	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	3	0.27
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	3	0.27
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	3	0.27
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	3	0.27
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	3	0.27
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	3	0.27
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	3	0.27
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	3	0.27
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	3	0.27
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	2	0.27
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	2	0.27
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	2	0.27
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	2	0.27
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	2	0.27
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	2	0.27
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	2	0.27
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	2	0.27
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	2	0.27
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG21	3	0.27
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG22	3	0.27
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG23	3	0.27
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG21	3	0.27
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG22	3	0.27
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG23	3	0.27
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG21	3	0.27
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG22	3	0.27
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG23	3	0.27
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	1	0.27
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	1	0.27
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	1	0.27
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	1	0.27
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	1	0.27
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	1	0.27
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	1	0.27
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	1	0.27
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	1	0.27
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG21	8	0.27
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG22	8	0.27
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG23	8	0.27
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	1	0.27
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	1	0.27
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	6	0.27
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	6	0.27
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	6	0.27
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB1	6	0.27
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB2	6	0.27
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB3	6	0.27
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	3	0.27
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	3	0.27
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	3	0.27
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD21	7	0.27
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD22	7	0.27
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD23	7	0.27
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	5	0.27
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	5	0.27
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	5	0.27
(1,221)	1:134:A:PHE:HE1	1:121:A:ALA:H	10	0.27
(1,221)	1:134:A:PHE:HE2	1:121:A:ALA:H	10	0.27
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	1	0.27
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	1	0.27
(1,190)	1:216:A:TYR:HE1	1:53:A:SER:H	5	0.27
(1,190)	1:216:A:TYR:HE2	1:53:A:SER:H	5	0.27
(1,102)	1:188:A:LEU:HD11	1:44:A:PHE:HD2	4	0.27
(1,102)	1:188:A:LEU:HD12	1:44:A:PHE:HD2	4	0.27
(1,102)	1:188:A:LEU:HD13	1:44:A:PHE:HD2	4	0.27
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	5	0.27
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	5	0.27
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	5	0.27
(1,97)	1:172:A:VAL:HG21	1:160:A:TYR:HE1	1	0.27
(1,97)	1:172:A:VAL:HG22	1:160:A:TYR:HE1	1	0.27
(1,97)	1:172:A:VAL:HG23	1:160:A:TYR:HE1	1	0.27
(1,816)	1:117:A:ALA:H	1:119:A:MET:H	7	0.26
(1,704)	1:141:A:ALA:H	1:142:A:TYR:H	2	0.26
(1,628)	1:222:A:VAL:HG11	1:220:A:LEU:HD21	7	0.26
(1,628)	1:222:A:VAL:HG11	1:220:A:LEU:HD22	7	0.26
(1,628)	1:222:A:VAL:HG11	1:220:A:LEU:HD23	7	0.26
(1,628)	1:222:A:VAL:HG12	1:220:A:LEU:HD21	7	0.26
(1,628)	1:222:A:VAL:HG12	1:220:A:LEU:HD22	7	0.26
(1,628)	1:222:A:VAL:HG12	1:220:A:LEU:HD23	7	0.26
(1,628)	1:222:A:VAL:HG13	1:220:A:LEU:HD21	7	0.26
(1,628)	1:222:A:VAL:HG13	1:220:A:LEU:HD22	7	0.26
(1,628)	1:222:A:VAL:HG13	1:220:A:LEU:HD23	7	0.26
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	3	0.26
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	3	0.26
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	3	0.26
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	3	0.26
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	3	0.26
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	3	0.26
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	3	0.26
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	3	0.26
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG21	2	0.26
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG22	2	0.26
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG23	2	0.26
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG21	2	0.26
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG22	2	0.26
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG23	2	0.26
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG21	2	0.26
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG22	2	0.26
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG23	2	0.26
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG21	5	0.26
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG22	5	0.26
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG23	5	0.26
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG21	5	0.26
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG22	5	0.26
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG23	5	0.26
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG21	5	0.26
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG22	5	0.26
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG23	5	0.26
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	6	0.26
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	6	0.26
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	6	0.26
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	6	0.26
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	6	0.26
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	6	0.26
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	6	0.26
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	6	0.26
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	6	0.26
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD11	8	0.26
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD12	8	0.26
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD13	8	0.26
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD11	8	0.26
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD12	8	0.26
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD13	8	0.26
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD11	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD12	8	0.26
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD13	8	0.26
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG21	6	0.26
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG22	6	0.26
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG23	6	0.26
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG11	3	0.26
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG12	3	0.26
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG13	3	0.26
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB1	9	0.26
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB2	9	0.26
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB3	9	0.26
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	3	0.26
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	3	0.26
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	3	0.26
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG11	1	0.26
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG12	1	0.26
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG13	1	0.26
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	3	0.26
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	3	0.26
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	3	0.26
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD21	2	0.26
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD22	2	0.26
(1,347)	1:83:A:ASN:H	1:198:A:LEU:HD23	2	0.26
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD11	2	0.26
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD12	2	0.26
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD13	2	0.26
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	7	0.26
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	7	0.26
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	7	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	3	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	3	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	3	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	4	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	4	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	4	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	9	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	9	0.26
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	9	0.26
(1,278)	1:203:A:ILE:H	1:203:A:ILE:HD11	6	0.26
(1,278)	1:203:A:ILE:H	1:203:A:ILE:HD12	6	0.26
(1,278)	1:203:A:ILE:H	1:203:A:ILE:HD13	6	0.26
(1,259)	1:143:A:LEU:H	1:143:A:LEU:HD11	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:143:A:LEU:H	1:143:A:LEU:HD12	7	0.26
(1,259)	1:143:A:LEU:H	1:143:A:LEU:HD13	7	0.26
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE1	5	0.26
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE2	5	0.26
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE3	5	0.26
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	7	0.26
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	7	0.26
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	7	0.26
(1,102)	1:188:A:LEU:HD11	1:44:A:PHE:HD2	6	0.26
(1,102)	1:188:A:LEU:HD12	1:44:A:PHE:HD2	6	0.26
(1,102)	1:188:A:LEU:HD13	1:44:A:PHE:HD2	6	0.26
(1,819)	1:125:A:GLY:H	1:123:A:GLN:H	5	0.25
(1,671)	1:73:A:GLY:H	1:74:A:LYS:H	2	0.25
(1,671)	1:73:A:GLY:H	1:74:A:LYS:H	6	0.25
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD21	5	0.25
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD22	5	0.25
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD23	5	0.25
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD21	5	0.25
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD22	5	0.25
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD23	5	0.25
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD21	5	0.25
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD22	5	0.25
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD23	5	0.25
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	3	0.25
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	3	0.25
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	3	0.25
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	3	0.25
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	3	0.25
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	3	0.25
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	3	0.25
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	3	0.25
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	3	0.25
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	4	0.25
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	4	0.25
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	4	0.25
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	4	0.25
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	4	0.25
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	4	0.25
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	4	0.25
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	4	0.25
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	4	0.25
(1,515)	1:122:A:LEU:HD11	1:32:A:LEU:HD21	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:122:A:LEU:HD11	1:32:A:LEU:HD22	5	0.25
(1,515)	1:122:A:LEU:HD11	1:32:A:LEU:HD23	5	0.25
(1,515)	1:122:A:LEU:HD12	1:32:A:LEU:HD21	5	0.25
(1,515)	1:122:A:LEU:HD12	1:32:A:LEU:HD22	5	0.25
(1,515)	1:122:A:LEU:HD12	1:32:A:LEU:HD23	5	0.25
(1,515)	1:122:A:LEU:HD13	1:32:A:LEU:HD21	5	0.25
(1,515)	1:122:A:LEU:HD13	1:32:A:LEU:HD22	5	0.25
(1,515)	1:122:A:LEU:HD13	1:32:A:LEU:HD23	5	0.25
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB1	5	0.25
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB2	5	0.25
(1,439)	1:190:A:LEU:H	1:145:A:ALA:HB3	5	0.25
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	9	0.25
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	9	0.25
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	9	0.25
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG21	6	0.25
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG22	6	0.25
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG23	6	0.25
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG21	10	0.25
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG22	10	0.25
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG23	10	0.25
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD11	4	0.25
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD12	4	0.25
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD13	4	0.25
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD11	5	0.25
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD12	5	0.25
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD13	5	0.25
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG21	4	0.25
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG22	4	0.25
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG23	4	0.25
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG21	6	0.25
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG22	6	0.25
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG23	6	0.25
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	2	0.25
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	2	0.25
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	2	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG21	5	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG22	5	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG23	5	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG21	9	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG22	9	0.25
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG23	9	0.25
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG11	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG12	3	0.25
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG13	3	0.25
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	8	0.25
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	8	0.25
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	8	0.25
(1,226)	1:134:A:PHE:HD1	1:130:A:MET:H	10	0.25
(1,226)	1:134:A:PHE:HD2	1:130:A:MET:H	10	0.25
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG21	8	0.25
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG22	8	0.25
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG23	8	0.25
(1,97)	1:172:A:VAL:HG21	1:160:A:TYR:HE1	8	0.25
(1,97)	1:172:A:VAL:HG22	1:160:A:TYR:HE1	8	0.25
(1,97)	1:172:A:VAL:HG23	1:160:A:TYR:HE1	8	0.25
(1,85)	1:152:A:THR:HG21	1:160:A:TYR:HE2	9	0.25
(1,85)	1:152:A:THR:HG22	1:160:A:TYR:HE2	9	0.25
(1,85)	1:152:A:THR:HG23	1:160:A:TYR:HE2	9	0.25
(1,81)	1:148:A:VAL:HG11	1:142:A:TYR:HE2	7	0.25
(1,81)	1:148:A:VAL:HG12	1:142:A:TYR:HE2	7	0.25
(1,81)	1:148:A:VAL:HG13	1:142:A:TYR:HE2	7	0.25
(1,964)	1:183:A:GLY:H	1:153:A:LYS:H	7	0.24
(1,851)	1:214:A:ILE:H	1:216:A:TYR:H	7	0.24
(1,747)	1:195:A:THR:H	1:196:A:GLU:H	10	0.24
(1,730)	1:176:A:THR:H	1:177:A:GLY:H	2	0.24
(1,629)	1:222:A:VAL:HG21	1:220:A:LEU:HD21	9	0.24
(1,629)	1:222:A:VAL:HG21	1:220:A:LEU:HD22	9	0.24
(1,629)	1:222:A:VAL:HG21	1:220:A:LEU:HD23	9	0.24
(1,629)	1:222:A:VAL:HG22	1:220:A:LEU:HD21	9	0.24
(1,629)	1:222:A:VAL:HG22	1:220:A:LEU:HD22	9	0.24
(1,629)	1:222:A:VAL:HG22	1:220:A:LEU:HD23	9	0.24
(1,629)	1:222:A:VAL:HG23	1:220:A:LEU:HD21	9	0.24
(1,629)	1:222:A:VAL:HG23	1:220:A:LEU:HD22	9	0.24
(1,629)	1:222:A:VAL:HG23	1:220:A:LEU:HD23	9	0.24
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	8	0.24
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	8	0.24
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	8	0.24
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	8	0.24
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	8	0.24
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	8	0.24
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	8	0.24
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	8	0.24
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	8	0.24
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG11	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG12	3	0.24
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG13	3	0.24
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG11	3	0.24
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG12	3	0.24
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG13	3	0.24
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG11	3	0.24
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG12	3	0.24
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG13	3	0.24
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB1	1	0.24
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB2	1	0.24
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB3	1	0.24
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB1	1	0.24
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB2	1	0.24
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB3	1	0.24
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB1	1	0.24
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB2	1	0.24
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB3	1	0.24
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG21	4	0.24
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG22	4	0.24
(1,573)	1:92:A:VAL:HG21	1:94:A:THR:HG23	4	0.24
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG21	4	0.24
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG22	4	0.24
(1,573)	1:92:A:VAL:HG22	1:94:A:THR:HG23	4	0.24
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG21	4	0.24
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG22	4	0.24
(1,573)	1:92:A:VAL:HG23	1:94:A:THR:HG23	4	0.24
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	10	0.24
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	10	0.24
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	10	0.24
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	10	0.24
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	10	0.24
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	10	0.24
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	10	0.24
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	10	0.24
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	10	0.24
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	1	0.24
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	1	0.24
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	1	0.24
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	1	0.24
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	1	0.24
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	1	0.24
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	1	0.24
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	1	0.24
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD21	7	0.24
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD22	7	0.24
(1,516)	1:122:A:LEU:HD21	1:32:A:LEU:HD23	7	0.24
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD21	7	0.24
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD22	7	0.24
(1,516)	1:122:A:LEU:HD22	1:32:A:LEU:HD23	7	0.24
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD21	7	0.24
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD22	7	0.24
(1,516)	1:122:A:LEU:HD23	1:32:A:LEU:HD23	7	0.24
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD11	10	0.24
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD12	10	0.24
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD13	10	0.24
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG21	5	0.24
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG22	5	0.24
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG23	5	0.24
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD11	8	0.24
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD12	8	0.24
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD13	8	0.24
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG11	7	0.24
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG12	7	0.24
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG13	7	0.24
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD11	10	0.24
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD12	10	0.24
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD13	10	0.24
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG21	9	0.24
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG22	9	0.24
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG23	9	0.24
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD11	2	0.24
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD12	2	0.24
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD13	2	0.24
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	7	0.24
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	7	0.24
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD21	9	0.24
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD22	9	0.24
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD23	9	0.24
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG21	4	0.24
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG22	4	0.24
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG23	4	0.24
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	2	0.24
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	2	0.24
(1,108)	1:214:A:ILE:HD11	1:216:A:TYR:HE1	7	0.24
(1,108)	1:214:A:ILE:HD11	1:216:A:TYR:HE2	7	0.24
(1,108)	1:214:A:ILE:HD12	1:216:A:TYR:HE1	7	0.24
(1,108)	1:214:A:ILE:HD12	1:216:A:TYR:HE2	7	0.24
(1,108)	1:214:A:ILE:HD13	1:216:A:TYR:HE1	7	0.24
(1,108)	1:214:A:ILE:HD13	1:216:A:TYR:HE2	7	0.24
(1,102)	1:188:A:LEU:HD11	1:44:A:PHE:HD2	8	0.24
(1,102)	1:188:A:LEU:HD12	1:44:A:PHE:HD2	8	0.24
(1,102)	1:188:A:LEU:HD13	1:44:A:PHE:HD2	8	0.24
(1,85)	1:152:A:THR:HG21	1:160:A:TYR:HE2	4	0.24
(1,85)	1:152:A:THR:HG22	1:160:A:TYR:HE2	4	0.24
(1,85)	1:152:A:THR:HG23	1:160:A:TYR:HE2	4	0.24
(1,70)	1:141:A:ALA:HB1	1:138:A:PHE:HD1	6	0.24
(1,70)	1:141:A:ALA:HB1	1:138:A:PHE:HD2	6	0.24
(1,70)	1:141:A:ALA:HB2	1:138:A:PHE:HD1	6	0.24
(1,70)	1:141:A:ALA:HB2	1:138:A:PHE:HD2	6	0.24
(1,70)	1:141:A:ALA:HB3	1:138:A:PHE:HD1	6	0.24
(1,70)	1:141:A:ALA:HB3	1:138:A:PHE:HD2	6	0.24
(1,948)	1:146:A:GLU:H	1:191:A:LYS:H	6	0.23
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	10	0.23
(1,849)	1:212:A:GLN:H	1:214:A:ILE:H	4	0.23
(1,831)	1:192:A:GLU:H	1:194:A:GLN:H	6	0.23
(1,823)	1:141:A:ALA:H	1:143:A:LEU:H	1	0.23
(1,671)	1:73:A:GLY:H	1:74:A:LYS:H	8	0.23
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG11	1	0.23
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG12	1	0.23
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG13	1	0.23
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG11	1	0.23
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG12	1	0.23
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG13	1	0.23
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG11	1	0.23
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG12	1	0.23
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG13	1	0.23
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD21	4	0.23
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD22	4	0.23
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD23	4	0.23
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD21	4	0.23
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD22	4	0.23
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD23	4	0.23
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD21	4	0.23
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD22	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD23	4	0.23
(1,581)	1:98:A:MET:HE1	1:184:A:THR:HG21	3	0.23
(1,581)	1:98:A:MET:HE1	1:184:A:THR:HG22	3	0.23
(1,581)	1:98:A:MET:HE1	1:184:A:THR:HG23	3	0.23
(1,581)	1:98:A:MET:HE2	1:184:A:THR:HG21	3	0.23
(1,581)	1:98:A:MET:HE2	1:184:A:THR:HG22	3	0.23
(1,581)	1:98:A:MET:HE2	1:184:A:THR:HG23	3	0.23
(1,581)	1:98:A:MET:HE3	1:184:A:THR:HG21	3	0.23
(1,581)	1:98:A:MET:HE3	1:184:A:THR:HG22	3	0.23
(1,581)	1:98:A:MET:HE3	1:184:A:THR:HG23	3	0.23
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE1	8	0.23
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE2	8	0.23
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE3	8	0.23
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE1	8	0.23
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE2	8	0.23
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE3	8	0.23
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE1	8	0.23
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE2	8	0.23
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE3	8	0.23
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	2	0.23
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	2	0.23
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	2	0.23
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	2	0.23
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	2	0.23
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	2	0.23
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	2	0.23
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	2	0.23
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	2	0.23
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	4	0.23
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	4	0.23
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	4	0.23
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	4	0.23
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	4	0.23
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	4	0.23
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	4	0.23
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	4	0.23
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	4	0.23
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	4	0.23
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	4	0.23
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	4	0.23
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	4	0.23
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	4	0.23
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	4	0.23
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	4	0.23
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	4	0.23
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD21	4	0.23
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD22	4	0.23
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD23	4	0.23
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG21	3	0.23
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG22	3	0.23
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG23	3	0.23
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB1	8	0.23
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB2	8	0.23
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB3	8	0.23
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	3	0.23
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	3	0.23
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	3	0.23
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	7	0.23
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	7	0.23
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	7	0.23
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG21	4	0.23
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG22	4	0.23
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG23	4	0.23
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD11	4	0.23
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD12	4	0.23
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD13	4	0.23
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	6	0.23
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	6	0.23
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	6	0.23
(1,226)	1:134:A:PHE:HD1	1:130:A:MET:H	5	0.23
(1,226)	1:134:A:PHE:HD2	1:130:A:MET:H	5	0.23
(1,192)	1:216:A:TYR:HE1	1:57:A:ASP:H	9	0.23
(1,192)	1:216:A:TYR:HE2	1:57:A:ASP:H	9	0.23
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	8	0.23
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	8	0.23
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	8	0.23
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	10	0.23
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	10	0.23
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	10	0.23
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG21	9	0.23
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG22	9	0.23
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG23	9	0.23
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD11	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD12	4	0.23
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD13	4	0.23
(1,102)	1:188:A:LEU:HD11	1:44:A:PHE:HD2	1	0.23
(1,102)	1:188:A:LEU:HD12	1:44:A:PHE:HD2	1	0.23
(1,102)	1:188:A:LEU:HD13	1:44:A:PHE:HD2	1	0.23
(1,91)	1:172:A:VAL:HG11	1:20:A:PHE:HD1	8	0.23
(1,91)	1:172:A:VAL:HG12	1:20:A:PHE:HD1	8	0.23
(1,91)	1:172:A:VAL:HG13	1:20:A:PHE:HD1	8	0.23
(1,85)	1:152:A:THR:HG21	1:160:A:TYR:HE2	2	0.23
(1,85)	1:152:A:THR:HG22	1:160:A:TYR:HE2	2	0.23
(1,85)	1:152:A:THR:HG23	1:160:A:TYR:HE2	2	0.23
(1,85)	1:152:A:THR:HG21	1:160:A:TYR:HE2	7	0.23
(1,85)	1:152:A:THR:HG22	1:160:A:TYR:HE2	7	0.23
(1,85)	1:152:A:THR:HG23	1:160:A:TYR:HE2	7	0.23
(1,880)	1:99:A:THR:H	1:102:A:ASP:H	4	0.22
(1,829)	1:180:A:MET:H	1:182:A:ARG:H	10	0.22
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD11	2	0.22
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD12	2	0.22
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD13	2	0.22
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD11	2	0.22
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD12	2	0.22
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD13	2	0.22
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD11	2	0.22
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD12	2	0.22
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD13	2	0.22
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG11	5	0.22
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG12	5	0.22
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG13	5	0.22
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG11	5	0.22
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG12	5	0.22
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG13	5	0.22
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG11	5	0.22
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG12	5	0.22
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG13	5	0.22
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	2	0.22
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	2	0.22
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	2	0.22
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	2	0.22
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	2	0.22
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	2	0.22
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	2	0.22
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	2	0.22
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD21	6	0.22
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD22	6	0.22
(1,586)	1:150:A:VAL:HG11	1:103:A:LEU:HD23	6	0.22
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD21	6	0.22
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD22	6	0.22
(1,586)	1:150:A:VAL:HG12	1:103:A:LEU:HD23	6	0.22
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD21	6	0.22
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD22	6	0.22
(1,586)	1:150:A:VAL:HG13	1:103:A:LEU:HD23	6	0.22
(1,549)	1:56:A:LEU:HD21	1:94:A:THR:HG21	2	0.22
(1,549)	1:56:A:LEU:HD21	1:94:A:THR:HG22	2	0.22
(1,549)	1:56:A:LEU:HD21	1:94:A:THR:HG23	2	0.22
(1,549)	1:56:A:LEU:HD22	1:94:A:THR:HG21	2	0.22
(1,549)	1:56:A:LEU:HD22	1:94:A:THR:HG22	2	0.22
(1,549)	1:56:A:LEU:HD22	1:94:A:THR:HG23	2	0.22
(1,549)	1:56:A:LEU:HD23	1:94:A:THR:HG21	2	0.22
(1,549)	1:56:A:LEU:HD23	1:94:A:THR:HG22	2	0.22
(1,549)	1:56:A:LEU:HD23	1:94:A:THR:HG23	2	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD11	4	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD12	4	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD13	4	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD11	4	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD12	4	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD13	4	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD11	4	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD12	4	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD13	4	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD11	9	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD12	9	0.22
(1,522)	1:89:A:LEU:HD11	1:45:A:LEU:HD13	9	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD11	9	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD12	9	0.22
(1,522)	1:89:A:LEU:HD12	1:45:A:LEU:HD13	9	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD11	9	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD12	9	0.22
(1,522)	1:89:A:LEU:HD13	1:45:A:LEU:HD13	9	0.22
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD11	6	0.22
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD12	6	0.22
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD13	6	0.22
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	8	0.22
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	8	0.22
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD11	7	0.22
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD12	7	0.22
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD13	7	0.22
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	1	0.22
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	1	0.22
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	1	0.22
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	8	0.22
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	8	0.22
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	8	0.22
(1,317)	1:62:A:GLU:H	1:59:A:ILE:HD11	4	0.22
(1,317)	1:62:A:GLU:H	1:59:A:ILE:HD12	4	0.22
(1,317)	1:62:A:GLU:H	1:59:A:ILE:HD13	4	0.22
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG11	1	0.22
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG12	1	0.22
(1,280)	1:207:A:VAL:H	1:207:A:VAL:HG13	1	0.22
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	7	0.22
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	7	0.22
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	7	0.22
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD11	5	0.22
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD12	5	0.22
(1,241)	1:56:A:LEU:H	1:56:A:LEU:HD13	5	0.22
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD11	2	0.22
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD12	2	0.22
(1,238)	1:48:A:LEU:H	1:48:A:LEU:HD13	2	0.22
(1,222)	1:134:A:PHE:HD1	1:121:A:ALA:H	4	0.22
(1,222)	1:134:A:PHE:HD2	1:121:A:ALA:H	4	0.22
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	5	0.22
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	5	0.22
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD21	9	0.22
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD22	9	0.22
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD23	9	0.22
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	6	0.22
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	6	0.22
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	6	0.22
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB1	10	0.22
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB2	10	0.22
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB3	10	0.22
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB1	1	0.22
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB2	1	0.22
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB3	1	0.22
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG21	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG22	1	0.22
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG23	1	0.22
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	4	0.22
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	4	0.22
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	4	0.22
(1,81)	1:148:A:VAL:HG11	1:142:A:TYR:HE2	6	0.22
(1,81)	1:148:A:VAL:HG12	1:142:A:TYR:HE2	6	0.22
(1,81)	1:148:A:VAL:HG13	1:142:A:TYR:HE2	6	0.22
(1,890)	1:198:A:LEU:H	1:195:A:THR:H	2	0.21
(1,872)	1:65:A:THR:H	1:62:A:GLU:H	4	0.21
(1,773)	1:224:A:LYS:H	1:223:A:GLU:H	8	0.21
(1,773)	1:224:A:LYS:H	1:223:A:GLU:H	9	0.21
(1,728)	1:174:A:THR:H	1:175:A:ASP:H	5	0.21
(1,703)	1:137:A:GLY:H	1:138:A:PHE:H	4	0.21
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG11	9	0.21
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG12	9	0.21
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG13	9	0.21
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG11	9	0.21
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG12	9	0.21
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG13	9	0.21
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG11	9	0.21
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG12	9	0.21
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG13	9	0.21
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	8	0.21
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	8	0.21
(1,602)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	8	0.21
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	8	0.21
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	8	0.21
(1,602)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	8	0.21
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	8	0.21
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	8	0.21
(1,602)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	8	0.21
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG21	3	0.21
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG22	3	0.21
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG23	3	0.21
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG21	3	0.21
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG22	3	0.21
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG23	3	0.21
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG21	3	0.21
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG22	3	0.21
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG23	3	0.21
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	5	0.21
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	5	0.21
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	5	0.21
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	5	0.21
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	5	0.21
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	5	0.21
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	5	0.21
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	5	0.21
(1,555)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	6	0.21
(1,555)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	6	0.21
(1,555)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	6	0.21
(1,555)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	6	0.21
(1,555)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	6	0.21
(1,555)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	6	0.21
(1,555)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	6	0.21
(1,555)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	6	0.21
(1,555)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	6	0.21
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	10	0.21
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	10	0.21
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	10	0.21
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	10	0.21
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	10	0.21
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	10	0.21
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	10	0.21
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	10	0.21
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	10	0.21
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE1	10	0.21
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE2	10	0.21
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE3	10	0.21
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD11	5	0.21
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD12	5	0.21
(1,346)	1:83:A:ASN:H	1:198:A:LEU:HD13	5	0.21
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG11	8	0.21
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG12	8	0.21
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG13	8	0.21
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD11	3	0.21
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD12	3	0.21
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD13	3	0.21
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD21	5	0.21
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD22	5	0.21
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD23	5	0.21
(1,231)	1:118:A:PHE:HE1	1:131:A:ILE:H	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:118:A:PHE:HE2	1:131:A:ILE:H	10	0.21
(1,230)	1:134:A:PHE:HD1	1:131:A:ILE:H	8	0.21
(1,230)	1:134:A:PHE:HD2	1:131:A:ILE:H	8	0.21
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG11	6	0.21
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG12	6	0.21
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG13	6	0.21
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB1	5	0.21
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB2	5	0.21
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB3	5	0.21
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	4	0.21
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	4	0.21
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	4	0.21
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	6	0.21
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	6	0.21
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	6	0.21
(1,145)	1:126:A:ALA:H	1:122:A:LEU:HD11	3	0.21
(1,145)	1:126:A:ALA:H	1:122:A:LEU:HD12	3	0.21
(1,145)	1:126:A:ALA:H	1:122:A:LEU:HD13	3	0.21
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	5	0.21
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	5	0.21
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	5	0.21
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	6	0.21
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	6	0.21
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	6	0.21
(1,81)	1:148:A:VAL:HG11	1:142:A:TYR:HE2	9	0.21
(1,81)	1:148:A:VAL:HG12	1:142:A:TYR:HE2	9	0.21
(1,81)	1:148:A:VAL:HG13	1:142:A:TYR:HE2	9	0.21
(1,14)	1:32:A:LEU:HD21	1:118:A:PHE:HE2	10	0.21
(1,14)	1:32:A:LEU:HD22	1:118:A:PHE:HE2	10	0.21
(1,14)	1:32:A:LEU:HD23	1:118:A:PHE:HE2	10	0.21
(2,106)	1:49:A:ILE:H	1:45:A:LEU:O	9	0.2
(1,942)	1:97:A:GLY:H	1:183:A:GLY:H	4	0.2
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	8	0.2
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	9	0.2
(1,827)	1:164:A:SER:H	1:166:A:ALA:H	8	0.2
(1,730)	1:176:A:THR:H	1:177:A:GLY:H	3	0.2
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG21	10	0.2
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG22	10	0.2
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG23	10	0.2
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG21	10	0.2
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG22	10	0.2
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG23	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG21	10	0.2
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG22	10	0.2
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG23	10	0.2
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD11	9	0.2
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD12	9	0.2
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD13	9	0.2
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD11	9	0.2
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD12	9	0.2
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD13	9	0.2
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD11	9	0.2
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD12	9	0.2
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD13	9	0.2
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG21	4	0.2
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG22	4	0.2
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG23	4	0.2
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG21	4	0.2
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG22	4	0.2
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG23	4	0.2
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG21	4	0.2
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG22	4	0.2
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG23	4	0.2
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	10	0.2
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	10	0.2
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	10	0.2
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	10	0.2
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	10	0.2
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	10	0.2
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	10	0.2
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	10	0.2
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	10	0.2
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	3	0.2
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	3	0.2
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	3	0.2
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	3	0.2
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	3	0.2
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	3	0.2
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	3	0.2
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	3	0.2
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	3	0.2
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG21	8	0.2
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG22	8	0.2
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG23	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG21	8	0.2
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG22	8	0.2
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG23	8	0.2
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG21	8	0.2
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG22	8	0.2
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG23	8	0.2
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	7	0.2
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	7	0.2
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	7	0.2
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG21	9	0.2
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG22	9	0.2
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG23	9	0.2
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG11	9	0.2
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG12	9	0.2
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG13	9	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD11	1	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD12	1	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD13	1	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD11	8	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD12	8	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD13	8	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD11	10	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD12	10	0.2
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD13	10	0.2
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD11	9	0.2
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD12	9	0.2
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD13	9	0.2
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB1	6	0.2
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB2	6	0.2
(1,297)	1:26:A:ILE:H	1:24:A:ALA:HB3	6	0.2
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG21	8	0.2
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG22	8	0.2
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG23	8	0.2
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG21	3	0.2
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG22	3	0.2
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG23	3	0.2
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD11	4	0.2
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD12	4	0.2
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD13	4	0.2
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD21	1	0.2
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD22	1	0.2
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD23	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:134:A:PHE:HD1	1:121:A:ALA:H	7	0.2
(1,222)	1:134:A:PHE:HD2	1:121:A:ALA:H	7	0.2
(1,212)	1:170:A:PHE:HE1	1:22:A:PHE:H	1	0.2
(1,212)	1:170:A:PHE:HE2	1:22:A:PHE:H	1	0.2
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	4	0.2
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	4	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD21	2	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD22	2	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD23	2	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD21	8	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD22	8	0.2
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD23	8	0.2
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE1	5	0.2
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE2	5	0.2
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE3	5	0.2
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE1	9	0.2
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE2	9	0.2
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE3	9	0.2
(1,70)	1:141:A:ALA:HB1	1:138:A:PHE:HD1	9	0.2
(1,70)	1:141:A:ALA:HB1	1:138:A:PHE:HD2	9	0.2
(1,70)	1:141:A:ALA:HB2	1:138:A:PHE:HD1	9	0.2
(1,70)	1:141:A:ALA:HB2	1:138:A:PHE:HD2	9	0.2
(1,70)	1:141:A:ALA:HB3	1:138:A:PHE:HD1	9	0.2
(1,70)	1:141:A:ALA:HB3	1:138:A:PHE:HD2	9	0.2
(1,69)	1:130:A:MET:HE1	1:134:A:PHE:HE1	9	0.2
(1,69)	1:130:A:MET:HE1	1:134:A:PHE:HE2	9	0.2
(1,69)	1:130:A:MET:HE2	1:134:A:PHE:HE1	9	0.2
(1,69)	1:130:A:MET:HE2	1:134:A:PHE:HE2	9	0.2
(1,69)	1:130:A:MET:HE3	1:134:A:PHE:HE1	9	0.2
(1,69)	1:130:A:MET:HE3	1:134:A:PHE:HE2	9	0.2
(1,63)	1:126:A:ALA:HB1	1:118:A:PHE:HD1	10	0.2
(1,63)	1:126:A:ALA:HB2	1:118:A:PHE:HD1	10	0.2
(1,63)	1:126:A:ALA:HB3	1:118:A:PHE:HD1	10	0.2
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	10	0.2
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	10	0.2
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	10	0.2
(1,16)	1:30:A:MET:HE1	1:139:A:TYR:HD1	1	0.2
(1,16)	1:30:A:MET:HE2	1:139:A:TYR:HD1	1	0.2
(1,16)	1:30:A:MET:HE3	1:139:A:TYR:HD1	1	0.2
(2,150)	1:211:A:SER:H	1:207:A:VAL:O	7	0.19
(2,104)	1:48:A:LEU:H	1:44:A:PHE:O	8	0.19
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,887)	1:127:A:ASP:H	1:130:A:MET:H	3	0.19
(1,874)	1:66:A:ASP:H	1:69:A:LYS:H	2	0.19
(1,825)	1:144:A:VAL:H	1:142:A:TYR:H	7	0.19
(1,772)	1:223:A:GLU:H	1:222:A:VAL:H	5	0.19
(1,722)	1:167:A:GLY:H	1:168:A:GLY:H	6	0.19
(1,671)	1:73:A:GLY:H	1:74:A:LYS:H	10	0.19
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG11	5	0.19
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG12	5	0.19
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG13	5	0.19
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG11	5	0.19
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG12	5	0.19
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG13	5	0.19
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG11	5	0.19
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG12	5	0.19
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG13	5	0.19
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	8	0.19
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	8	0.19
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	8	0.19
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	8	0.19
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	8	0.19
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	8	0.19
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	8	0.19
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	8	0.19
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	8	0.19
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG21	9	0.19
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG22	9	0.19
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG23	9	0.19
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG21	9	0.19
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG22	9	0.19
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG23	9	0.19
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG21	9	0.19
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG22	9	0.19
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG23	9	0.19
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB1	9	0.19
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB2	9	0.19
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB3	9	0.19
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB1	9	0.19
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB2	9	0.19
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB3	9	0.19
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB1	9	0.19
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB2	9	0.19
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB3	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:104:A:ILE:HD11	1:172:A:VAL:HG21	9	0.19
(1,591)	1:104:A:ILE:HD11	1:172:A:VAL:HG22	9	0.19
(1,591)	1:104:A:ILE:HD11	1:172:A:VAL:HG23	9	0.19
(1,591)	1:104:A:ILE:HD12	1:172:A:VAL:HG21	9	0.19
(1,591)	1:104:A:ILE:HD12	1:172:A:VAL:HG22	9	0.19
(1,591)	1:104:A:ILE:HD12	1:172:A:VAL:HG23	9	0.19
(1,591)	1:104:A:ILE:HD13	1:172:A:VAL:HG21	9	0.19
(1,591)	1:104:A:ILE:HD13	1:172:A:VAL:HG22	9	0.19
(1,591)	1:104:A:ILE:HD13	1:172:A:VAL:HG23	9	0.19
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	10	0.19
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	10	0.19
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	10	0.19
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	10	0.19
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	10	0.19
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	10	0.19
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	10	0.19
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	10	0.19
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	10	0.19
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	6	0.19
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	6	0.19
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	6	0.19
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	6	0.19
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	6	0.19
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	6	0.19
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	6	0.19
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	6	0.19
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	6	0.19
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	4	0.19
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	4	0.19
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	4	0.19
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	4	0.19
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	4	0.19
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	4	0.19
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	4	0.19
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	4	0.19
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	4	0.19
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	10	0.19
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	10	0.19
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	10	0.19
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	10	0.19
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	10	0.19
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	10	0.19
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	10	0.19
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	10	0.19
(1,545)	1:56:A:LEU:HD11	1:76:A:LEU:HD11	3	0.19
(1,545)	1:56:A:LEU:HD11	1:76:A:LEU:HD12	3	0.19
(1,545)	1:56:A:LEU:HD11	1:76:A:LEU:HD13	3	0.19
(1,545)	1:56:A:LEU:HD12	1:76:A:LEU:HD11	3	0.19
(1,545)	1:56:A:LEU:HD12	1:76:A:LEU:HD12	3	0.19
(1,545)	1:56:A:LEU:HD12	1:76:A:LEU:HD13	3	0.19
(1,545)	1:56:A:LEU:HD13	1:76:A:LEU:HD11	3	0.19
(1,545)	1:56:A:LEU:HD13	1:76:A:LEU:HD12	3	0.19
(1,545)	1:56:A:LEU:HD13	1:76:A:LEU:HD13	3	0.19
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD21	9	0.19
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD22	9	0.19
(1,472)	1:221:A:PHE:H	1:220:A:LEU:HD23	9	0.19
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG11	10	0.19
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG12	10	0.19
(1,440)	1:191:A:LYS:H	1:144:A:VAL:HG13	10	0.19
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG21	2	0.19
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG22	2	0.19
(1,430)	1:188:A:LEU:H	1:148:A:VAL:HG23	2	0.19
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD11	4	0.19
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD12	4	0.19
(1,333)	1:79:A:ASN:H	1:81:A:ILE:HD13	4	0.19
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG21	4	0.19
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG22	4	0.19
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG23	4	0.19
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG21	2	0.19
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG22	2	0.19
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG23	2	0.19
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	2	0.19
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	2	0.19
(1,189)	1:197:A:TYR:HD1	1:195:A:THR:H	2	0.19
(1,189)	1:197:A:TYR:HD2	1:195:A:THR:H	2	0.19
(1,187)	1:160:A:TYR:HD1	1:159:A:GLN:H	9	0.19
(1,187)	1:160:A:TYR:HD2	1:159:A:GLN:H	9	0.19
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD11	3	0.19
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD12	3	0.19
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD13	3	0.19
(1,152)	1:44:A:PHE:H	1:144:A:VAL:HG11	7	0.19
(1,152)	1:44:A:PHE:H	1:144:A:VAL:HG12	7	0.19
(1,152)	1:44:A:PHE:H	1:144:A:VAL:HG13	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	1	0.19
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	1	0.19
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	1	0.19
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD11	6	0.19
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD12	6	0.19
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD13	6	0.19
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	7	0.19
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	7	0.19
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	7	0.19
(1,98)	1:172:A:VAL:HG21	1:170:A:PHE:HE1	3	0.19
(1,98)	1:172:A:VAL:HG22	1:170:A:PHE:HE1	3	0.19
(1,98)	1:172:A:VAL:HG23	1:170:A:PHE:HE1	3	0.19
(1,98)	1:172:A:VAL:HG21	1:170:A:PHE:HE1	6	0.19
(1,98)	1:172:A:VAL:HG22	1:170:A:PHE:HE1	6	0.19
(1,98)	1:172:A:VAL:HG23	1:170:A:PHE:HE1	6	0.19
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	5	0.19
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	5	0.19
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	5	0.19
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	5	0.19
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	5	0.19
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	5	0.19
(1,81)	1:148:A:VAL:HG11	1:142:A:TYR:HE2	10	0.19
(1,81)	1:148:A:VAL:HG12	1:142:A:TYR:HE2	10	0.19
(1,81)	1:148:A:VAL:HG13	1:142:A:TYR:HE2	10	0.19
(1,79)	1:144:A:VAL:HG21	1:44:A:PHE:HE1	9	0.19
(1,79)	1:144:A:VAL:HG21	1:44:A:PHE:HE2	9	0.19
(1,79)	1:144:A:VAL:HG22	1:44:A:PHE:HE1	9	0.19
(1,79)	1:144:A:VAL:HG22	1:44:A:PHE:HE2	9	0.19
(1,79)	1:144:A:VAL:HG23	1:44:A:PHE:HE1	9	0.19
(1,79)	1:144:A:VAL:HG23	1:44:A:PHE:HE2	9	0.19
(1,77)	1:144:A:VAL:HG11	1:197:A:TYR:HD2	9	0.19
(1,77)	1:144:A:VAL:HG12	1:197:A:TYR:HD2	9	0.19
(1,77)	1:144:A:VAL:HG13	1:197:A:TYR:HD2	9	0.19
(1,68)	1:130:A:MET:HE1	1:134:A:PHE:HD2	6	0.19
(1,68)	1:130:A:MET:HE2	1:134:A:PHE:HD2	6	0.19
(1,68)	1:130:A:MET:HE3	1:134:A:PHE:HD2	6	0.19
(1,64)	1:126:A:ALA:HB1	1:118:A:PHE:HE1	8	0.19
(1,64)	1:126:A:ALA:HB2	1:118:A:PHE:HE1	8	0.19
(1,64)	1:126:A:ALA:HB3	1:118:A:PHE:HE1	8	0.19
(1,16)	1:30:A:MET:HE1	1:139:A:TYR:HD1	10	0.19
(1,16)	1:30:A:MET:HE2	1:139:A:TYR:HD1	10	0.19
(1,16)	1:30:A:MET:HE3	1:139:A:TYR:HD1	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	5	0.18
(1,966)	1:154:A:HIS:H	1:183:A:GLY:H	4	0.18
(1,950)	1:147:A:LYS:H	1:191:A:LYS:H	10	0.18
(1,924)	1:81:A:ILE:H	1:92:A:VAL:H	7	0.18
(1,874)	1:66:A:ASP:H	1:69:A:LYS:H	3	0.18
(1,804)	1:68:A:SER:H	1:70:A:LEU:H	5	0.18
(1,703)	1:137:A:GLY:H	1:138:A:PHE:H	2	0.18
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	7	0.18
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	7	0.18
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	7	0.18
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	7	0.18
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	7	0.18
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	7	0.18
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	7	0.18
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	7	0.18
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	7	0.18
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG21	3	0.18
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG22	3	0.18
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG23	3	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG21	3	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG22	3	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG23	3	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG21	3	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG22	3	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG23	3	0.18
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG21	8	0.18
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG22	8	0.18
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG23	8	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG21	8	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG22	8	0.18
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG23	8	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG21	8	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG22	8	0.18
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG23	8	0.18
(1,608)	1:149:A:THR:HG21	1:187:A:ILE:HD11	1	0.18
(1,608)	1:149:A:THR:HG21	1:187:A:ILE:HD12	1	0.18
(1,608)	1:149:A:THR:HG21	1:187:A:ILE:HD13	1	0.18
(1,608)	1:149:A:THR:HG22	1:187:A:ILE:HD11	1	0.18
(1,608)	1:149:A:THR:HG22	1:187:A:ILE:HD12	1	0.18
(1,608)	1:149:A:THR:HG22	1:187:A:ILE:HD13	1	0.18
(1,608)	1:149:A:THR:HG23	1:187:A:ILE:HD11	1	0.18
(1,608)	1:149:A:THR:HG23	1:187:A:ILE:HD12	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:149:A:THR:HG23	1:187:A:ILE:HD13	1	0.18
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB1	10	0.18
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB2	10	0.18
(1,597)	1:148:A:VAL:HG11	1:141:A:ALA:HB3	10	0.18
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB1	10	0.18
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB2	10	0.18
(1,597)	1:148:A:VAL:HG12	1:141:A:ALA:HB3	10	0.18
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB1	10	0.18
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB2	10	0.18
(1,597)	1:148:A:VAL:HG13	1:141:A:ALA:HB3	10	0.18
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG11	6	0.18
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG12	6	0.18
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG13	6	0.18
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG11	6	0.18
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG12	6	0.18
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG13	6	0.18
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG11	6	0.18
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG12	6	0.18
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG13	6	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE1	1	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE2	1	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE3	1	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE1	1	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE2	1	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE3	1	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE1	1	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE2	1	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE3	1	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE1	2	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE2	2	0.18
(1,578)	1:107:A:LEU:HD21	1:98:A:MET:HE3	2	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE1	2	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE2	2	0.18
(1,578)	1:107:A:LEU:HD22	1:98:A:MET:HE3	2	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE1	2	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE2	2	0.18
(1,578)	1:107:A:LEU:HD23	1:98:A:MET:HE3	2	0.18
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	3	0.18
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	3	0.18
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	3	0.18
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	3	0.18
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	3	0.18
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	3	0.18
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	3	0.18
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	3	0.18
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	5	0.18
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	5	0.18
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	5	0.18
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	5	0.18
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	5	0.18
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	5	0.18
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	5	0.18
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	5	0.18
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	5	0.18
(1,554)	1:76:A:LEU:HD21	1:70:A:LEU:HD11	5	0.18
(1,554)	1:76:A:LEU:HD21	1:70:A:LEU:HD12	5	0.18
(1,554)	1:76:A:LEU:HD21	1:70:A:LEU:HD13	5	0.18
(1,554)	1:76:A:LEU:HD22	1:70:A:LEU:HD11	5	0.18
(1,554)	1:76:A:LEU:HD22	1:70:A:LEU:HD12	5	0.18
(1,554)	1:76:A:LEU:HD22	1:70:A:LEU:HD13	5	0.18
(1,554)	1:76:A:LEU:HD23	1:70:A:LEU:HD11	5	0.18
(1,554)	1:76:A:LEU:HD23	1:70:A:LEU:HD12	5	0.18
(1,554)	1:76:A:LEU:HD23	1:70:A:LEU:HD13	5	0.18
(1,552)	1:64:A:LEU:HD11	1:65:A:THR:HG21	10	0.18
(1,552)	1:64:A:LEU:HD11	1:65:A:THR:HG22	10	0.18
(1,552)	1:64:A:LEU:HD11	1:65:A:THR:HG23	10	0.18
(1,552)	1:64:A:LEU:HD12	1:65:A:THR:HG21	10	0.18
(1,552)	1:64:A:LEU:HD12	1:65:A:THR:HG22	10	0.18
(1,552)	1:64:A:LEU:HD12	1:65:A:THR:HG23	10	0.18
(1,552)	1:64:A:LEU:HD13	1:65:A:THR:HG21	10	0.18
(1,552)	1:64:A:LEU:HD13	1:65:A:THR:HG22	10	0.18
(1,552)	1:64:A:LEU:HD13	1:65:A:THR:HG23	10	0.18
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG21	8	0.18
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG22	8	0.18
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG23	8	0.18
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG21	8	0.18
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG22	8	0.18
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG23	8	0.18
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG21	8	0.18
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG22	8	0.18
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG23	8	0.18
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	3	0.18
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	3	0.18
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	3	0.18
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	3	0.18
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	3	0.18
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	3	0.18
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	3	0.18
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	3	0.18
(1,528)	1:45:A:LEU:HD21	1:206:A:ILE:HD11	4	0.18
(1,528)	1:45:A:LEU:HD21	1:206:A:ILE:HD12	4	0.18
(1,528)	1:45:A:LEU:HD21	1:206:A:ILE:HD13	4	0.18
(1,528)	1:45:A:LEU:HD22	1:206:A:ILE:HD11	4	0.18
(1,528)	1:45:A:LEU:HD22	1:206:A:ILE:HD12	4	0.18
(1,528)	1:45:A:LEU:HD22	1:206:A:ILE:HD13	4	0.18
(1,528)	1:45:A:LEU:HD23	1:206:A:ILE:HD11	4	0.18
(1,528)	1:45:A:LEU:HD23	1:206:A:ILE:HD12	4	0.18
(1,528)	1:45:A:LEU:HD23	1:206:A:ILE:HD13	4	0.18
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	3	0.18
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	3	0.18
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	3	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	3	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	3	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	3	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	3	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	3	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	3	0.18
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	10	0.18
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	10	0.18
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	10	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	10	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	10	0.18
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	10	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	10	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	10	0.18
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	10	0.18
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD11	9	0.18
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD12	9	0.18
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD13	9	0.18
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD11	8	0.18
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD12	8	0.18
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD13	8	0.18
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG11	9	0.18
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG12	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG13	9	0.18
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG21	3	0.18
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG22	3	0.18
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG23	3	0.18
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG21	2	0.18
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG22	2	0.18
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG23	2	0.18
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG21	5	0.18
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG22	5	0.18
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG23	5	0.18
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG21	9	0.18
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG22	9	0.18
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG23	9	0.18
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	2	0.18
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	2	0.18
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	2	0.18
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	4	0.18
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	4	0.18
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	4	0.18
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD11	4	0.18
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD12	4	0.18
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD13	4	0.18
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG21	1	0.18
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG22	1	0.18
(1,291)	1:18:A:GLU:H	1:174:A:THR:HG23	1	0.18
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG21	10	0.18
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG22	10	0.18
(1,289)	1:18:A:GLU:H	1:17:A:VAL:HG23	10	0.18
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD21	4	0.18
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD22	4	0.18
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD23	4	0.18
(1,219)	1:134:A:PHE:HD1	1:117:A:ALA:H	8	0.18
(1,219)	1:134:A:PHE:HD2	1:117:A:ALA:H	8	0.18
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	8	0.18
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	8	0.18
(1,189)	1:197:A:TYR:HD1	1:195:A:THR:H	7	0.18
(1,189)	1:197:A:TYR:HD2	1:195:A:THR:H	7	0.18
(1,187)	1:160:A:TYR:HD1	1:159:A:GLN:H	1	0.18
(1,187)	1:160:A:TYR:HD2	1:159:A:GLN:H	1	0.18
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG21	5	0.18
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG22	5	0.18
(1,166)	1:177:A:GLY:H	1:176:A:THR:HG23	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG11	4	0.18
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG12	4	0.18
(1,163)	1:104:A:ILE:H	1:172:A:VAL:HG13	4	0.18
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB1	3	0.18
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB2	3	0.18
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB3	3	0.18
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	4	0.18
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	4	0.18
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	4	0.18
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	5	0.18
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	5	0.18
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	5	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG21	6	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG22	6	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG23	6	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG21	8	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG22	8	0.18
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG23	8	0.18
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD11	6	0.18
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD12	6	0.18
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD13	6	0.18
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	9	0.18
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	9	0.18
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	9	0.18
(1,110)	1:219:A:THR:HG21	1:221:A:PHE:HE1	9	0.18
(1,110)	1:219:A:THR:HG22	1:221:A:PHE:HE1	9	0.18
(1,110)	1:219:A:THR:HG23	1:221:A:PHE:HE1	9	0.18
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	1	0.18
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	1	0.18
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	1	0.18
(1,70)	1:141:A:ALA:HB1	1:138:A:PHE:HD1	4	0.18
(1,70)	1:141:A:ALA:HB1	1:138:A:PHE:HD2	4	0.18
(1,70)	1:141:A:ALA:HB2	1:138:A:PHE:HD1	4	0.18
(1,70)	1:141:A:ALA:HB2	1:138:A:PHE:HD2	4	0.18
(1,70)	1:141:A:ALA:HB3	1:138:A:PHE:HD1	4	0.18
(1,70)	1:141:A:ALA:HB3	1:138:A:PHE:HD2	4	0.18
(1,52)	1:109:A:THR:HG21	1:139:A:TYR:HD2	6	0.18
(1,52)	1:109:A:THR:HG22	1:139:A:TYR:HD2	6	0.18
(1,52)	1:109:A:THR:HG23	1:139:A:TYR:HD2	6	0.18
(1,52)	1:109:A:THR:HG21	1:139:A:TYR:HD2	8	0.18
(1,52)	1:109:A:THR:HG22	1:139:A:TYR:HD2	8	0.18
(1,52)	1:109:A:THR:HG23	1:139:A:TYR:HD2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:107:A:LEU:HD11	1:139:A:TYR:HE1	6	0.18
(1,48)	1:107:A:LEU:HD11	1:139:A:TYR:HE2	6	0.18
(1,48)	1:107:A:LEU:HD12	1:139:A:TYR:HE1	6	0.18
(1,48)	1:107:A:LEU:HD12	1:139:A:TYR:HE2	6	0.18
(1,48)	1:107:A:LEU:HD13	1:139:A:TYR:HE1	6	0.18
(1,48)	1:107:A:LEU:HD13	1:139:A:TYR:HE2	6	0.18
(2,126)	1:59:A:ILE:H	1:55:A:ALA:O	5	0.17
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	5	0.17
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	9	0.17
(1,948)	1:146:A:GLU:H	1:191:A:LYS:H	3	0.17
(1,890)	1:198:A:LEU:H	1:195:A:THR:H	9	0.17
(1,883)	1:117:A:ALA:H	1:120:A:GLU:H	9	0.17
(1,882)	1:117:A:ALA:H	1:114:A:GLY:H	2	0.17
(1,831)	1:192:A:GLU:H	1:194:A:GLN:H	2	0.17
(1,816)	1:117:A:ALA:H	1:119:A:MET:H	9	0.17
(1,811)	1:86:A:ASP:H	1:88:A:THR:H	4	0.17
(1,744)	1:192:A:GLU:H	1:193:A:ASP:H	10	0.17
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	6	0.17
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	6	0.17
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	6	0.17
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	6	0.17
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	6	0.17
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	6	0.17
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	6	0.17
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	6	0.17
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	6	0.17
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG11	10	0.17
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG12	10	0.17
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG13	10	0.17
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG11	10	0.17
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG12	10	0.17
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG13	10	0.17
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG11	10	0.17
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG12	10	0.17
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG13	10	0.17
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD11	6	0.17
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD12	6	0.17
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD13	6	0.17
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD11	6	0.17
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD12	6	0.17
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD13	6	0.17
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD11	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD12	6	0.17
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD13	6	0.17
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	1	0.17
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	1	0.17
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	1	0.17
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	1	0.17
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	1	0.17
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	1	0.17
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	1	0.17
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	1	0.17
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	1	0.17
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG21	7	0.17
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG22	7	0.17
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG23	7	0.17
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG21	7	0.17
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG22	7	0.17
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG23	7	0.17
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG21	7	0.17
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG22	7	0.17
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG23	7	0.17
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG11	6	0.17
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG12	6	0.17
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG13	6	0.17
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG11	6	0.17
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG12	6	0.17
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG13	6	0.17
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG11	2	0.17
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG12	2	0.17
(1,425)	1:187:A:ILE:H	1:150:A:VAL:HG13	2	0.17
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE1	8	0.17
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE2	8	0.17
(1,419)	1:185:A:LYS:H	1:180:A:MET:HE3	8	0.17
(1,406)	1:170:A:PHE:H	1:19:A:THR:HG21	4	0.17
(1,406)	1:170:A:PHE:H	1:19:A:THR:HG22	4	0.17
(1,406)	1:170:A:PHE:H	1:19:A:THR:HG23	4	0.17
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG21	2	0.17
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG22	2	0.17
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG23	2	0.17
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG21	2	0.17
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG22	2	0.17
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG23	2	0.17
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG21	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG22	8	0.17
(1,389)	1:151:A:ILE:H	1:150:A:VAL:HG23	8	0.17
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	6	0.17
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	6	0.17
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	6	0.17
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD21	7	0.17
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD22	7	0.17
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD23	7	0.17
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	8	0.17
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	8	0.17
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	8	0.17
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	10	0.17
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	10	0.17
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	10	0.17
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB1	1	0.17
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB2	1	0.17
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB3	1	0.17
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD11	10	0.17
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD12	10	0.17
(1,279)	1:206:A:ILE:H	1:206:A:ILE:HD13	10	0.17
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	8	0.17
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	8	0.17
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	8	0.17
(1,251)	1:80:A:LEU:H	1:80:A:LEU:HD21	5	0.17
(1,251)	1:80:A:LEU:H	1:80:A:LEU:HD22	5	0.17
(1,251)	1:80:A:LEU:H	1:80:A:LEU:HD23	5	0.17
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD21	1	0.17
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD22	1	0.17
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD23	1	0.17
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD21	9	0.17
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD22	9	0.17
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD23	9	0.17
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	10	0.17
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	10	0.17
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB1	7	0.17
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB2	7	0.17
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB3	7	0.17
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	10	0.17
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	10	0.17
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	10	0.17
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	7	0.17
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	7	0.17
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	7	0.17
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	7	0.17
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	7	0.17
(1,65)	1:126:A:ALA:HB1	1:134:A:PHE:HE1	7	0.17
(1,65)	1:126:A:ALA:HB1	1:134:A:PHE:HE2	7	0.17
(1,65)	1:126:A:ALA:HB2	1:134:A:PHE:HE1	7	0.17
(1,65)	1:126:A:ALA:HB2	1:134:A:PHE:HE2	7	0.17
(1,65)	1:126:A:ALA:HB3	1:134:A:PHE:HE1	7	0.17
(1,65)	1:126:A:ALA:HB3	1:134:A:PHE:HE2	7	0.17
(1,32)	1:81:A:ILE:HD11	1:221:A:PHE:HD1	1	0.17
(1,32)	1:81:A:ILE:HD11	1:221:A:PHE:HD2	1	0.17
(1,32)	1:81:A:ILE:HD12	1:221:A:PHE:HD1	1	0.17
(1,32)	1:81:A:ILE:HD12	1:221:A:PHE:HD2	1	0.17
(1,32)	1:81:A:ILE:HD13	1:221:A:PHE:HD1	1	0.17
(1,32)	1:81:A:ILE:HD13	1:221:A:PHE:HD2	1	0.17
(1,14)	1:32:A:LEU:HD21	1:118:A:PHE:HE2	8	0.17
(1,14)	1:32:A:LEU:HD22	1:118:A:PHE:HE2	8	0.17
(1,14)	1:32:A:LEU:HD23	1:118:A:PHE:HE2	8	0.17
(2,118)	1:55:A:ALA:H	1:51:A:ASN:O	10	0.16
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	1	0.16
(1,823)	1:141:A:ALA:H	1:143:A:LEU:H	6	0.16
(1,816)	1:117:A:ALA:H	1:119:A:MET:H	6	0.16
(1,744)	1:192:A:GLU:H	1:193:A:ASP:H	2	0.16
(1,722)	1:167:A:GLY:H	1:168:A:GLY:H	7	0.16
(1,721)	1:168:A:GLY:H	1:169:A:SER:H	5	0.16
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	5	0.16
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	5	0.16
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	5	0.16
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	5	0.16
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	5	0.16
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	5	0.16
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	5	0.16
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	5	0.16
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	5	0.16
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG11	6	0.16
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG12	6	0.16
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG13	6	0.16
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG11	6	0.16
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG12	6	0.16
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG13	6	0.16
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG11	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG12	6	0.16
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG13	6	0.16
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG11	7	0.16
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG12	7	0.16
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG13	7	0.16
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG11	7	0.16
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG12	7	0.16
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG13	7	0.16
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG11	7	0.16
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG12	7	0.16
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG13	7	0.16
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG21	2	0.16
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG22	2	0.16
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG23	2	0.16
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG21	2	0.16
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG22	2	0.16
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG23	2	0.16
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG21	2	0.16
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG22	2	0.16
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG23	2	0.16
(1,594)	1:126:A:ALA:HB1	1:130:A:MET:HE1	9	0.16
(1,594)	1:126:A:ALA:HB1	1:130:A:MET:HE2	9	0.16
(1,594)	1:126:A:ALA:HB1	1:130:A:MET:HE3	9	0.16
(1,594)	1:126:A:ALA:HB2	1:130:A:MET:HE1	9	0.16
(1,594)	1:126:A:ALA:HB2	1:130:A:MET:HE2	9	0.16
(1,594)	1:126:A:ALA:HB2	1:130:A:MET:HE3	9	0.16
(1,594)	1:126:A:ALA:HB3	1:130:A:MET:HE1	9	0.16
(1,594)	1:126:A:ALA:HB3	1:130:A:MET:HE2	9	0.16
(1,594)	1:126:A:ALA:HB3	1:130:A:MET:HE3	9	0.16
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD11	4	0.16
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD12	4	0.16
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD13	4	0.16
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD11	4	0.16
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD12	4	0.16
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD13	4	0.16
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD11	4	0.16
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD12	4	0.16
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD13	4	0.16
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG21	9	0.16
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG22	9	0.16
(1,587)	1:103:A:LEU:HD21	1:152:A:THR:HG23	9	0.16
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG21	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG22	9	0.16
(1,587)	1:103:A:LEU:HD22	1:152:A:THR:HG23	9	0.16
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG21	9	0.16
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG22	9	0.16
(1,587)	1:103:A:LEU:HD23	1:152:A:THR:HG23	9	0.16
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	9	0.16
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	9	0.16
(1,567)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	9	0.16
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	9	0.16
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	9	0.16
(1,567)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	9	0.16
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	9	0.16
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	9	0.16
(1,567)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	9	0.16
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG21	3	0.16
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG22	3	0.16
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG23	3	0.16
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG21	3	0.16
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG22	3	0.16
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG23	3	0.16
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG21	3	0.16
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG22	3	0.16
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG23	3	0.16
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG21	9	0.16
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG22	9	0.16
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG23	9	0.16
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG21	9	0.16
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG22	9	0.16
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG23	9	0.16
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG21	9	0.16
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG22	9	0.16
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG23	9	0.16
(1,559)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	4	0.16
(1,559)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	4	0.16
(1,559)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	4	0.16
(1,559)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	4	0.16
(1,559)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	4	0.16
(1,559)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	4	0.16
(1,559)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	4	0.16
(1,559)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	4	0.16
(1,559)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	4	0.16
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	10	0.16
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	10	0.16
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	10	0.16
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	10	0.16
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	10	0.16
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	10	0.16
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	10	0.16
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	10	0.16
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG21	5	0.16
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG22	5	0.16
(1,534)	1:48:A:LEU:HD11	1:186:A:VAL:HG23	5	0.16
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG21	5	0.16
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG22	5	0.16
(1,534)	1:48:A:LEU:HD12	1:186:A:VAL:HG23	5	0.16
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG21	5	0.16
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG22	5	0.16
(1,534)	1:48:A:LEU:HD13	1:186:A:VAL:HG23	5	0.16
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	7	0.16
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	7	0.16
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	7	0.16
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	7	0.16
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	7	0.16
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	7	0.16
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	7	0.16
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	7	0.16
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	7	0.16
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG21	9	0.16
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG22	9	0.16
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG23	9	0.16
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG21	9	0.16
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG22	9	0.16
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG23	9	0.16
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG21	9	0.16
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG22	9	0.16
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG23	9	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG21	4	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG22	4	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG23	4	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG21	10	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG22	10	0.16
(1,469)	1:220:A:LEU:H	1:219:A:THR:HG23	10	0.16
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD11	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD12	4	0.16
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD13	4	0.16
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD11	9	0.16
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD12	9	0.16
(1,467)	1:216:A:TYR:H	1:214:A:ILE:HD13	9	0.16
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG21	6	0.16
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG22	6	0.16
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG23	6	0.16
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG21	10	0.16
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG22	10	0.16
(1,444)	1:192:A:GLU:H	1:195:A:THR:HG23	10	0.16
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD21	2	0.16
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD22	2	0.16
(1,437)	1:189:A:HIS:H	1:188:A:LEU:HD23	2	0.16
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG21	4	0.16
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG22	4	0.16
(1,426)	1:187:A:ILE:H	1:150:A:VAL:HG23	4	0.16
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD11	10	0.16
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD12	10	0.16
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD13	10	0.16
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG21	6	0.16
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG22	6	0.16
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG23	6	0.16
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB1	7	0.16
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB2	7	0.16
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB3	7	0.16
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE1	5	0.16
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE2	5	0.16
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE3	5	0.16
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE1	6	0.16
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE2	6	0.16
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE3	6	0.16
(1,364)	1:96:A:ILE:H	1:55:A:ALA:HB1	2	0.16
(1,364)	1:96:A:ILE:H	1:55:A:ALA:HB2	2	0.16
(1,364)	1:96:A:ILE:H	1:55:A:ALA:HB3	2	0.16
(1,363)	1:93:A:ASP:H	1:180:A:MET:HE1	6	0.16
(1,363)	1:93:A:ASP:H	1:180:A:MET:HE2	6	0.16
(1,363)	1:93:A:ASP:H	1:180:A:MET:HE3	6	0.16
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG21	4	0.16
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG22	4	0.16
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG23	4	0.16
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG11	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG12	2	0.16
(1,343)	1:81:A:ILE:H	1:92:A:VAL:HG13	2	0.16
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG11	5	0.16
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG12	5	0.16
(1,335)	1:79:A:ASN:H	1:92:A:VAL:HG13	5	0.16
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD11	1	0.16
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD12	1	0.16
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD13	1	0.16
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD11	9	0.16
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD12	9	0.16
(1,334)	1:79:A:ASN:H	1:80:A:LEU:HD13	9	0.16
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD21	5	0.16
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD22	5	0.16
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD23	5	0.16
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD11	8	0.16
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD12	8	0.16
(1,283)	1:218:A:ILE:H	1:218:A:ILE:HD13	8	0.16
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	5	0.16
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	5	0.16
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	5	0.16
(1,217)	1:221:A:PHE:HE1	1:220:A:LEU:H	10	0.16
(1,217)	1:221:A:PHE:HE2	1:220:A:LEU:H	10	0.16
(1,192)	1:216:A:TYR:HE1	1:57:A:ASP:H	8	0.16
(1,192)	1:216:A:TYR:HE2	1:57:A:ASP:H	8	0.16
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD11	5	0.16
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD12	5	0.16
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD13	5	0.16
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	3	0.16
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	3	0.16
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	3	0.16
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	5	0.16
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	5	0.16
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	5	0.16
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB1	3	0.16
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB2	3	0.16
(1,147)	1:123:A:GLN:H	1:126:A:ALA:HB3	3	0.16
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB1	7	0.16
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB2	7	0.16
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB3	7	0.16
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD11	8	0.16
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD12	8	0.16
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD13	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG21	10	0.16
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG22	10	0.16
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG23	10	0.16
(1,117)	1:34:A:ILE:H	1:32:A:LEU:HD21	9	0.16
(1,117)	1:34:A:ILE:H	1:32:A:LEU:HD22	9	0.16
(1,117)	1:34:A:ILE:H	1:32:A:LEU:HD23	9	0.16
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE1	8	0.16
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE2	8	0.16
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE3	8	0.16
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	8	0.16
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	8	0.16
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	8	0.16
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	8	0.16
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	8	0.16
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	8	0.16
(1,80)	1:144:A:VAL:HG21	1:197:A:TYR:HD2	7	0.16
(1,80)	1:144:A:VAL:HG22	1:197:A:TYR:HD2	7	0.16
(1,80)	1:144:A:VAL:HG23	1:197:A:TYR:HD2	7	0.16
(1,77)	1:144:A:VAL:HG11	1:197:A:TYR:HD2	10	0.16
(1,77)	1:144:A:VAL:HG12	1:197:A:TYR:HD2	10	0.16
(1,77)	1:144:A:VAL:HG13	1:197:A:TYR:HD2	10	0.16
(1,63)	1:126:A:ALA:HB1	1:118:A:PHE:HD1	6	0.16
(1,63)	1:126:A:ALA:HB2	1:118:A:PHE:HD1	6	0.16
(1,63)	1:126:A:ALA:HB3	1:118:A:PHE:HD1	6	0.16
(1,48)	1:107:A:LEU:HD11	1:139:A:TYR:HE1	9	0.16
(1,48)	1:107:A:LEU:HD11	1:139:A:TYR:HE2	9	0.16
(1,48)	1:107:A:LEU:HD12	1:139:A:TYR:HE1	9	0.16
(1,48)	1:107:A:LEU:HD12	1:139:A:TYR:HE2	9	0.16
(1,48)	1:107:A:LEU:HD13	1:139:A:TYR:HE1	9	0.16
(1,48)	1:107:A:LEU:HD13	1:139:A:TYR:HE2	9	0.16
(1,43)	1:103:A:LEU:HD21	1:160:A:TYR:HE1	4	0.16
(1,43)	1:103:A:LEU:HD21	1:160:A:TYR:HE2	4	0.16
(1,43)	1:103:A:LEU:HD22	1:160:A:TYR:HE1	4	0.16
(1,43)	1:103:A:LEU:HD22	1:160:A:TYR:HE2	4	0.16
(1,43)	1:103:A:LEU:HD23	1:160:A:TYR:HE1	4	0.16
(1,43)	1:103:A:LEU:HD23	1:160:A:TYR:HE2	4	0.16
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	3	0.16
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	3	0.16
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	3	0.16
(1,27)	1:64:A:LEU:HD11	1:61:A:TYR:HD1	9	0.16
(1,27)	1:64:A:LEU:HD12	1:61:A:TYR:HD1	9	0.16
(1,27)	1:64:A:LEU:HD13	1:61:A:TYR:HD1	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:34:A:ILE:HD11	1:142:A:TYR:HE1	1	0.16
(1,21)	1:34:A:ILE:HD11	1:142:A:TYR:HE2	1	0.16
(1,21)	1:34:A:ILE:HD12	1:142:A:TYR:HE1	1	0.16
(1,21)	1:34:A:ILE:HD12	1:142:A:TYR:HE2	1	0.16
(1,21)	1:34:A:ILE:HD13	1:142:A:TYR:HE1	1	0.16
(1,21)	1:34:A:ILE:HD13	1:142:A:TYR:HE2	1	0.16
(1,7)	1:29:A:LEU:HD11	1:139:A:TYR:HD2	2	0.16
(1,7)	1:29:A:LEU:HD12	1:139:A:TYR:HD2	2	0.16
(1,7)	1:29:A:LEU:HD13	1:139:A:TYR:HD2	2	0.16
(2,132)	1:62:A:GLU:H	1:58:A:LYS:O	6	0.15
(2,126)	1:59:A:ILE:H	1:55:A:ALA:O	8	0.15
(2,108)	1:50:A:SER:H	1:46:A:ARG:O	3	0.15
(2,108)	1:50:A:SER:H	1:46:A:ARG:O	8	0.15
(1,958)	1:185:A:LYS:H	1:151:A:ILE:H	6	0.15
(1,902)	1:211:A:SER:H	1:214:A:ILE:H	3	0.15
(1,885)	1:121:A:ALA:H	1:124:A:ALA:H	5	0.15
(1,875)	1:68:A:SER:H	1:71:A:ASP:H	5	0.15
(1,829)	1:180:A:MET:H	1:182:A:ARG:H	3	0.15
(1,828)	1:167:A:GLY:H	1:169:A:SER:H	5	0.15
(1,767)	1:215:A:GLY:H	1:216:A:TYR:H	6	0.15
(1,767)	1:215:A:GLY:H	1:216:A:TYR:H	7	0.15
(1,744)	1:192:A:GLU:H	1:193:A:ASP:H	9	0.15
(1,731)	1:177:A:GLY:H	1:178:A:GLU:H	8	0.15
(1,715)	1:158:A:GLU:H	1:159:A:GLN:H	2	0.15
(1,701)	1:129:A:SER:H	1:130:A:MET:H	5	0.15
(1,665)	1:66:A:ASP:H	1:65:A:THR:H	8	0.15
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	9	0.15
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	9	0.15
(1,623)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	9	0.15
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	9	0.15
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	9	0.15
(1,623)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	9	0.15
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	9	0.15
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	9	0.15
(1,623)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	9	0.15
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG21	2	0.15
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG22	2	0.15
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG23	2	0.15
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG21	2	0.15
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG22	2	0.15
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG23	2	0.15
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG21	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG22	2	0.15
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG23	2	0.15
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG21	9	0.15
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG22	9	0.15
(1,618)	1:190:A:LEU:HD21	1:195:A:THR:HG23	9	0.15
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG21	9	0.15
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG22	9	0.15
(1,618)	1:190:A:LEU:HD22	1:195:A:THR:HG23	9	0.15
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG21	9	0.15
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG22	9	0.15
(1,618)	1:190:A:LEU:HD23	1:195:A:THR:HG23	9	0.15
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG11	7	0.15
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG12	7	0.15
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG13	7	0.15
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG11	7	0.15
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG12	7	0.15
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG13	7	0.15
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG11	7	0.15
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG12	7	0.15
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG13	7	0.15
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG21	5	0.15
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG22	5	0.15
(1,610)	1:150:A:VAL:HG21	1:184:A:THR:HG23	5	0.15
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG21	5	0.15
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG22	5	0.15
(1,610)	1:150:A:VAL:HG22	1:184:A:THR:HG23	5	0.15
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG21	5	0.15
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG22	5	0.15
(1,610)	1:150:A:VAL:HG23	1:184:A:THR:HG23	5	0.15
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD11	2	0.15
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD12	2	0.15
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD13	2	0.15
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD11	2	0.15
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD12	2	0.15
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD13	2	0.15
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD11	2	0.15
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD12	2	0.15
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD13	2	0.15
(1,592)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	6	0.15
(1,592)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	6	0.15
(1,592)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	6	0.15
(1,592)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	6	0.15
(1,592)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	6	0.15
(1,592)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	6	0.15
(1,592)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	6	0.15
(1,592)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	6	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD11	1	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD12	1	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD13	1	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD11	1	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD12	1	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD13	1	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD11	1	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD12	1	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD13	1	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD11	5	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD12	5	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD13	5	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD11	5	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD12	5	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD13	5	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD11	5	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD12	5	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD13	5	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD11	8	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD12	8	0.15
(1,590)	1:172:A:VAL:HG11	1:104:A:ILE:HD13	8	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD11	8	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD12	8	0.15
(1,590)	1:172:A:VAL:HG12	1:104:A:ILE:HD13	8	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD11	8	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD12	8	0.15
(1,590)	1:172:A:VAL:HG13	1:104:A:ILE:HD13	8	0.15
(1,576)	1:98:A:MET:HE1	1:103:A:LEU:HD21	6	0.15
(1,576)	1:98:A:MET:HE1	1:103:A:LEU:HD22	6	0.15
(1,576)	1:98:A:MET:HE1	1:103:A:LEU:HD23	6	0.15
(1,576)	1:98:A:MET:HE2	1:103:A:LEU:HD21	6	0.15
(1,576)	1:98:A:MET:HE2	1:103:A:LEU:HD22	6	0.15
(1,576)	1:98:A:MET:HE2	1:103:A:LEU:HD23	6	0.15
(1,576)	1:98:A:MET:HE3	1:103:A:LEU:HD21	6	0.15
(1,576)	1:98:A:MET:HE3	1:103:A:LEU:HD22	6	0.15
(1,576)	1:98:A:MET:HE3	1:103:A:LEU:HD23	6	0.15
(1,575)	1:98:A:MET:HE1	1:103:A:LEU:HD11	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:98:A:MET:HE1	1:103:A:LEU:HD12	3	0.15
(1,575)	1:98:A:MET:HE1	1:103:A:LEU:HD13	3	0.15
(1,575)	1:98:A:MET:HE2	1:103:A:LEU:HD11	3	0.15
(1,575)	1:98:A:MET:HE2	1:103:A:LEU:HD12	3	0.15
(1,575)	1:98:A:MET:HE2	1:103:A:LEU:HD13	3	0.15
(1,575)	1:98:A:MET:HE3	1:103:A:LEU:HD11	3	0.15
(1,575)	1:98:A:MET:HE3	1:103:A:LEU:HD12	3	0.15
(1,575)	1:98:A:MET:HE3	1:103:A:LEU:HD13	3	0.15
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	6	0.15
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	6	0.15
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	6	0.15
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	6	0.15
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	6	0.15
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	6	0.15
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	6	0.15
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	6	0.15
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	6	0.15
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	10	0.15
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	10	0.15
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	10	0.15
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	10	0.15
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	10	0.15
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	10	0.15
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	10	0.15
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	10	0.15
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	10	0.15
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	6	0.15
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	6	0.15
(1,546)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	6	0.15
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	6	0.15
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	6	0.15
(1,546)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	6	0.15
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	6	0.15
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	6	0.15
(1,546)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	6	0.15
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD11	2	0.15
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD12	2	0.15
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD13	2	0.15
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD11	2	0.15
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD12	2	0.15
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD13	2	0.15
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD11	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD12	2	0.15
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD13	2	0.15
(1,538)	1:48:A:LEU:HD21	1:188:A:LEU:HD11	2	0.15
(1,538)	1:48:A:LEU:HD21	1:188:A:LEU:HD12	2	0.15
(1,538)	1:48:A:LEU:HD21	1:188:A:LEU:HD13	2	0.15
(1,538)	1:48:A:LEU:HD22	1:188:A:LEU:HD11	2	0.15
(1,538)	1:48:A:LEU:HD22	1:188:A:LEU:HD12	2	0.15
(1,538)	1:48:A:LEU:HD22	1:188:A:LEU:HD13	2	0.15
(1,538)	1:48:A:LEU:HD23	1:188:A:LEU:HD11	2	0.15
(1,538)	1:48:A:LEU:HD23	1:188:A:LEU:HD12	2	0.15
(1,538)	1:48:A:LEU:HD23	1:188:A:LEU:HD13	2	0.15
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	5	0.15
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	5	0.15
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	5	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	5	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	5	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	5	0.15
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	5	0.15
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	5	0.15
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	5	0.15
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	10	0.15
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	10	0.15
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	10	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	10	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	10	0.15
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	10	0.15
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	10	0.15
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	10	0.15
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	10	0.15
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB1	10	0.15
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB2	10	0.15
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB3	10	0.15
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB1	10	0.15
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB2	10	0.15
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB3	10	0.15
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB1	10	0.15
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB2	10	0.15
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB3	10	0.15
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	5	0.15
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	5	0.15
(1,524)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	5	0.15
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	5	0.15
(1,524)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	5	0.15
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	5	0.15
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	5	0.15
(1,524)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	5	0.15
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE1	10	0.15
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE2	10	0.15
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE3	10	0.15
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE1	10	0.15
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE2	10	0.15
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE3	10	0.15
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE1	10	0.15
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE2	10	0.15
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE3	10	0.15
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE1	7	0.15
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE2	7	0.15
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE3	7	0.15
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE1	7	0.15
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE2	7	0.15
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE3	7	0.15
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE1	7	0.15
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE2	7	0.15
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE3	7	0.15
(1,456)	1:204:A:LYS:H	1:203:A:ILE:HD11	2	0.15
(1,456)	1:204:A:LYS:H	1:203:A:ILE:HD12	2	0.15
(1,456)	1:204:A:LYS:H	1:203:A:ILE:HD13	2	0.15
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD11	7	0.15
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD12	7	0.15
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD13	7	0.15
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG21	6	0.15
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG22	6	0.15
(1,382)	1:145:A:ALA:H	1:144:A:VAL:HG23	6	0.15
(1,358)	1:91:A:ILE:H	1:92:A:VAL:HG11	6	0.15
(1,358)	1:91:A:ILE:H	1:92:A:VAL:HG12	6	0.15
(1,358)	1:91:A:ILE:H	1:92:A:VAL:HG13	6	0.15
(1,349)	1:84:A:LYS:H	1:198:A:LEU:HD21	5	0.15
(1,349)	1:84:A:LYS:H	1:198:A:LEU:HD22	5	0.15
(1,349)	1:84:A:LYS:H	1:198:A:LEU:HD23	5	0.15
(1,328)	1:77:A:HIS:H	1:56:A:LEU:HD11	9	0.15
(1,328)	1:77:A:HIS:H	1:56:A:LEU:HD12	9	0.15
(1,328)	1:77:A:HIS:H	1:56:A:LEU:HD13	9	0.15
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD21	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD22	6	0.15
(1,326)	1:75:A:GLU:H	1:76:A:LEU:HD23	6	0.15
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	1	0.15
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	1	0.15
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	1	0.15
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	2	0.15
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	2	0.15
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	2	0.15
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB1	3	0.15
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB2	3	0.15
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB3	3	0.15
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	1	0.15
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	1	0.15
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	1	0.15
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	4	0.15
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	4	0.15
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	4	0.15
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG11	8	0.15
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG12	8	0.15
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG13	8	0.15
(1,204)	1:22:A:PHE:HD1	1:26:A:ILE:H	8	0.15
(1,204)	1:22:A:PHE:HD2	1:26:A:ILE:H	8	0.15
(1,167)	1:184:A:THR:H	1:180:A:MET:HE1	8	0.15
(1,167)	1:184:A:THR:H	1:180:A:MET:HE2	8	0.15
(1,167)	1:184:A:THR:H	1:180:A:MET:HE3	8	0.15
(1,164)	1:159:A:GLN:H	1:174:A:THR:HG21	10	0.15
(1,164)	1:159:A:GLN:H	1:174:A:THR:HG22	10	0.15
(1,164)	1:159:A:GLN:H	1:174:A:THR:HG23	10	0.15
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB1	4	0.15
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB2	4	0.15
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB3	4	0.15
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD11	5	0.15
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD12	5	0.15
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD13	5	0.15
(1,106)	1:206:A:ILE:HD11	1:44:A:PHE:HE1	4	0.15
(1,106)	1:206:A:ILE:HD11	1:44:A:PHE:HE2	4	0.15
(1,106)	1:206:A:ILE:HD12	1:44:A:PHE:HE1	4	0.15
(1,106)	1:206:A:ILE:HD12	1:44:A:PHE:HE2	4	0.15
(1,106)	1:206:A:ILE:HD13	1:44:A:PHE:HE1	4	0.15
(1,106)	1:206:A:ILE:HD13	1:44:A:PHE:HE2	4	0.15
(1,98)	1:172:A:VAL:HG21	1:170:A:PHE:HE1	7	0.15
(1,98)	1:172:A:VAL:HG22	1:170:A:PHE:HE1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:172:A:VAL:HG23	1:170:A:PHE:HE1	7	0.15
(1,85)	1:152:A:THR:HG21	1:160:A:TYR:HE2	3	0.15
(1,85)	1:152:A:THR:HG22	1:160:A:TYR:HE2	3	0.15
(1,85)	1:152:A:THR:HG23	1:160:A:TYR:HE2	3	0.15
(1,85)	1:152:A:THR:HG21	1:160:A:TYR:HE2	8	0.15
(1,85)	1:152:A:THR:HG22	1:160:A:TYR:HE2	8	0.15
(1,85)	1:152:A:THR:HG23	1:160:A:TYR:HE2	8	0.15
(1,72)	1:143:A:LEU:HD11	1:38:A:TYR:HD2	2	0.15
(1,72)	1:143:A:LEU:HD12	1:38:A:TYR:HD2	2	0.15
(1,72)	1:143:A:LEU:HD13	1:38:A:TYR:HD2	2	0.15
(1,55)	1:119:A:MET:HE1	1:118:A:PHE:HD2	5	0.15
(1,55)	1:119:A:MET:HE2	1:118:A:PHE:HD2	5	0.15
(1,55)	1:119:A:MET:HE3	1:118:A:PHE:HD2	5	0.15
(1,49)	1:107:A:LEU:HD11	1:142:A:TYR:HE2	6	0.15
(1,49)	1:107:A:LEU:HD12	1:142:A:TYR:HE2	6	0.15
(1,49)	1:107:A:LEU:HD13	1:142:A:TYR:HE2	6	0.15
(1,38)	1:91:A:ILE:HD11	1:44:A:PHE:HD1	1	0.15
(1,38)	1:91:A:ILE:HD11	1:44:A:PHE:HD2	1	0.15
(1,38)	1:91:A:ILE:HD12	1:44:A:PHE:HD1	1	0.15
(1,38)	1:91:A:ILE:HD12	1:44:A:PHE:HD2	1	0.15
(1,38)	1:91:A:ILE:HD13	1:44:A:PHE:HD1	1	0.15
(1,38)	1:91:A:ILE:HD13	1:44:A:PHE:HD2	1	0.15
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	5	0.15
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	5	0.15
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	5	0.15
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE1	10	0.15
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE2	10	0.15
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE1	10	0.15
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE2	10	0.15
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE1	10	0.15
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE2	10	0.15
(1,15)	1:30:A:MET:HE1	1:22:A:PHE:HE1	3	0.15
(1,15)	1:30:A:MET:HE1	1:22:A:PHE:HE2	3	0.15
(1,15)	1:30:A:MET:HE2	1:22:A:PHE:HE1	3	0.15
(1,15)	1:30:A:MET:HE2	1:22:A:PHE:HE2	3	0.15
(1,15)	1:30:A:MET:HE3	1:22:A:PHE:HE1	3	0.15
(1,15)	1:30:A:MET:HE3	1:22:A:PHE:HE2	3	0.15
(1,13)	1:32:A:LEU:HD21	1:118:A:PHE:HD2	3	0.15
(1,13)	1:32:A:LEU:HD22	1:118:A:PHE:HD2	3	0.15
(1,13)	1:32:A:LEU:HD23	1:118:A:PHE:HD2	3	0.15
(1,11)	1:32:A:LEU:HD11	1:118:A:PHE:HD2	1	0.15
(1,11)	1:32:A:LEU:HD12	1:118:A:PHE:HD2	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:32:A:LEU:HD13	1:118:A:PHE:HD2	1	0.15
(2,146)	1:209:A:LYS:H	1:205:A:GLU:O	7	0.14
(2,132)	1:62:A:GLU:H	1:58:A:LYS:O	8	0.14
(2,80)	1:190:A:LEU:H	1:87:A:ARG:O	8	0.14
(1,967)	1:159:A:GLN:H	1:175:A:ASP:H	10	0.14
(1,923)	1:90:A:THR:H	1:81:A:ILE:H	4	0.14
(1,884)	1:120:A:GLU:H	1:123:A:GLN:H	7	0.14
(1,823)	1:141:A:ALA:H	1:143:A:LEU:H	9	0.14
(1,816)	1:117:A:ALA:H	1:119:A:MET:H	10	0.14
(1,806)	1:72:A:SER:H	1:70:A:LEU:H	4	0.14
(1,730)	1:176:A:THR:H	1:177:A:GLY:H	5	0.14
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD11	5	0.14
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD12	5	0.14
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD13	5	0.14
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD11	5	0.14
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD12	5	0.14
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD13	5	0.14
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD11	5	0.14
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD12	5	0.14
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD13	5	0.14
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	5	0.14
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	5	0.14
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	5	0.14
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	5	0.14
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	5	0.14
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	5	0.14
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	5	0.14
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	5	0.14
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	5	0.14
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD11	3	0.14
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD12	3	0.14
(1,596)	1:136:A:VAL:HG11	1:131:A:ILE:HD13	3	0.14
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD11	3	0.14
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD12	3	0.14
(1,596)	1:136:A:VAL:HG12	1:131:A:ILE:HD13	3	0.14
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD11	3	0.14
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD12	3	0.14
(1,596)	1:136:A:VAL:HG13	1:131:A:ILE:HD13	3	0.14
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	4	0.14
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	4	0.14
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	4	0.14
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	4	0.14
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	4	0.14
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	4	0.14
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	4	0.14
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	4	0.14
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	10	0.14
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	10	0.14
(1,566)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	10	0.14
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	10	0.14
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	10	0.14
(1,566)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	10	0.14
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	10	0.14
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	10	0.14
(1,566)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	10	0.14
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	2	0.14
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	2	0.14
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	2	0.14
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	2	0.14
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	2	0.14
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	2	0.14
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	2	0.14
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	2	0.14
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	2	0.14
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB1	5	0.14
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB2	5	0.14
(1,533)	1:48:A:LEU:HD11	1:141:A:ALA:HB3	5	0.14
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB1	5	0.14
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB2	5	0.14
(1,533)	1:48:A:LEU:HD12	1:141:A:ALA:HB3	5	0.14
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB1	5	0.14
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB2	5	0.14
(1,533)	1:48:A:LEU:HD13	1:141:A:ALA:HB3	5	0.14
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD11	7	0.14
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD12	7	0.14
(1,512)	1:122:A:LEU:HD11	1:32:A:LEU:HD13	7	0.14
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD11	7	0.14
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD12	7	0.14
(1,512)	1:122:A:LEU:HD12	1:32:A:LEU:HD13	7	0.14
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD11	7	0.14
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD12	7	0.14
(1,512)	1:122:A:LEU:HD13	1:32:A:LEU:HD13	7	0.14
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG21	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG22	4	0.14
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG23	4	0.14
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG21	4	0.14
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG22	4	0.14
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG23	4	0.14
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG21	4	0.14
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG22	4	0.14
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG23	4	0.14
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG11	1	0.14
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG12	1	0.14
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG13	1	0.14
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG11	5	0.14
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG12	5	0.14
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG13	5	0.14
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD21	4	0.14
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD22	4	0.14
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD23	4	0.14
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD11	6	0.14
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD12	6	0.14
(1,446)	1:194:A:GLN:H	1:190:A:LEU:HD13	6	0.14
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD21	7	0.14
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD22	7	0.14
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD23	7	0.14
(1,421)	1:186:A:VAL:H	1:90:A:THR:HG21	5	0.14
(1,421)	1:186:A:VAL:H	1:90:A:THR:HG22	5	0.14
(1,421)	1:186:A:VAL:H	1:90:A:THR:HG23	5	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG21	1	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG22	1	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG23	1	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG21	4	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG22	4	0.14
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG23	4	0.14
(1,404)	1:163:A:GLU:H	1:172:A:VAL:HG11	3	0.14
(1,404)	1:163:A:GLU:H	1:172:A:VAL:HG12	3	0.14
(1,404)	1:163:A:GLU:H	1:172:A:VAL:HG13	3	0.14
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE1	10	0.14
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE2	10	0.14
(1,378)	1:127:A:ASP:H	1:130:A:MET:HE3	10	0.14
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB1	3	0.14
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB2	3	0.14
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB3	3	0.14
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB1	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB2	4	0.14
(1,375)	1:126:A:ALA:H	1:124:A:ALA:HB3	4	0.14
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB1	3	0.14
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB2	3	0.14
(1,374)	1:125:A:GLY:H	1:124:A:ALA:HB3	3	0.14
(1,372)	1:123:A:GLN:H	1:122:A:LEU:HD21	7	0.14
(1,372)	1:123:A:GLN:H	1:122:A:LEU:HD22	7	0.14
(1,372)	1:123:A:GLN:H	1:122:A:LEU:HD23	7	0.14
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB1	2	0.14
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB2	2	0.14
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB3	2	0.14
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG21	7	0.14
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG22	7	0.14
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG23	7	0.14
(1,321)	1:66:A:ASP:H	1:65:A:THR:HG21	8	0.14
(1,321)	1:66:A:ASP:H	1:65:A:THR:HG22	8	0.14
(1,321)	1:66:A:ASP:H	1:65:A:THR:HG23	8	0.14
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	6	0.14
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	6	0.14
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	6	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	5	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	5	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	5	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	7	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	7	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	7	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	8	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	8	0.14
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	8	0.14
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG21	5	0.14
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG22	5	0.14
(1,287)	1:222:A:VAL:H	1:222:A:VAL:HG23	5	0.14
(1,187)	1:160:A:TYR:HD1	1:159:A:GLN:H	10	0.14
(1,187)	1:160:A:TYR:HD2	1:159:A:GLN:H	10	0.14
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB1	3	0.14
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB2	3	0.14
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB3	3	0.14
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB1	9	0.14
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB2	9	0.14
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB3	9	0.14
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB1	2	0.14
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:125:A:GLY:H	1:126:A:ALA:HB3	2	0.14
(1,134)	1:86:A:ASP:H	1:88:A:THR:HG21	6	0.14
(1,134)	1:86:A:ASP:H	1:88:A:THR:HG22	6	0.14
(1,134)	1:86:A:ASP:H	1:88:A:THR:HG23	6	0.14
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD21	4	0.14
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD22	4	0.14
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD23	4	0.14
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD11	2	0.14
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD12	2	0.14
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD13	2	0.14
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE1	7	0.14
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE2	7	0.14
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE3	7	0.14
(1,113)	1:168:A:GLY:H	1:27:A:ALA:HB1	1	0.14
(1,113)	1:168:A:GLY:H	1:27:A:ALA:HB2	1	0.14
(1,113)	1:168:A:GLY:H	1:27:A:ALA:HB3	1	0.14
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	2	0.14
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	2	0.14
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	2	0.14
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	3	0.14
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	3	0.14
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	3	0.14
(1,106)	1:206:A:ILE:HD11	1:44:A:PHE:HE1	1	0.14
(1,106)	1:206:A:ILE:HD11	1:44:A:PHE:HE2	1	0.14
(1,106)	1:206:A:ILE:HD12	1:44:A:PHE:HE1	1	0.14
(1,106)	1:206:A:ILE:HD12	1:44:A:PHE:HE2	1	0.14
(1,106)	1:206:A:ILE:HD13	1:44:A:PHE:HE1	1	0.14
(1,106)	1:206:A:ILE:HD13	1:44:A:PHE:HE2	1	0.14
(1,87)	1:166:A:ALA:HB1	1:142:A:TYR:HD1	7	0.14
(1,87)	1:166:A:ALA:HB1	1:142:A:TYR:HD2	7	0.14
(1,87)	1:166:A:ALA:HB2	1:142:A:TYR:HD1	7	0.14
(1,87)	1:166:A:ALA:HB2	1:142:A:TYR:HD2	7	0.14
(1,87)	1:166:A:ALA:HB3	1:142:A:TYR:HD1	7	0.14
(1,87)	1:166:A:ALA:HB3	1:142:A:TYR:HD2	7	0.14
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	4	0.14
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	4	0.14
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	4	0.14
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	4	0.14
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	4	0.14
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	4	0.14
(1,77)	1:144:A:VAL:HG11	1:197:A:TYR:HD2	6	0.14
(1,77)	1:144:A:VAL:HG12	1:197:A:TYR:HD2	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:144:A:VAL:HG13	1:197:A:TYR:HD2	6	0.14
(1,68)	1:130:A:MET:HE1	1:134:A:PHE:HD2	9	0.14
(1,68)	1:130:A:MET:HE2	1:134:A:PHE:HD2	9	0.14
(1,68)	1:130:A:MET:HE3	1:134:A:PHE:HD2	9	0.14
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	2	0.14
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	2	0.14
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	2	0.14
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	4	0.14
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	4	0.14
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	4	0.14
(2,126)	1:59:A:ILE:H	1:55:A:ALA:O	4	0.13
(2,112)	1:52:A:SER:H	1:48:A:LEU:O	2	0.13
(2,32)	1:89:A:LEU:H	1:188:A:LEU:O	1	0.13
(2,2)	1:18:A:GLU:H	1:172:A:VAL:O	6	0.13
(1,966)	1:154:A:HIS:H	1:183:A:GLY:H	2	0.13
(1,961)	1:160:A:TYR:H	1:152:A:THR:H	6	0.13
(1,939)	1:93:A:ASP:H	1:186:A:VAL:H	6	0.13
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	2	0.13
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	7	0.13
(1,910)	1:58:A:LYS:H	1:96:A:ILE:H	4	0.13
(1,888)	1:154:A:HIS:H	1:157:A:ASP:H	2	0.13
(1,879)	1:85:A:GLN:H	1:88:A:THR:H	4	0.13
(1,831)	1:192:A:GLU:H	1:194:A:GLN:H	5	0.13
(1,763)	1:212:A:GLN:H	1:211:A:SER:H	2	0.13
(1,743)	1:191:A:LYS:H	1:192:A:GLU:H	2	0.13
(1,743)	1:191:A:LYS:H	1:192:A:GLU:H	10	0.13
(1,707)	1:144:A:VAL:H	1:145:A:ALA:H	2	0.13
(1,672)	1:74:A:LYS:H	1:75:A:GLU:H	1	0.13
(1,667)	1:69:A:LYS:H	1:70:A:LEU:H	10	0.13
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD11	6	0.13
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD12	6	0.13
(1,625)	1:214:A:ILE:HD11	1:218:A:ILE:HD13	6	0.13
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD11	6	0.13
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD12	6	0.13
(1,625)	1:214:A:ILE:HD12	1:218:A:ILE:HD13	6	0.13
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD11	6	0.13
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD12	6	0.13
(1,625)	1:214:A:ILE:HD13	1:218:A:ILE:HD13	6	0.13
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG21	3	0.13
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG22	3	0.13
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG23	3	0.13
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG21	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG22	3	0.13
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG23	3	0.13
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG21	3	0.13
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG22	3	0.13
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG23	3	0.13
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG21	2	0.13
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG22	2	0.13
(1,609)	1:150:A:VAL:HG11	1:186:A:VAL:HG23	2	0.13
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG21	2	0.13
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG22	2	0.13
(1,609)	1:150:A:VAL:HG12	1:186:A:VAL:HG23	2	0.13
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG21	2	0.13
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG22	2	0.13
(1,609)	1:150:A:VAL:HG13	1:186:A:VAL:HG23	2	0.13
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB1	6	0.13
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB2	6	0.13
(1,607)	1:149:A:THR:HG21	1:161:A:ALA:HB3	6	0.13
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB1	6	0.13
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB2	6	0.13
(1,607)	1:149:A:THR:HG22	1:161:A:ALA:HB3	6	0.13
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB1	6	0.13
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB2	6	0.13
(1,607)	1:149:A:THR:HG23	1:161:A:ALA:HB3	6	0.13
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	9	0.13
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	9	0.13
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	9	0.13
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	9	0.13
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	9	0.13
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	9	0.13
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	9	0.13
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	9	0.13
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	9	0.13
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	10	0.13
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	10	0.13
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	10	0.13
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	10	0.13
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	10	0.13
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	10	0.13
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	10	0.13
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	10	0.13
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	10	0.13
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD11	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD12	9	0.13
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD13	9	0.13
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD11	9	0.13
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD12	9	0.13
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD13	9	0.13
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD11	9	0.13
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD12	9	0.13
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD13	9	0.13
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD11	10	0.13
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD12	10	0.13
(1,541)	1:207:A:VAL:HG21	1:49:A:ILE:HD13	10	0.13
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD11	10	0.13
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD12	10	0.13
(1,541)	1:207:A:VAL:HG22	1:49:A:ILE:HD13	10	0.13
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD11	10	0.13
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD12	10	0.13
(1,541)	1:207:A:VAL:HG23	1:49:A:ILE:HD13	10	0.13
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	1	0.13
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	1	0.13
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	1	0.13
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	1	0.13
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	1	0.13
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	1	0.13
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	1	0.13
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	1	0.13
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	1	0.13
(1,520)	1:45:A:LEU:HD11	1:49:A:ILE:HD11	8	0.13
(1,520)	1:45:A:LEU:HD11	1:49:A:ILE:HD12	8	0.13
(1,520)	1:45:A:LEU:HD11	1:49:A:ILE:HD13	8	0.13
(1,520)	1:45:A:LEU:HD12	1:49:A:ILE:HD11	8	0.13
(1,520)	1:45:A:LEU:HD12	1:49:A:ILE:HD12	8	0.13
(1,520)	1:45:A:LEU:HD12	1:49:A:ILE:HD13	8	0.13
(1,520)	1:45:A:LEU:HD13	1:49:A:ILE:HD11	8	0.13
(1,520)	1:45:A:LEU:HD13	1:49:A:ILE:HD12	8	0.13
(1,520)	1:45:A:LEU:HD13	1:49:A:ILE:HD13	8	0.13
(1,504)	1:29:A:LEU:HD11	1:131:A:ILE:HD11	8	0.13
(1,504)	1:29:A:LEU:HD11	1:131:A:ILE:HD12	8	0.13
(1,504)	1:29:A:LEU:HD11	1:131:A:ILE:HD13	8	0.13
(1,504)	1:29:A:LEU:HD12	1:131:A:ILE:HD11	8	0.13
(1,504)	1:29:A:LEU:HD12	1:131:A:ILE:HD12	8	0.13
(1,504)	1:29:A:LEU:HD12	1:131:A:ILE:HD13	8	0.13
(1,504)	1:29:A:LEU:HD13	1:131:A:ILE:HD11	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:29:A:LEU:HD13	1:131:A:ILE:HD12	8	0.13
(1,504)	1:29:A:LEU:HD13	1:131:A:ILE:HD13	8	0.13
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD11	8	0.13
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD12	8	0.13
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD13	8	0.13
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD11	9	0.13
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD12	9	0.13
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD13	9	0.13
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG11	7	0.13
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG12	7	0.13
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG13	7	0.13
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG11	1	0.13
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG12	1	0.13
(1,460)	1:208:A:LYS:H	1:207:A:VAL:HG13	1	0.13
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD21	3	0.13
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD22	3	0.13
(1,459)	1:208:A:LYS:H	1:45:A:LEU:HD23	3	0.13
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD11	8	0.13
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD12	8	0.13
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD13	8	0.13
(1,453)	1:199:A:GLU:H	1:198:A:LEU:HD11	5	0.13
(1,453)	1:199:A:GLU:H	1:198:A:LEU:HD12	5	0.13
(1,453)	1:199:A:GLU:H	1:198:A:LEU:HD13	5	0.13
(1,441)	1:191:A:LYS:H	1:144:A:VAL:HG21	7	0.13
(1,441)	1:191:A:LYS:H	1:144:A:VAL:HG22	7	0.13
(1,441)	1:191:A:LYS:H	1:144:A:VAL:HG23	7	0.13
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG21	5	0.13
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG22	5	0.13
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG23	5	0.13
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG21	7	0.13
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG22	7	0.13
(1,417)	1:185:A:LYS:H	1:92:A:VAL:HG23	7	0.13
(1,415)	1:182:A:ARG:H	1:180:A:MET:HE1	10	0.13
(1,415)	1:182:A:ARG:H	1:180:A:MET:HE2	10	0.13
(1,415)	1:182:A:ARG:H	1:180:A:MET:HE3	10	0.13
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG21	1	0.13
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG22	1	0.13
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG23	1	0.13
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG21	7	0.13
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG22	7	0.13
(1,403)	1:163:A:GLU:H	1:171:A:THR:HG23	7	0.13
(1,399)	1:162:A:TRP:H	1:150:A:VAL:HG21	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:162:A:TRP:H	1:150:A:VAL:HG22	9	0.13
(1,399)	1:162:A:TRP:H	1:150:A:VAL:HG23	9	0.13
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG21	1	0.13
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG22	1	0.13
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG23	1	0.13
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG11	7	0.13
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG12	7	0.13
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG13	7	0.13
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	8	0.13
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	8	0.13
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	8	0.13
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG21	10	0.13
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG22	10	0.13
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG23	10	0.13
(1,384)	1:147:A:LYS:H	1:148:A:VAL:HG11	2	0.13
(1,384)	1:147:A:LYS:H	1:148:A:VAL:HG12	2	0.13
(1,384)	1:147:A:LYS:H	1:148:A:VAL:HG13	2	0.13
(1,380)	1:143:A:LEU:H	1:144:A:VAL:HG21	2	0.13
(1,380)	1:143:A:LEU:H	1:144:A:VAL:HG22	2	0.13
(1,380)	1:143:A:LEU:H	1:144:A:VAL:HG23	2	0.13
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB1	9	0.13
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB2	9	0.13
(1,370)	1:123:A:GLN:H	1:121:A:ALA:HB3	9	0.13
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG21	3	0.13
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG22	3	0.13
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG23	3	0.13
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD11	4	0.13
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD12	4	0.13
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD13	4	0.13
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD11	2	0.13
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD12	2	0.13
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD13	2	0.13
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG21	5	0.13
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG22	5	0.13
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG23	5	0.13
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD11	7	0.13
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD12	7	0.13
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD13	7	0.13
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD11	2	0.13
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD12	2	0.13
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD13	2	0.13
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	1	0.13
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	1	0.13
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	9	0.13
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	9	0.13
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	9	0.13
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB1	10	0.13
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB2	10	0.13
(1,306)	1:56:A:LEU:H	1:55:A:ALA:HB3	10	0.13
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	4	0.13
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	4	0.13
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	4	0.13
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	9	0.13
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	9	0.13
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	9	0.13
(1,230)	1:134:A:PHE:HD1	1:131:A:ILE:H	3	0.13
(1,230)	1:134:A:PHE:HD2	1:131:A:ILE:H	3	0.13
(1,229)	1:118:A:PHE:HD1	1:131:A:ILE:H	3	0.13
(1,229)	1:118:A:PHE:HD2	1:131:A:ILE:H	3	0.13
(1,204)	1:22:A:PHE:HD1	1:26:A:ILE:H	9	0.13
(1,204)	1:22:A:PHE:HD2	1:26:A:ILE:H	9	0.13
(1,194)	1:77:A:HIS:HE1	1:76:A:LEU:H	10	0.13
(1,191)	1:216:A:TYR:HE1	1:54:A:ASP:H	2	0.13
(1,191)	1:216:A:TYR:HE2	1:54:A:ASP:H	2	0.13
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD11	4	0.13
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD12	4	0.13
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD13	4	0.13
(1,181)	1:53:A:SER:H	1:214:A:ILE:HD11	5	0.13
(1,181)	1:53:A:SER:H	1:214:A:ILE:HD12	5	0.13
(1,181)	1:53:A:SER:H	1:214:A:ILE:HD13	5	0.13
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB1	9	0.13
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB2	9	0.13
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB3	9	0.13
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB1	5	0.13
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB2	5	0.13
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB3	5	0.13
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB1	7	0.13
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB2	7	0.13
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB3	7	0.13
(1,141)	1:162:A:TRP:H	1:103:A:LEU:HD11	4	0.13
(1,141)	1:162:A:TRP:H	1:103:A:LEU:HD12	4	0.13
(1,141)	1:162:A:TRP:H	1:103:A:LEU:HD13	4	0.13
(1,139)	1:93:A:ASP:H	1:94:A:THR:HG21	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:93:A:ASP:H	1:94:A:THR:HG22	6	0.13
(1,139)	1:93:A:ASP:H	1:94:A:THR:HG23	6	0.13
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD11	4	0.13
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD12	4	0.13
(1,120)	1:46:A:ARG:H	1:45:A:LEU:HD13	4	0.13
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD11	3	0.13
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD12	3	0.13
(1,118)	1:35:A:ASN:H	1:32:A:LEU:HD13	3	0.13
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	7	0.13
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	7	0.13
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	7	0.13
(1,110)	1:219:A:THR:HG21	1:221:A:PHE:HE1	2	0.13
(1,110)	1:219:A:THR:HG22	1:221:A:PHE:HE1	2	0.13
(1,110)	1:219:A:THR:HG23	1:221:A:PHE:HE1	2	0.13
(1,104)	1:188:A:LEU:HD21	1:44:A:PHE:HE2	1	0.13
(1,104)	1:188:A:LEU:HD22	1:44:A:PHE:HE2	1	0.13
(1,104)	1:188:A:LEU:HD23	1:44:A:PHE:HE2	1	0.13
(1,98)	1:172:A:VAL:HG21	1:170:A:PHE:HE1	2	0.13
(1,98)	1:172:A:VAL:HG22	1:170:A:PHE:HE1	2	0.13
(1,98)	1:172:A:VAL:HG23	1:170:A:PHE:HE1	2	0.13
(1,97)	1:172:A:VAL:HG21	1:160:A:TYR:HE1	4	0.13
(1,97)	1:172:A:VAL:HG22	1:160:A:TYR:HE1	4	0.13
(1,97)	1:172:A:VAL:HG23	1:160:A:TYR:HE1	4	0.13
(1,77)	1:144:A:VAL:HG11	1:197:A:TYR:HD2	4	0.13
(1,77)	1:144:A:VAL:HG12	1:197:A:TYR:HD2	4	0.13
(1,77)	1:144:A:VAL:HG13	1:197:A:TYR:HD2	4	0.13
(1,74)	1:143:A:LEU:HD21	1:38:A:TYR:HE2	4	0.13
(1,74)	1:143:A:LEU:HD22	1:38:A:TYR:HE2	4	0.13
(1,74)	1:143:A:LEU:HD23	1:38:A:TYR:HE2	4	0.13
(1,45)	1:104:A:ILE:HD11	1:20:A:PHE:HE1	10	0.13
(1,45)	1:104:A:ILE:HD11	1:20:A:PHE:HE2	10	0.13
(1,45)	1:104:A:ILE:HD12	1:20:A:PHE:HE1	10	0.13
(1,45)	1:104:A:ILE:HD12	1:20:A:PHE:HE2	10	0.13
(1,45)	1:104:A:ILE:HD13	1:20:A:PHE:HE1	10	0.13
(1,45)	1:104:A:ILE:HD13	1:20:A:PHE:HE2	10	0.13
(1,43)	1:103:A:LEU:HD21	1:160:A:TYR:HE1	6	0.13
(1,43)	1:103:A:LEU:HD21	1:160:A:TYR:HE2	6	0.13
(1,43)	1:103:A:LEU:HD22	1:160:A:TYR:HE1	6	0.13
(1,43)	1:103:A:LEU:HD22	1:160:A:TYR:HE2	6	0.13
(1,43)	1:103:A:LEU:HD23	1:160:A:TYR:HE1	6	0.13
(1,43)	1:103:A:LEU:HD23	1:160:A:TYR:HE2	6	0.13
(1,13)	1:32:A:LEU:HD21	1:118:A:PHE:HD2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:32:A:LEU:HD22	1:118:A:PHE:HD2	7	0.13
(1,13)	1:32:A:LEU:HD23	1:118:A:PHE:HD2	7	0.13
(1,7)	1:29:A:LEU:HD11	1:139:A:TYR:HD2	6	0.13
(1,7)	1:29:A:LEU:HD12	1:139:A:TYR:HD2	6	0.13
(1,7)	1:29:A:LEU:HD13	1:139:A:TYR:HD2	6	0.13
(2,138)	1:205:A:GLU:H	1:201:A:ARG:O	10	0.12
(2,126)	1:59:A:ILE:H	1:55:A:ALA:O	2	0.12
(2,125)	1:59:A:ILE:N	1:55:A:ALA:O	5	0.12
(2,79)	1:190:A:LEU:N	1:87:A:ARG:O	8	0.12
(1,967)	1:159:A:GLN:H	1:175:A:ASP:H	6	0.12
(1,966)	1:154:A:HIS:H	1:183:A:GLY:H	8	0.12
(1,952)	1:148:A:VAL:H	1:166:A:ALA:H	1	0.12
(1,942)	1:97:A:GLY:H	1:183:A:GLY:H	3	0.12
(1,939)	1:93:A:ASP:H	1:186:A:VAL:H	4	0.12
(1,909)	1:55:A:ALA:H	1:96:A:ILE:H	9	0.12
(1,875)	1:68:A:SER:H	1:71:A:ASP:H	6	0.12
(1,875)	1:68:A:SER:H	1:71:A:ASP:H	8	0.12
(1,873)	1:66:A:ASP:H	1:63:A:SER:H	7	0.12
(1,827)	1:164:A:SER:H	1:166:A:ALA:H	9	0.12
(1,820)	1:124:A:ALA:H	1:126:A:ALA:H	10	0.12
(1,773)	1:224:A:LYS:H	1:223:A:GLU:H	3	0.12
(1,745)	1:193:A:ASP:H	1:194:A:GLN:H	10	0.12
(1,721)	1:168:A:GLY:H	1:169:A:SER:H	9	0.12
(1,672)	1:74:A:LYS:H	1:75:A:GLU:H	9	0.12
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG21	6	0.12
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG22	6	0.12
(1,619)	1:198:A:LEU:HD21	1:195:A:THR:HG23	6	0.12
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG21	6	0.12
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG22	6	0.12
(1,619)	1:198:A:LEU:HD22	1:195:A:THR:HG23	6	0.12
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG21	6	0.12
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG22	6	0.12
(1,619)	1:198:A:LEU:HD23	1:195:A:THR:HG23	6	0.12
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD21	3	0.12
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD22	3	0.12
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD23	3	0.12
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD21	3	0.12
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD22	3	0.12
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD23	3	0.12
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD21	3	0.12
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD22	3	0.12
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD23	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG11	2	0.12
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG12	2	0.12
(1,614)	1:188:A:LEU:HD11	1:186:A:VAL:HG13	2	0.12
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG11	2	0.12
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG12	2	0.12
(1,614)	1:188:A:LEU:HD12	1:186:A:VAL:HG13	2	0.12
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG11	2	0.12
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG12	2	0.12
(1,614)	1:188:A:LEU:HD13	1:186:A:VAL:HG13	2	0.12
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD21	10	0.12
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD22	10	0.12
(1,605)	1:148:A:VAL:HG21	1:188:A:LEU:HD23	10	0.12
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD21	10	0.12
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD22	10	0.12
(1,605)	1:148:A:VAL:HG22	1:188:A:LEU:HD23	10	0.12
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD21	10	0.12
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD22	10	0.12
(1,605)	1:148:A:VAL:HG23	1:188:A:LEU:HD23	10	0.12
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG11	1	0.12
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG12	1	0.12
(1,585)	1:103:A:LEU:HD11	1:172:A:VAL:HG13	1	0.12
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG11	1	0.12
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG12	1	0.12
(1,585)	1:103:A:LEU:HD12	1:172:A:VAL:HG13	1	0.12
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG11	1	0.12
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG12	1	0.12
(1,585)	1:103:A:LEU:HD13	1:172:A:VAL:HG13	1	0.12
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	5	0.12
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	5	0.12
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	5	0.12
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	5	0.12
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	5	0.12
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	5	0.12
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	5	0.12
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	5	0.12
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	5	0.12
(1,579)	1:150:A:VAL:HG11	1:98:A:MET:HE1	1	0.12
(1,579)	1:150:A:VAL:HG11	1:98:A:MET:HE2	1	0.12
(1,579)	1:150:A:VAL:HG11	1:98:A:MET:HE3	1	0.12
(1,579)	1:150:A:VAL:HG12	1:98:A:MET:HE1	1	0.12
(1,579)	1:150:A:VAL:HG12	1:98:A:MET:HE2	1	0.12
(1,579)	1:150:A:VAL:HG12	1:98:A:MET:HE3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:150:A:VAL:HG13	1:98:A:MET:HE1	1	0.12
(1,579)	1:150:A:VAL:HG13	1:98:A:MET:HE2	1	0.12
(1,579)	1:150:A:VAL:HG13	1:98:A:MET:HE3	1	0.12
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE1	3	0.12
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE2	3	0.12
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE3	3	0.12
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE1	3	0.12
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE2	3	0.12
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE3	3	0.12
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE1	3	0.12
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE2	3	0.12
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE3	3	0.12
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG21	1	0.12
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG22	1	0.12
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG23	1	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG21	1	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG22	1	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG23	1	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG21	1	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG22	1	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG23	1	0.12
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG21	10	0.12
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG22	10	0.12
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG23	10	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG21	10	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG22	10	0.12
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG23	10	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG21	10	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG22	10	0.12
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG23	10	0.12
(1,560)	1:80:A:LEU:HD21	1:218:A:ILE:HD11	2	0.12
(1,560)	1:80:A:LEU:HD21	1:218:A:ILE:HD12	2	0.12
(1,560)	1:80:A:LEU:HD21	1:218:A:ILE:HD13	2	0.12
(1,560)	1:80:A:LEU:HD22	1:218:A:ILE:HD11	2	0.12
(1,560)	1:80:A:LEU:HD22	1:218:A:ILE:HD12	2	0.12
(1,560)	1:80:A:LEU:HD22	1:218:A:ILE:HD13	2	0.12
(1,560)	1:80:A:LEU:HD23	1:218:A:ILE:HD11	2	0.12
(1,560)	1:80:A:LEU:HD23	1:218:A:ILE:HD12	2	0.12
(1,560)	1:80:A:LEU:HD23	1:218:A:ILE:HD13	2	0.12
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD11	5	0.12
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD12	5	0.12
(1,551)	1:70:A:LEU:HD11	1:59:A:ILE:HD13	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD11	5	0.12
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD12	5	0.12
(1,551)	1:70:A:LEU:HD12	1:59:A:ILE:HD13	5	0.12
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD11	5	0.12
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD12	5	0.12
(1,551)	1:70:A:LEU:HD13	1:59:A:ILE:HD13	5	0.12
(1,540)	1:207:A:VAL:HG11	1:49:A:ILE:HD11	5	0.12
(1,540)	1:207:A:VAL:HG11	1:49:A:ILE:HD12	5	0.12
(1,540)	1:207:A:VAL:HG11	1:49:A:ILE:HD13	5	0.12
(1,540)	1:207:A:VAL:HG12	1:49:A:ILE:HD11	5	0.12
(1,540)	1:207:A:VAL:HG12	1:49:A:ILE:HD12	5	0.12
(1,540)	1:207:A:VAL:HG12	1:49:A:ILE:HD13	5	0.12
(1,540)	1:207:A:VAL:HG13	1:49:A:ILE:HD11	5	0.12
(1,540)	1:207:A:VAL:HG13	1:49:A:ILE:HD12	5	0.12
(1,540)	1:207:A:VAL:HG13	1:49:A:ILE:HD13	5	0.12
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	8	0.12
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	8	0.12
(1,536)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	8	0.12
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	8	0.12
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	8	0.12
(1,536)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	8	0.12
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	8	0.12
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	8	0.12
(1,536)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	8	0.12
(1,517)	1:33:A:ILE:HD11	1:131:A:ILE:HD11	4	0.12
(1,517)	1:33:A:ILE:HD11	1:131:A:ILE:HD12	4	0.12
(1,517)	1:33:A:ILE:HD11	1:131:A:ILE:HD13	4	0.12
(1,517)	1:33:A:ILE:HD12	1:131:A:ILE:HD11	4	0.12
(1,517)	1:33:A:ILE:HD12	1:131:A:ILE:HD12	4	0.12
(1,517)	1:33:A:ILE:HD12	1:131:A:ILE:HD13	4	0.12
(1,517)	1:33:A:ILE:HD13	1:131:A:ILE:HD11	4	0.12
(1,517)	1:33:A:ILE:HD13	1:131:A:ILE:HD12	4	0.12
(1,517)	1:33:A:ILE:HD13	1:131:A:ILE:HD13	4	0.12
(1,509)	1:34:A:ILE:HD11	1:30:A:MET:HE1	7	0.12
(1,509)	1:34:A:ILE:HD11	1:30:A:MET:HE2	7	0.12
(1,509)	1:34:A:ILE:HD11	1:30:A:MET:HE3	7	0.12
(1,509)	1:34:A:ILE:HD12	1:30:A:MET:HE1	7	0.12
(1,509)	1:34:A:ILE:HD12	1:30:A:MET:HE2	7	0.12
(1,509)	1:34:A:ILE:HD12	1:30:A:MET:HE3	7	0.12
(1,509)	1:34:A:ILE:HD13	1:30:A:MET:HE1	7	0.12
(1,509)	1:34:A:ILE:HD13	1:30:A:MET:HE2	7	0.12
(1,509)	1:34:A:ILE:HD13	1:30:A:MET:HE3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:214:A:ILE:H	1:218:A:ILE:HD11	2	0.12
(1,466)	1:214:A:ILE:H	1:218:A:ILE:HD12	2	0.12
(1,466)	1:214:A:ILE:H	1:218:A:ILE:HD13	2	0.12
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD11	2	0.12
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD12	2	0.12
(1,465)	1:213:A:PHE:H	1:218:A:ILE:HD13	2	0.12
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD11	9	0.12
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD12	9	0.12
(1,458)	1:207:A:VAL:H	1:45:A:LEU:HD13	9	0.12
(1,451)	1:197:A:TYR:H	1:195:A:THR:HG21	6	0.12
(1,451)	1:197:A:TYR:H	1:195:A:THR:HG22	6	0.12
(1,451)	1:197:A:TYR:H	1:195:A:THR:HG23	6	0.12
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD11	4	0.12
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD12	4	0.12
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD13	4	0.12
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD11	6	0.12
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD12	6	0.12
(1,449)	1:196:A:GLU:H	1:198:A:LEU:HD13	6	0.12
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD21	6	0.12
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD22	6	0.12
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD23	6	0.12
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD11	1	0.12
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD12	1	0.12
(1,408)	1:172:A:VAL:H	1:104:A:ILE:HD13	1	0.12
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG21	6	0.12
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG22	6	0.12
(1,392)	1:151:A:ILE:H	1:186:A:VAL:HG23	6	0.12
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG21	9	0.12
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG22	9	0.12
(1,391)	1:151:A:ILE:H	1:184:A:THR:HG23	9	0.12
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG21	6	0.12
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG22	6	0.12
(1,387)	1:151:A:ILE:H	1:149:A:THR:HG23	6	0.12
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB1	5	0.12
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB2	5	0.12
(1,377)	1:127:A:ASP:H	1:126:A:ALA:HB3	5	0.12
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE1	7	0.12
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE2	7	0.12
(1,369)	1:120:A:GLU:H	1:119:A:MET:HE3	7	0.12
(1,366)	1:101:A:ALA:H	1:99:A:THR:HG21	9	0.12
(1,366)	1:101:A:ALA:H	1:99:A:THR:HG22	9	0.12
(1,366)	1:101:A:ALA:H	1:99:A:THR:HG23	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG21	6	0.12
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG22	6	0.12
(1,357)	1:91:A:ILE:H	1:90:A:THR:HG23	6	0.12
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD21	1	0.12
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD22	1	0.12
(1,352)	1:87:A:ARG:H	1:198:A:LEU:HD23	1	0.12
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD11	3	0.12
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD12	3	0.12
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD13	3	0.12
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD11	10	0.12
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD12	10	0.12
(1,350)	1:85:A:GLN:H	1:198:A:LEU:HD13	10	0.12
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD11	9	0.12
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD12	9	0.12
(1,344)	1:81:A:ILE:H	1:220:A:LEU:HD13	9	0.12
(1,340)	1:81:A:ILE:H	1:80:A:LEU:HD21	4	0.12
(1,340)	1:81:A:ILE:H	1:80:A:LEU:HD22	4	0.12
(1,340)	1:81:A:ILE:H	1:80:A:LEU:HD23	4	0.12
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD11	6	0.12
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD12	6	0.12
(1,315)	1:61:A:TYR:H	1:64:A:LEU:HD13	6	0.12
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD11	5	0.12
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD12	5	0.12
(1,308)	1:58:A:LYS:H	1:96:A:ILE:HD13	5	0.12
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD21	5	0.12
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD22	5	0.12
(1,301)	1:44:A:PHE:H	1:143:A:LEU:HD23	5	0.12
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD11	5	0.12
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD12	5	0.12
(1,300)	1:43:A:ILE:H	1:143:A:LEU:HD13	5	0.12
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	3	0.12
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	3	0.12
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	3	0.12
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB1	6	0.12
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB2	6	0.12
(1,299)	1:28:A:GLN:H	1:27:A:ALA:HB3	6	0.12
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB1	10	0.12
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB2	10	0.12
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB3	10	0.12
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	3	0.12
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	3	0.12
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:143:A:LEU:H	1:143:A:LEU:HD21	3	0.12
(1,260)	1:143:A:LEU:H	1:143:A:LEU:HD22	3	0.12
(1,260)	1:143:A:LEU:H	1:143:A:LEU:HD23	3	0.12
(1,243)	1:59:A:ILE:H	1:59:A:ILE:HD11	6	0.12
(1,243)	1:59:A:ILE:H	1:59:A:ILE:HD12	6	0.12
(1,243)	1:59:A:ILE:H	1:59:A:ILE:HD13	6	0.12
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG11	6	0.12
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG12	6	0.12
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG13	6	0.12
(1,232)	1:134:A:PHE:HE1	1:131:A:ILE:H	3	0.12
(1,232)	1:134:A:PHE:HE2	1:131:A:ILE:H	3	0.12
(1,230)	1:134:A:PHE:HD1	1:131:A:ILE:H	5	0.12
(1,230)	1:134:A:PHE:HD2	1:131:A:ILE:H	5	0.12
(1,229)	1:118:A:PHE:HD1	1:131:A:ILE:H	5	0.12
(1,229)	1:118:A:PHE:HD2	1:131:A:ILE:H	5	0.12
(1,227)	1:118:A:PHE:HE1	1:130:A:MET:H	6	0.12
(1,227)	1:118:A:PHE:HE2	1:130:A:MET:H	6	0.12
(1,212)	1:170:A:PHE:HE1	1:22:A:PHE:H	6	0.12
(1,212)	1:170:A:PHE:HE2	1:22:A:PHE:H	6	0.12
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD11	10	0.12
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD12	10	0.12
(1,177)	1:202:A:ARG:H	1:203:A:ILE:HD13	10	0.12
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB1	7	0.12
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB2	7	0.12
(1,160)	1:168:A:GLY:H	1:166:A:ALA:HB3	7	0.12
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB1	2	0.12
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB2	2	0.12
(1,159)	1:175:A:ASP:H	1:161:A:ALA:HB3	2	0.12
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB1	9	0.12
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB2	9	0.12
(1,151)	1:143:A:LEU:H	1:141:A:ALA:HB3	9	0.12
(1,142)	1:104:A:ILE:H	1:103:A:LEU:HD21	1	0.12
(1,142)	1:104:A:ILE:H	1:103:A:LEU:HD22	1	0.12
(1,142)	1:104:A:ILE:H	1:103:A:LEU:HD23	1	0.12
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG21	4	0.12
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG22	4	0.12
(1,136)	1:89:A:LEU:H	1:88:A:THR:HG23	4	0.12
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD21	6	0.12
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD22	6	0.12
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD23	6	0.12
(1,123)	1:49:A:ILE:H	1:48:A:LEU:HD21	8	0.12
(1,123)	1:49:A:ILE:H	1:48:A:LEU:HD22	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:49:A:ILE:H	1:48:A:LEU:HD23	8	0.12
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE1	10	0.12
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE2	10	0.12
(1,114)	1:166:A:ALA:H	1:30:A:MET:HE3	10	0.12
(1,104)	1:188:A:LEU:HD21	1:44:A:PHE:HE2	5	0.12
(1,104)	1:188:A:LEU:HD22	1:44:A:PHE:HE2	5	0.12
(1,104)	1:188:A:LEU:HD23	1:44:A:PHE:HE2	5	0.12
(1,99)	1:174:A:THR:HG21	1:160:A:TYR:HE1	6	0.12
(1,99)	1:174:A:THR:HG22	1:160:A:TYR:HE1	6	0.12
(1,99)	1:174:A:THR:HG23	1:160:A:TYR:HE1	6	0.12
(1,98)	1:172:A:VAL:HG21	1:170:A:PHE:HE1	5	0.12
(1,98)	1:172:A:VAL:HG22	1:170:A:PHE:HE1	5	0.12
(1,98)	1:172:A:VAL:HG23	1:170:A:PHE:HE1	5	0.12
(1,96)	1:172:A:VAL:HG21	1:20:A:PHE:HE1	3	0.12
(1,96)	1:172:A:VAL:HG22	1:20:A:PHE:HE1	3	0.12
(1,96)	1:172:A:VAL:HG23	1:20:A:PHE:HE1	3	0.12
(1,89)	1:171:A:THR:HG21	1:20:A:PHE:HD1	2	0.12
(1,89)	1:171:A:THR:HG22	1:20:A:PHE:HD1	2	0.12
(1,89)	1:171:A:THR:HG23	1:20:A:PHE:HD1	2	0.12
(1,86)	1:166:A:ALA:HB1	1:22:A:PHE:HE2	7	0.12
(1,86)	1:166:A:ALA:HB2	1:22:A:PHE:HE2	7	0.12
(1,86)	1:166:A:ALA:HB3	1:22:A:PHE:HE2	7	0.12
(1,86)	1:166:A:ALA:HB1	1:22:A:PHE:HE2	10	0.12
(1,86)	1:166:A:ALA:HB2	1:22:A:PHE:HE2	10	0.12
(1,86)	1:166:A:ALA:HB3	1:22:A:PHE:HE2	10	0.12
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE1	2	0.12
(1,84)	1:148:A:VAL:HG21	1:142:A:TYR:HE2	2	0.12
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE1	2	0.12
(1,84)	1:148:A:VAL:HG22	1:142:A:TYR:HE2	2	0.12
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE1	2	0.12
(1,84)	1:148:A:VAL:HG23	1:142:A:TYR:HE2	2	0.12
(1,81)	1:148:A:VAL:HG11	1:142:A:TYR:HE2	4	0.12
(1,81)	1:148:A:VAL:HG12	1:142:A:TYR:HE2	4	0.12
(1,81)	1:148:A:VAL:HG13	1:142:A:TYR:HE2	4	0.12
(1,77)	1:144:A:VAL:HG11	1:197:A:TYR:HD2	2	0.12
(1,77)	1:144:A:VAL:HG12	1:197:A:TYR:HD2	2	0.12
(1,77)	1:144:A:VAL:HG13	1:197:A:TYR:HD2	2	0.12
(1,65)	1:126:A:ALA:HB1	1:134:A:PHE:HE1	9	0.12
(1,65)	1:126:A:ALA:HB1	1:134:A:PHE:HE2	9	0.12
(1,65)	1:126:A:ALA:HB2	1:134:A:PHE:HE1	9	0.12
(1,65)	1:126:A:ALA:HB2	1:134:A:PHE:HE2	9	0.12
(1,65)	1:126:A:ALA:HB3	1:134:A:PHE:HE1	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:126:A:ALA:HB3	1:134:A:PHE:HE2	9	0.12
(1,36)	1:89:A:LEU:HD21	1:44:A:PHE:HD1	7	0.12
(1,36)	1:89:A:LEU:HD21	1:44:A:PHE:HD2	7	0.12
(1,36)	1:89:A:LEU:HD22	1:44:A:PHE:HD1	7	0.12
(1,36)	1:89:A:LEU:HD22	1:44:A:PHE:HD2	7	0.12
(1,36)	1:89:A:LEU:HD23	1:44:A:PHE:HD1	7	0.12
(1,36)	1:89:A:LEU:HD23	1:44:A:PHE:HD2	7	0.12
(1,33)	1:81:A:ILE:HD11	1:221:A:PHE:HE1	2	0.12
(1,33)	1:81:A:ILE:HD11	1:221:A:PHE:HE2	2	0.12
(1,33)	1:81:A:ILE:HD12	1:221:A:PHE:HE1	2	0.12
(1,33)	1:81:A:ILE:HD12	1:221:A:PHE:HE2	2	0.12
(1,33)	1:81:A:ILE:HD13	1:221:A:PHE:HE1	2	0.12
(1,33)	1:81:A:ILE:HD13	1:221:A:PHE:HE2	2	0.12
(1,30)	1:76:A:LEU:HD11	1:216:A:TYR:HD1	5	0.12
(1,30)	1:76:A:LEU:HD12	1:216:A:TYR:HD1	5	0.12
(1,30)	1:76:A:LEU:HD13	1:216:A:TYR:HD1	5	0.12
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE1	3	0.12
(1,26)	1:56:A:LEU:HD21	1:216:A:TYR:HE2	3	0.12
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE1	3	0.12
(1,26)	1:56:A:LEU:HD22	1:216:A:TYR:HE2	3	0.12
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE1	3	0.12
(1,26)	1:56:A:LEU:HD23	1:216:A:TYR:HE2	3	0.12
(1,15)	1:30:A:MET:HE1	1:22:A:PHE:HE1	6	0.12
(1,15)	1:30:A:MET:HE1	1:22:A:PHE:HE2	6	0.12
(1,15)	1:30:A:MET:HE2	1:22:A:PHE:HE1	6	0.12
(1,15)	1:30:A:MET:HE2	1:22:A:PHE:HE2	6	0.12
(1,15)	1:30:A:MET:HE3	1:22:A:PHE:HE1	6	0.12
(1,15)	1:30:A:MET:HE3	1:22:A:PHE:HE2	6	0.12
(1,11)	1:32:A:LEU:HD11	1:118:A:PHE:HD2	7	0.12
(1,11)	1:32:A:LEU:HD12	1:118:A:PHE:HD2	7	0.12
(1,11)	1:32:A:LEU:HD13	1:118:A:PHE:HD2	7	0.12
(2,148)	1:210:A:HIS:H	1:206:A:ILE:O	1	0.11
(2,144)	1:208:A:LYS:H	1:204:A:LYS:O	5	0.11
(2,126)	1:59:A:ILE:H	1:55:A:ALA:O	7	0.11
(2,125)	1:59:A:ILE:N	1:55:A:ALA:O	8	0.11
(2,110)	1:51:A:ASN:H	1:47:A:GLU:O	10	0.11
(2,108)	1:50:A:SER:H	1:46:A:ARG:O	9	0.11
(2,66)	1:160:A:TYR:H	1:152:A:THR:O	6	0.11
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	2	0.11
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	10	0.11
(2,22)	1:221:A:PHE:H	1:80:A:LEU:O	9	0.11
(1,973)	1:163:A:GLU:H	1:171:A:THR:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:183:A:GLY:H	1:153:A:LYS:H	8	0.11
(1,950)	1:147:A:LYS:H	1:191:A:LYS:H	2	0.11
(1,913)	1:94:A:THR:H	1:77:A:HIS:H	3	0.11
(1,889)	1:191:A:LYS:H	1:194:A:GLN:H	9	0.11
(1,883)	1:117:A:ALA:H	1:120:A:GLU:H	3	0.11
(1,846)	1:210:A:HIS:H	1:208:A:LYS:H	7	0.11
(1,834)	1:196:A:GLU:H	1:194:A:GLN:H	3	0.11
(1,829)	1:180:A:MET:H	1:182:A:ARG:H	1	0.11
(1,829)	1:180:A:MET:H	1:182:A:ARG:H	9	0.11
(1,828)	1:167:A:GLY:H	1:169:A:SER:H	7	0.11
(1,828)	1:167:A:GLY:H	1:169:A:SER:H	10	0.11
(1,783)	1:44:A:PHE:H	1:46:A:ARG:H	4	0.11
(1,783)	1:44:A:PHE:H	1:46:A:ARG:H	5	0.11
(1,762)	1:211:A:SER:H	1:210:A:HIS:H	4	0.11
(1,722)	1:167:A:GLY:H	1:168:A:GLY:H	9	0.11
(1,705)	1:143:A:LEU:H	1:142:A:TYR:H	1	0.11
(1,695)	1:119:A:MET:H	1:120:A:GLU:H	5	0.11
(1,676)	1:83:A:ASN:H	1:84:A:LYS:H	9	0.11
(1,671)	1:73:A:GLY:H	1:74:A:LYS:H	3	0.11
(1,667)	1:69:A:LYS:H	1:70:A:LEU:H	2	0.11
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	2	0.11
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	2	0.11
(1,626)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	2	0.11
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	2	0.11
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	2	0.11
(1,626)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	2	0.11
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	2	0.11
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	2	0.11
(1,626)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	2	0.11
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG11	2	0.11
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG12	2	0.11
(1,615)	1:188:A:LEU:HD21	1:186:A:VAL:HG13	2	0.11
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG11	2	0.11
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG12	2	0.11
(1,615)	1:188:A:LEU:HD22	1:186:A:VAL:HG13	2	0.11
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG11	2	0.11
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG12	2	0.11
(1,615)	1:188:A:LEU:HD23	1:186:A:VAL:HG13	2	0.11
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	1	0.11
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	1	0.11
(1,612)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	1	0.11
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	1	0.11
(1,612)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	1	0.11
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	1	0.11
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	1	0.11
(1,612)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	1	0.11
(1,595)	1:128:A:ILE:HD11	1:143:A:LEU:HD11	10	0.11
(1,595)	1:128:A:ILE:HD11	1:143:A:LEU:HD12	10	0.11
(1,595)	1:128:A:ILE:HD11	1:143:A:LEU:HD13	10	0.11
(1,595)	1:128:A:ILE:HD12	1:143:A:LEU:HD11	10	0.11
(1,595)	1:128:A:ILE:HD12	1:143:A:LEU:HD12	10	0.11
(1,595)	1:128:A:ILE:HD12	1:143:A:LEU:HD13	10	0.11
(1,595)	1:128:A:ILE:HD13	1:143:A:LEU:HD11	10	0.11
(1,595)	1:128:A:ILE:HD13	1:143:A:LEU:HD12	10	0.11
(1,595)	1:128:A:ILE:HD13	1:143:A:LEU:HD13	10	0.11
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE1	5	0.11
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE2	5	0.11
(1,574)	1:92:A:VAL:HG21	1:180:A:MET:HE3	5	0.11
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE1	5	0.11
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE2	5	0.11
(1,574)	1:92:A:VAL:HG22	1:180:A:MET:HE3	5	0.11
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE1	5	0.11
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE2	5	0.11
(1,574)	1:92:A:VAL:HG23	1:180:A:MET:HE3	5	0.11
(1,571)	1:91:A:ILE:HD11	1:188:A:LEU:HD21	8	0.11
(1,571)	1:91:A:ILE:HD11	1:188:A:LEU:HD22	8	0.11
(1,571)	1:91:A:ILE:HD11	1:188:A:LEU:HD23	8	0.11
(1,571)	1:91:A:ILE:HD12	1:188:A:LEU:HD21	8	0.11
(1,571)	1:91:A:ILE:HD12	1:188:A:LEU:HD22	8	0.11
(1,571)	1:91:A:ILE:HD12	1:188:A:LEU:HD23	8	0.11
(1,571)	1:91:A:ILE:HD13	1:188:A:LEU:HD21	8	0.11
(1,571)	1:91:A:ILE:HD13	1:188:A:LEU:HD22	8	0.11
(1,571)	1:91:A:ILE:HD13	1:188:A:LEU:HD23	8	0.11
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	7	0.11
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	7	0.11
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	7	0.11
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	7	0.11
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	7	0.11
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	7	0.11
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	7	0.11
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	7	0.11
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	7	0.11
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	9	0.11
(1,568)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	9	0.11
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	9	0.11
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	9	0.11
(1,568)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	9	0.11
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	9	0.11
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	9	0.11
(1,568)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	9	0.11
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD11	7	0.11
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD12	7	0.11
(1,564)	1:89:A:LEU:HD11	1:190:A:LEU:HD13	7	0.11
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD11	7	0.11
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD12	7	0.11
(1,564)	1:89:A:LEU:HD12	1:190:A:LEU:HD13	7	0.11
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD11	7	0.11
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD12	7	0.11
(1,564)	1:89:A:LEU:HD13	1:190:A:LEU:HD13	7	0.11
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG21	5	0.11
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG22	5	0.11
(1,561)	1:81:A:ILE:HD11	1:90:A:THR:HG23	5	0.11
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG21	5	0.11
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG22	5	0.11
(1,561)	1:81:A:ILE:HD12	1:90:A:THR:HG23	5	0.11
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG21	5	0.11
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG22	5	0.11
(1,561)	1:81:A:ILE:HD13	1:90:A:THR:HG23	5	0.11
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	4	0.11
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	4	0.11
(1,557)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	4	0.11
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	4	0.11
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	4	0.11
(1,557)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	4	0.11
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	4	0.11
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	4	0.11
(1,557)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	4	0.11
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	8	0.11
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	8	0.11
(1,556)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	8	0.11
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	8	0.11
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	8	0.11
(1,556)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	8	0.11
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	8	0.11
(1,556)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	8	0.11
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	9	0.11
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	9	0.11
(1,553)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	9	0.11
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	9	0.11
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	9	0.11
(1,553)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	9	0.11
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	9	0.11
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	9	0.11
(1,553)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	9	0.11
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	2	0.11
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	2	0.11
(1,547)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	2	0.11
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	2	0.11
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	2	0.11
(1,547)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	2	0.11
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	2	0.11
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	2	0.11
(1,547)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	2	0.11
(1,535)	1:48:A:LEU:HD11	1:188:A:LEU:HD11	6	0.11
(1,535)	1:48:A:LEU:HD11	1:188:A:LEU:HD12	6	0.11
(1,535)	1:48:A:LEU:HD11	1:188:A:LEU:HD13	6	0.11
(1,535)	1:48:A:LEU:HD12	1:188:A:LEU:HD11	6	0.11
(1,535)	1:48:A:LEU:HD12	1:188:A:LEU:HD12	6	0.11
(1,535)	1:48:A:LEU:HD12	1:188:A:LEU:HD13	6	0.11
(1,535)	1:48:A:LEU:HD13	1:188:A:LEU:HD11	6	0.11
(1,535)	1:48:A:LEU:HD13	1:188:A:LEU:HD12	6	0.11
(1,535)	1:48:A:LEU:HD13	1:188:A:LEU:HD13	6	0.11
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD11	5	0.11
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD12	5	0.11
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD13	5	0.11
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD11	5	0.11
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD12	5	0.11
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD13	5	0.11
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD11	5	0.11
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD12	5	0.11
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD13	5	0.11
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE1	7	0.11
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE2	7	0.11
(1,511)	1:32:A:LEU:HD11	1:119:A:MET:HE3	7	0.11
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE1	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE2	7	0.11
(1,511)	1:32:A:LEU:HD12	1:119:A:MET:HE3	7	0.11
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE1	7	0.11
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE2	7	0.11
(1,511)	1:32:A:LEU:HD13	1:119:A:MET:HE3	7	0.11
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE1	5	0.11
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE2	5	0.11
(1,506)	1:29:A:LEU:HD21	1:119:A:MET:HE3	5	0.11
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE1	5	0.11
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE2	5	0.11
(1,506)	1:29:A:LEU:HD22	1:119:A:MET:HE3	5	0.11
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE1	5	0.11
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE2	5	0.11
(1,506)	1:29:A:LEU:HD23	1:119:A:MET:HE3	5	0.11
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG21	10	0.11
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG22	10	0.11
(1,502)	1:171:A:THR:HG21	1:19:A:THR:HG23	10	0.11
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG21	10	0.11
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG22	10	0.11
(1,502)	1:171:A:THR:HG22	1:19:A:THR:HG23	10	0.11
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG21	10	0.11
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG22	10	0.11
(1,502)	1:171:A:THR:HG23	1:19:A:THR:HG23	10	0.11
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD11	10	0.11
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD12	10	0.11
(1,474)	1:222:A:VAL:H	1:220:A:LEU:HD13	10	0.11
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG21	7	0.11
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG22	7	0.11
(1,470)	1:221:A:PHE:H	1:219:A:THR:HG23	7	0.11
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD11	7	0.11
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD12	7	0.11
(1,468)	1:216:A:TYR:H	1:218:A:ILE:HD13	7	0.11
(1,450)	1:197:A:TYR:H	1:190:A:LEU:HD21	7	0.11
(1,450)	1:197:A:TYR:H	1:190:A:LEU:HD22	7	0.11
(1,450)	1:197:A:TYR:H	1:190:A:LEU:HD23	7	0.11
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD21	1	0.11
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD22	1	0.11
(1,432)	1:188:A:LEU:H	1:190:A:LEU:HD23	1	0.11
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG11	2	0.11
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG12	2	0.11
(1,418)	1:185:A:LYS:H	1:150:A:VAL:HG13	2	0.11
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG11	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG12	3	0.11
(1,396)	1:161:A:ALA:H	1:172:A:VAL:HG13	3	0.11
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG21	5	0.11
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG22	5	0.11
(1,395)	1:160:A:TYR:H	1:152:A:THR:HG23	5	0.11
(1,376)	1:127:A:ASP:H	1:122:A:LEU:HD11	6	0.11
(1,376)	1:127:A:ASP:H	1:122:A:LEU:HD12	6	0.11
(1,376)	1:127:A:ASP:H	1:122:A:LEU:HD13	6	0.11
(1,371)	1:123:A:GLN:H	1:122:A:LEU:HD11	2	0.11
(1,371)	1:123:A:GLN:H	1:122:A:LEU:HD12	2	0.11
(1,371)	1:123:A:GLN:H	1:122:A:LEU:HD13	2	0.11
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD11	6	0.11
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD12	6	0.11
(1,345)	1:83:A:ASN:H	1:89:A:LEU:HD13	6	0.11
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG21	9	0.11
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG22	9	0.11
(1,338)	1:80:A:LEU:H	1:219:A:THR:HG23	9	0.11
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB1	2	0.11
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB2	2	0.11
(1,295)	1:22:A:PHE:H	1:21:A:ALA:HB3	2	0.11
(1,290)	1:18:A:GLU:H	1:172:A:VAL:HG21	3	0.11
(1,290)	1:18:A:GLU:H	1:172:A:VAL:HG22	3	0.11
(1,290)	1:18:A:GLU:H	1:172:A:VAL:HG23	3	0.11
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG11	2	0.11
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG12	2	0.11
(1,267)	1:172:A:VAL:H	1:172:A:VAL:HG13	2	0.11
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD21	7	0.11
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD22	7	0.11
(1,249)	1:76:A:LEU:H	1:76:A:LEU:HD23	7	0.11
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD21	4	0.11
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD22	4	0.11
(1,242)	1:56:A:LEU:H	1:56:A:LEU:HD23	4	0.11
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG11	10	0.11
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG12	10	0.11
(1,233)	1:17:A:VAL:H	1:17:A:VAL:HG13	10	0.11
(1,223)	1:118:A:PHE:HE1	1:127:A:ASP:H	8	0.11
(1,223)	1:118:A:PHE:HE2	1:127:A:ASP:H	8	0.11
(1,218)	1:221:A:PHE:HE1	1:222:A:VAL:H	1	0.11
(1,218)	1:221:A:PHE:HE2	1:222:A:VAL:H	1	0.11
(1,201)	1:20:A:PHE:HD1	1:21:A:ALA:H	9	0.11
(1,201)	1:20:A:PHE:HD2	1:21:A:ALA:H	9	0.11
(1,192)	1:216:A:TYR:HE1	1:57:A:ASP:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:216:A:TYR:HE2	1:57:A:ASP:H	4	0.11
(1,186)	1:160:A:TYR:HE1	1:159:A:GLN:H	8	0.11
(1,186)	1:160:A:TYR:HE2	1:159:A:GLN:H	8	0.11
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD21	4	0.11
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD22	4	0.11
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD23	4	0.11
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD21	8	0.11
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD22	8	0.11
(1,183)	1:203:A:ILE:H	1:220:A:LEU:HD23	8	0.11
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD11	9	0.11
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD12	9	0.11
(1,182)	1:215:A:GLY:H	1:214:A:ILE:HD13	9	0.11
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD11	2	0.11
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD12	2	0.11
(1,176)	1:201:A:ARG:H	1:203:A:ILE:HD13	2	0.11
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD21	5	0.11
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD22	5	0.11
(1,170)	1:141:A:ALA:H	1:188:A:LEU:HD23	5	0.11
(1,167)	1:184:A:THR:H	1:180:A:MET:HE1	1	0.11
(1,167)	1:184:A:THR:H	1:180:A:MET:HE2	1	0.11
(1,167)	1:184:A:THR:H	1:180:A:MET:HE3	1	0.11
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB1	2	0.11
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB2	2	0.11
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB3	2	0.11
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB1	10	0.11
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB2	10	0.11
(1,158)	1:173:A:ARG:H	1:161:A:ALA:HB3	10	0.11
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE1	6	0.11
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE2	6	0.11
(1,150)	1:131:A:ILE:H	1:130:A:MET:HE3	6	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB1	1	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB2	1	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB3	1	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB1	4	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB2	4	0.11
(1,146)	1:122:A:LEU:H	1:126:A:ALA:HB3	4	0.11
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB1	4	0.11
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB2	4	0.11
(1,144)	1:124:A:ALA:H	1:121:A:ALA:HB3	4	0.11
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD11	1	0.11
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD12	1	0.11
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD13	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD11	10	0.11
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD12	10	0.11
(1,138)	1:92:A:VAL:H	1:91:A:ILE:HD13	10	0.11
(1,135)	1:87:A:ARG:H	1:88:A:THR:HG21	2	0.11
(1,135)	1:87:A:ARG:H	1:88:A:THR:HG22	2	0.11
(1,135)	1:87:A:ARG:H	1:88:A:THR:HG23	2	0.11
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD21	3	0.11
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD22	3	0.11
(1,133)	1:92:A:VAL:H	1:80:A:LEU:HD23	3	0.11
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD21	9	0.11
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD22	9	0.11
(1,127)	1:216:A:TYR:H	1:56:A:LEU:HD23	9	0.11
(1,119)	1:31:A:SER:H	1:34:A:ILE:HD11	5	0.11
(1,119)	1:31:A:SER:H	1:34:A:ILE:HD12	5	0.11
(1,119)	1:31:A:SER:H	1:34:A:ILE:HD13	5	0.11
(1,110)	1:219:A:THR:HG21	1:221:A:PHE:HE1	8	0.11
(1,110)	1:219:A:THR:HG22	1:221:A:PHE:HE1	8	0.11
(1,110)	1:219:A:THR:HG23	1:221:A:PHE:HE1	8	0.11
(1,105)	1:190:A:LEU:HD21	1:197:A:TYR:HD2	5	0.11
(1,105)	1:190:A:LEU:HD22	1:197:A:TYR:HD2	5	0.11
(1,105)	1:190:A:LEU:HD23	1:197:A:TYR:HD2	5	0.11
(1,100)	1:186:A:VAL:HG21	1:138:A:PHE:HD1	3	0.11
(1,100)	1:186:A:VAL:HG22	1:138:A:PHE:HD1	3	0.11
(1,100)	1:186:A:VAL:HG23	1:138:A:PHE:HD1	3	0.11
(1,99)	1:174:A:THR:HG21	1:160:A:TYR:HE1	4	0.11
(1,99)	1:174:A:THR:HG22	1:160:A:TYR:HE1	4	0.11
(1,99)	1:174:A:THR:HG23	1:160:A:TYR:HE1	4	0.11
(1,83)	1:148:A:VAL:HG21	1:142:A:TYR:HD1	6	0.11
(1,83)	1:148:A:VAL:HG21	1:142:A:TYR:HD2	6	0.11
(1,83)	1:148:A:VAL:HG22	1:142:A:TYR:HD1	6	0.11
(1,83)	1:148:A:VAL:HG22	1:142:A:TYR:HD2	6	0.11
(1,83)	1:148:A:VAL:HG23	1:142:A:TYR:HD1	6	0.11
(1,83)	1:148:A:VAL:HG23	1:142:A:TYR:HD2	6	0.11
(1,81)	1:148:A:VAL:HG11	1:142:A:TYR:HE2	5	0.11
(1,81)	1:148:A:VAL:HG12	1:142:A:TYR:HE2	5	0.11
(1,81)	1:148:A:VAL:HG13	1:142:A:TYR:HE2	5	0.11
(1,79)	1:144:A:VAL:HG21	1:44:A:PHE:HE1	10	0.11
(1,79)	1:144:A:VAL:HG21	1:44:A:PHE:HE2	10	0.11
(1,79)	1:144:A:VAL:HG22	1:44:A:PHE:HE1	10	0.11
(1,79)	1:144:A:VAL:HG22	1:44:A:PHE:HE2	10	0.11
(1,79)	1:144:A:VAL:HG23	1:44:A:PHE:HE1	10	0.11
(1,79)	1:144:A:VAL:HG23	1:44:A:PHE:HE2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:128:A:ILE:HD11	1:38:A:TYR:HD1	3	0.11
(1,66)	1:128:A:ILE:HD11	1:38:A:TYR:HD2	3	0.11
(1,66)	1:128:A:ILE:HD12	1:38:A:TYR:HD1	3	0.11
(1,66)	1:128:A:ILE:HD12	1:38:A:TYR:HD2	3	0.11
(1,66)	1:128:A:ILE:HD13	1:38:A:TYR:HD1	3	0.11
(1,66)	1:128:A:ILE:HD13	1:38:A:TYR:HD2	3	0.11
(1,49)	1:107:A:LEU:HD11	1:142:A:TYR:HE2	1	0.11
(1,49)	1:107:A:LEU:HD12	1:142:A:TYR:HE2	1	0.11
(1,49)	1:107:A:LEU:HD13	1:142:A:TYR:HE2	1	0.11
(1,44)	1:104:A:ILE:HD11	1:20:A:PHE:HD1	7	0.11
(1,44)	1:104:A:ILE:HD11	1:20:A:PHE:HD2	7	0.11
(1,44)	1:104:A:ILE:HD12	1:20:A:PHE:HD1	7	0.11
(1,44)	1:104:A:ILE:HD12	1:20:A:PHE:HD2	7	0.11
(1,44)	1:104:A:ILE:HD13	1:20:A:PHE:HD1	7	0.11
(1,44)	1:104:A:ILE:HD13	1:20:A:PHE:HD2	7	0.11
(1,32)	1:81:A:ILE:HD11	1:221:A:PHE:HD1	2	0.11
(1,32)	1:81:A:ILE:HD11	1:221:A:PHE:HD2	2	0.11
(1,32)	1:81:A:ILE:HD12	1:221:A:PHE:HD1	2	0.11
(1,32)	1:81:A:ILE:HD12	1:221:A:PHE:HD2	2	0.11
(1,32)	1:81:A:ILE:HD13	1:221:A:PHE:HD1	2	0.11
(1,32)	1:81:A:ILE:HD13	1:221:A:PHE:HD2	2	0.11
(1,14)	1:32:A:LEU:HD21	1:118:A:PHE:HE2	3	0.11
(1,14)	1:32:A:LEU:HD22	1:118:A:PHE:HE2	3	0.11
(1,14)	1:32:A:LEU:HD23	1:118:A:PHE:HE2	3	0.11
(1,12)	1:32:A:LEU:HD11	1:118:A:PHE:HE2	1	0.11
(1,12)	1:32:A:LEU:HD12	1:118:A:PHE:HE2	1	0.11
(1,12)	1:32:A:LEU:HD13	1:118:A:PHE:HE2	1	0.11
(2,40)	1:93:A:ASP:H	1:184:A:THR:O	7	0.1
(1,875)	1:68:A:SER:H	1:71:A:ASP:H	3	0.1
(1,851)	1:214:A:ILE:H	1:216:A:TYR:H	9	0.1
(1,773)	1:224:A:LYS:H	1:223:A:GLU:H	7	0.1
(1,721)	1:168:A:GLY:H	1:169:A:SER:H	6	0.1
(1,703)	1:137:A:GLY:H	1:138:A:PHE:H	5	0.1
(1,698)	1:125:A:GLY:H	1:124:A:ALA:H	5	0.1
(1,660)	1:60:A:ARG:H	1:61:A:TYR:H	8	0.1
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD11	2	0.1
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD12	2	0.1
(1,620)	1:190:A:LEU:HD21	1:198:A:LEU:HD13	2	0.1
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD11	2	0.1
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD12	2	0.1
(1,620)	1:190:A:LEU:HD22	1:198:A:LEU:HD13	2	0.1
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD11	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD12	2	0.1
(1,620)	1:190:A:LEU:HD23	1:198:A:LEU:HD13	2	0.1
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD21	2	0.1
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD22	2	0.1
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD23	2	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD21	2	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD22	2	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD23	2	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD21	2	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD22	2	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD23	2	0.1
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD21	4	0.1
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD22	4	0.1
(1,617)	1:190:A:LEU:HD11	1:198:A:LEU:HD23	4	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD21	4	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD22	4	0.1
(1,617)	1:190:A:LEU:HD12	1:198:A:LEU:HD23	4	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD21	4	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD22	4	0.1
(1,617)	1:190:A:LEU:HD13	1:198:A:LEU:HD23	4	0.1
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	2	0.1
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	2	0.1
(1,583)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	2	0.1
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	2	0.1
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	2	0.1
(1,583)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	2	0.1
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	2	0.1
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	2	0.1
(1,583)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	2	0.1
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	1	0.1
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	1	0.1
(1,558)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	1	0.1
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	1	0.1
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	1	0.1
(1,558)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	1	0.1
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	1	0.1
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	1	0.1
(1,558)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	1	0.1
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG21	4	0.1
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG22	4	0.1
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG23	4	0.1
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG21	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG22	4	0.1
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG23	4	0.1
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG21	4	0.1
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG22	4	0.1
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG23	4	0.1
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG21	9	0.1
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG22	9	0.1
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG23	9	0.1
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG21	9	0.1
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG22	9	0.1
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG23	9	0.1
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG21	9	0.1
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG22	9	0.1
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG23	9	0.1
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD11	9	0.1
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD12	9	0.1
(1,525)	1:45:A:LEU:HD21	1:49:A:ILE:HD13	9	0.1
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD11	9	0.1
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD12	9	0.1
(1,525)	1:45:A:LEU:HD22	1:49:A:ILE:HD13	9	0.1
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD11	9	0.1
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD12	9	0.1
(1,525)	1:45:A:LEU:HD23	1:49:A:ILE:HD13	9	0.1
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG11	3	0.1
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG12	3	0.1
(1,462)	1:209:A:LYS:H	1:207:A:VAL:HG13	3	0.1
(1,420)	1:185:A:LYS:H	1:184:A:THR:HG21	9	0.1
(1,420)	1:185:A:LYS:H	1:184:A:THR:HG22	9	0.1
(1,420)	1:185:A:LYS:H	1:184:A:THR:HG23	9	0.1
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG21	9	0.1
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG22	9	0.1
(1,397)	1:162:A:TRP:H	1:149:A:THR:HG23	9	0.1
(1,332)	1:78:A:ILE:H	1:56:A:LEU:HD21	10	0.1
(1,332)	1:78:A:ILE:H	1:56:A:LEU:HD22	10	0.1
(1,332)	1:78:A:ILE:H	1:56:A:LEU:HD23	10	0.1
(1,218)	1:221:A:PHE:HE1	1:222:A:VAL:H	6	0.1
(1,218)	1:221:A:PHE:HE2	1:222:A:VAL:H	6	0.1
(1,195)	1:210:A:HIS:HE1	1:43:A:ILE:H	6	0.1
(1,194)	1:77:A:HIS:HE1	1:76:A:LEU:H	2	0.1
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB1	1	0.1
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB2	1	0.1
(1,112)	1:29:A:LEU:H	1:27:A:ALA:HB3	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:144:A:VAL:HG11	1:197:A:TYR:HD2	7	0.1
(1,77)	1:144:A:VAL:HG12	1:197:A:TYR:HD2	7	0.1
(1,77)	1:144:A:VAL:HG13	1:197:A:TYR:HD2	7	0.1
(1,54)	1:117:A:ALA:HB1	1:134:A:PHE:HD1	2	0.1
(1,54)	1:117:A:ALA:HB1	1:134:A:PHE:HD2	2	0.1
(1,54)	1:117:A:ALA:HB2	1:134:A:PHE:HD1	2	0.1
(1,54)	1:117:A:ALA:HB2	1:134:A:PHE:HD2	2	0.1
(1,54)	1:117:A:ALA:HB3	1:134:A:PHE:HD1	2	0.1
(1,54)	1:117:A:ALA:HB3	1:134:A:PHE:HD2	2	0.1
(1,44)	1:104:A:ILE:HD11	1:20:A:PHE:HD1	10	0.1
(1,44)	1:104:A:ILE:HD11	1:20:A:PHE:HD2	10	0.1
(1,44)	1:104:A:ILE:HD12	1:20:A:PHE:HD1	10	0.1
(1,44)	1:104:A:ILE:HD12	1:20:A:PHE:HD2	10	0.1
(1,44)	1:104:A:ILE:HD13	1:20:A:PHE:HD1	10	0.1
(1,44)	1:104:A:ILE:HD13	1:20:A:PHE:HD2	10	0.1
(1,35)	1:89:A:LEU:HD11	1:44:A:PHE:HE2	7	0.1
(1,35)	1:89:A:LEU:HD12	1:44:A:PHE:HE2	7	0.1
(1,35)	1:89:A:LEU:HD13	1:44:A:PHE:HE2	7	0.1
(1,31)	1:76:A:LEU:HD21	1:216:A:TYR:HE1	9	0.1
(1,31)	1:76:A:LEU:HD22	1:216:A:TYR:HE1	9	0.1
(1,31)	1:76:A:LEU:HD23	1:216:A:TYR:HE1	9	0.1
(1,29)	1:64:A:LEU:HD21	1:61:A:TYR:HD1	9	0.1
(1,29)	1:64:A:LEU:HD22	1:61:A:TYR:HD1	9	0.1
(1,29)	1:64:A:LEU:HD23	1:61:A:TYR:HD1	9	0.1
(1,9)	1:29:A:LEU:HD21	1:118:A:PHE:HE2	5	0.1
(1,9)	1:29:A:LEU:HD22	1:118:A:PHE:HE2	5	0.1
(1,9)	1:29:A:LEU:HD23	1:118:A:PHE:HE2	5	0.1

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

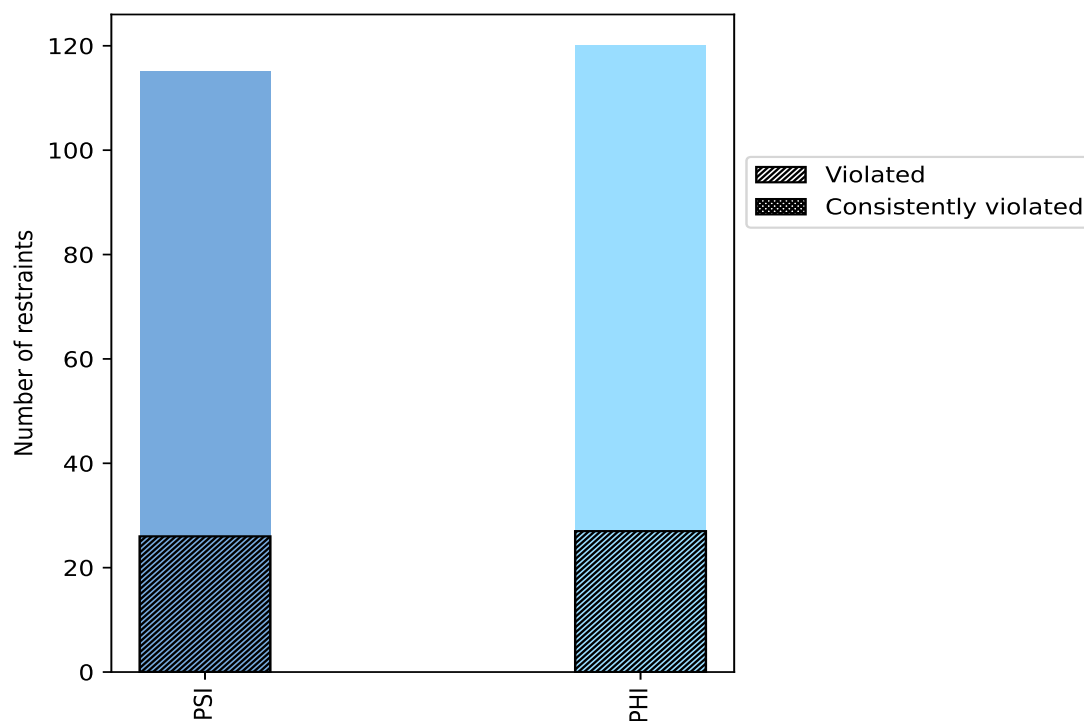
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	115	48.9	26	22.6	11.1	0	0.0	0.0
PHI	120	51.1	27	22.5	11.5	0	0.0	0.0
Total	235	100.0	53	22.6	22.6	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 [i](#)



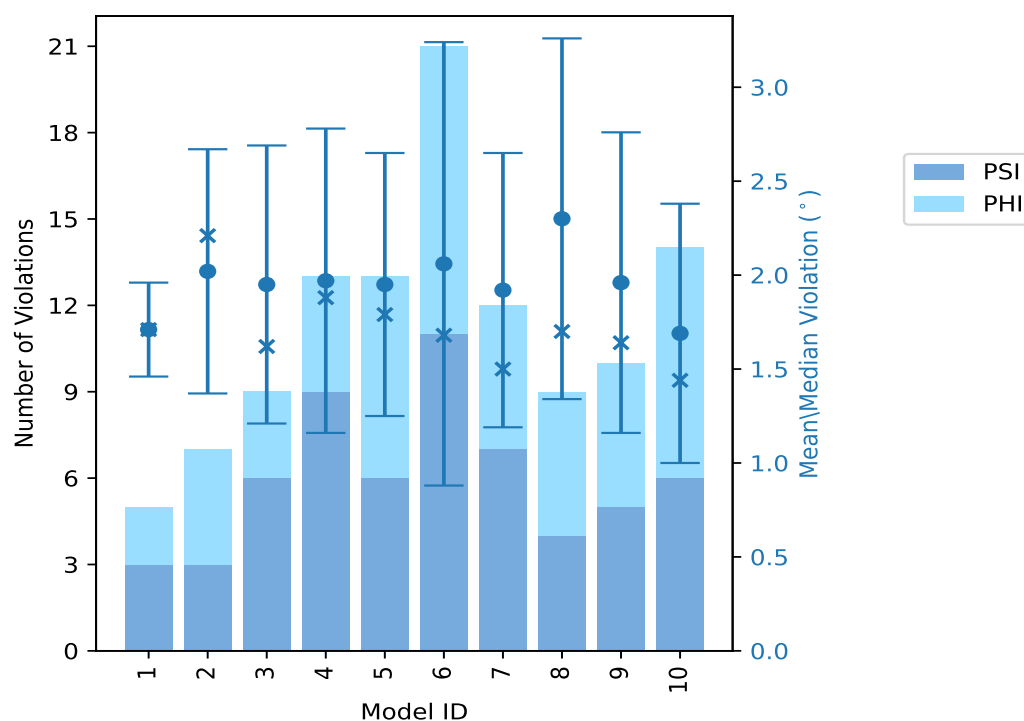
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [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	3	2	5	1.71	2.1	0.25	1.71
2	3	4	7	2.02	2.65	0.65	2.21
3	6	3	9	1.95	3.52	0.74	1.62
4	9	4	13	1.97	4.0	0.81	1.88
5	6	7	13	1.95	3.62	0.7	1.79
6	11	10	21	2.06	5.35	1.18	1.68
7	7	5	12	1.92	3.83	0.73	1.5
8	4	5	9	2.3	4.25	0.96	1.7
9	5	5	10	1.96	4.01	0.8	1.64
10	6	8	14	1.69	3.05	0.69	1.44

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

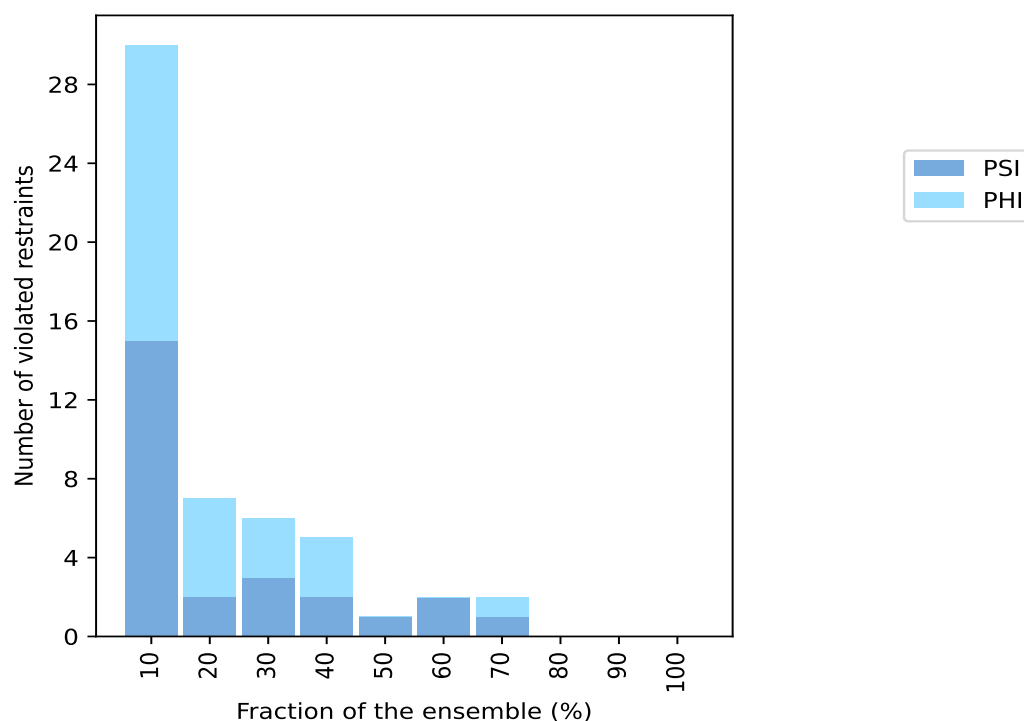
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
15	15	30	1	10.0
2	5	7	2	20.0
3	3	6	3	30.0
2	3	5	4	40.0
1	0	1	5	50.0
2	0	2	6	60.0
1	1	2	7	70.0
0	0	0	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

¹ Number of models with violations

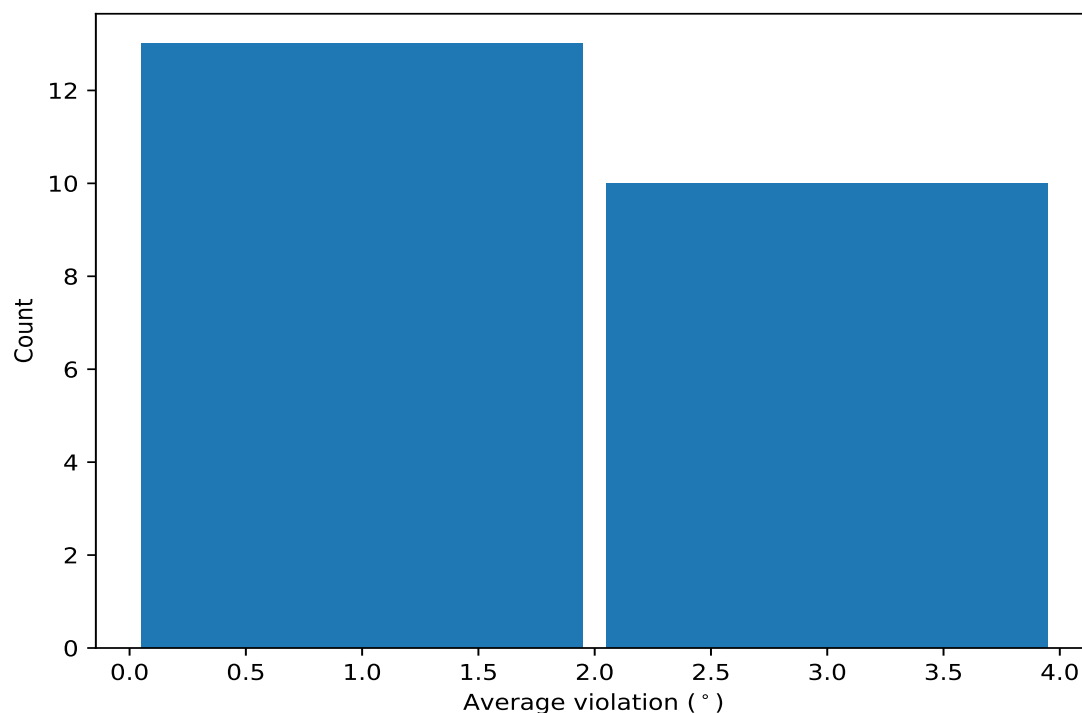
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,84)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	7	2.27	0.71	2.21
(1,15)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	7	1.68	0.63	1.69
(1,157)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	6	1.82	1.02	1.47
(1,175)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	6	1.66	0.4	1.68
(1,90)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:ASP:N	5	1.65	0.31	1.62
(1,187)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	4	2.51	1.59	1.85
(1,144)	1:148:A:VAL:C	1:149:A:THR:N	1:149:A:THR:CA	1:149:A:THR:C	4	2.04	0.51	2.23
(1,14)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:ILE:N	4	1.91	0.45	1.82
(1,200)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	4	1.86	0.64	1.66
(1,74)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:ASP:N	4	1.66	0.26	1.57
(1,186)	1:179:A:PRO:N	1:179:A:PRO:CA	1:179:A:PRO:C	1:180:A:MET:N	3	3.01	1.79	2.65
(1,3)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	3	2.91	0.88	2.89
(1,133)	1:129:A:SER:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	3	2.18	0.85	2.46

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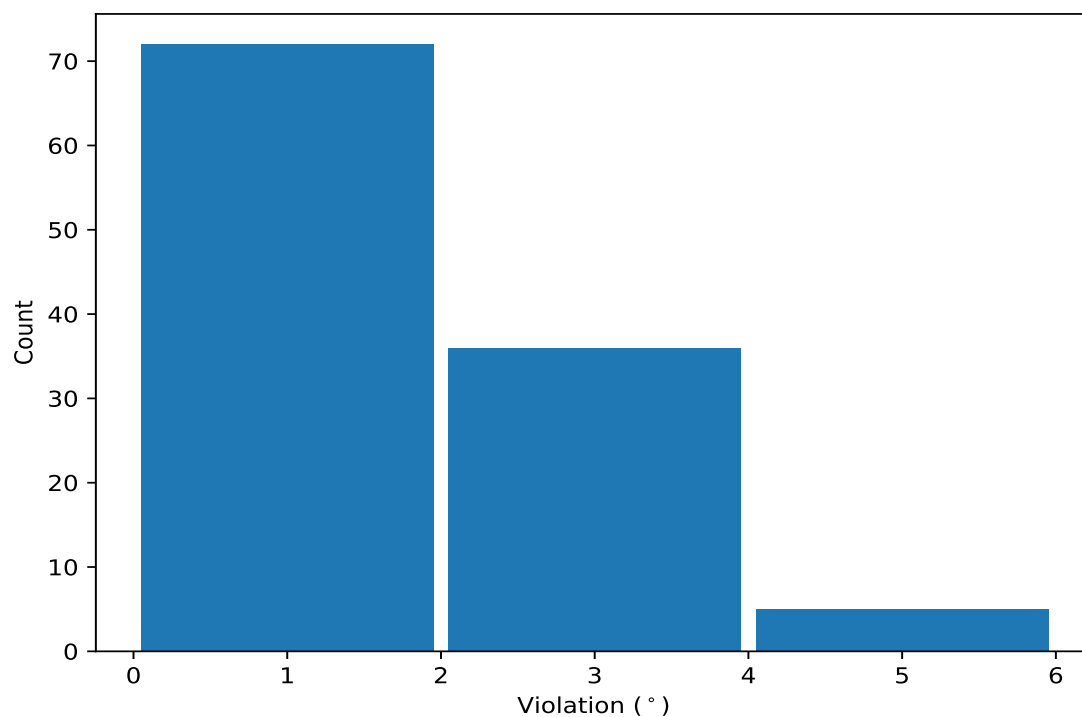
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,134)	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	1:131:A:ILE:N	3	2.16	1.09	1.84
(1,155)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	3	2.11	0.48	2.04
(1,154)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	3	1.87	0.58	1.71
(1,34)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:GLU:N	2	3.1	0.73	3.1
(1,73)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	2	2.22	0.52	2.22
(1,136)	1:142:A:TYR:C	1:143:A:LEU:N	1:143:A:LEU:CA	1:143:A:LEU:C	2	1.62	0.03	1.62
(1,142)	1:147:A:LYS:C	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	2	1.54	0.09	1.54
(1,161)	1:160:A:TYR:N	1:160:A:TYR:CA	1:160:A:TYR:C	1:161:A:ALA:N	2	1.46	0.02	1.46
(1,114)	1:100:A:LYS:C	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	2	1.27	0.24	1.27
(1,83)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	2	1.21	0.02	1.21

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:179:A:PRO:N	1:179:A:PRO:CA	1:179:A:PRO:C	1:180:A:MET:N	6	5.35
(1,187)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	6	5.14
(1,70)	1:67:A:PRO:N	1:67:A:PRO:CA	1:67:A:PRO:C	1:68:A:SER:N	8	4.25
(1,157)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	9	4.01
(1,3)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	4	4.0
(1,34)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:GLU:N	7	3.83
(1,134)	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	1:131:A:ILE:N	5	3.62
(1,84)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	8	3.53
(1,219)	1:210:A:HIS:N	1:210:A:HIS:CA	1:210:A:HIS:C	1:211:A:SER:N	3	3.52
(1,133)	1:129:A:SER:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	10	3.05
(1,123)	1:120:A:GLU:C	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	10	2.97
(1,84)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	3	2.97
(1,200)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	4	2.92
(1,104)	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	1:93:A:ASP:N	6	2.92
(1,3)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	6	2.89
(1,132)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:130:A:MET:N	10	2.79
(1,73)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	5	2.74
(1,155)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	4	2.73
(1,15)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	9	2.72
(1,233)	1:225:A:GLU:N	1:225:A:GLU:CA	1:225:A:GLU:C	1:226:A:ARG:N	5	2.67
(1,186)	1:179:A:PRO:N	1:179:A:PRO:CA	1:179:A:PRO:C	1:180:A:MET:N	2	2.65
(1,154)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	2	2.65
(1,14)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:ILE:N	8	2.61
(1,144)	1:148:A:VAL:C	1:149:A:THR:N	1:149:A:THR:CA	1:149:A:THR:C	8	2.52
(1,133)	1:129:A:SER:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	5	2.46
(1,135)	1:140:A:SER:C	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	7	2.45
(1,187)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	2	2.44
(1,15)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	7	2.44
(1,84)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	6	2.43
(1,34)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:GLU:N	6	2.38
(1,144)	1:148:A:VAL:C	1:149:A:THR:N	1:149:A:THR:CA	1:149:A:THR:C	7	2.3
(1,188)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	7	2.25
(1,84)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	2	2.21
(1,144)	1:148:A:VAL:C	1:149:A:THR:N	1:149:A:THR:CA	1:149:A:THR:C	6	2.16
(1,90)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:ASP:N	2	2.15
(1,195)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	3	2.14
(1,175)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	9	2.14
(1,175)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	4	2.11
(1,74)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:ASP:N	1	2.1
(1,155)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	6	2.04
(1,96)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	4	2.01
(1,14)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:ILE:N	6	1.95
(1,157)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	4	1.89
(1,229)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:PHE:N	4	1.88
(1,3)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	9	1.85
(1,134)	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	1:131:A:ILE:N	1	1.84
(1,175)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	5	1.83
(1,131)	1:128:A:ILE:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	5	1.81
(1,129)	1:127:A:ASP:C	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	10	1.79
(1,72)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:LYS:N	5	1.79
(1,90)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:ASP:N	4	1.78
(1,154)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	6	1.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,15)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1	1.71
(1,200)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	8	1.7
(1,73)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	10	1.7
(1,14)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:ILE:N	3	1.7
(1,15)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	5	1.69
(1,190)	1:183:A:GLY:C	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	6	1.68
(1,84)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	4	1.68
(1,136)	1:142:A:TYR:C	1:143:A:LEU:N	1:143:A:LEU:CA	1:143:A:LEU:C	9	1.65
(1,74)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:ASP:N	9	1.64
(1,142)	1:147:A:LYS:C	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	3	1.62
(1,90)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:ASP:N	9	1.62
(1,200)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	6	1.61
(1,157)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	8	1.59
(1,136)	1:142:A:TYR:C	1:143:A:LEU:N	1:143:A:LEU:CA	1:143:A:LEU:C	6	1.59
(1,125)	1:121:A:ALA:C	1:122:A:LEU:N	1:122:A:LEU:CA	1:122:A:LEU:C	8	1.58
(1,155)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	3	1.55
(1,230)	1:220:A:LEU:C	1:221:A:PHE:N	1:221:A:PHE:CA	1:221:A:PHE:C	6	1.54
(1,175)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	1	1.54
(1,84)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	5	1.53
(1,114)	1:100:A:LYS:C	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	10	1.52
(1,84)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	7	1.52
(1,103)	1:91:A:ILE:C	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	8	1.5
(1,74)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:ASP:N	10	1.5
(1,90)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:ASP:N	7	1.49
(1,161)	1:160:A:TYR:N	1:160:A:TYR:CA	1:160:A:TYR:C	1:161:A:ALA:N	5	1.48
(1,191)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	4	1.46
(1,142)	1:147:A:LYS:C	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	7	1.45
(1,161)	1:160:A:TYR:N	1:160:A:TYR:CA	1:160:A:TYR:C	1:161:A:ALA:N	3	1.44
(1,223)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	7	1.43
(1,74)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:ASP:N	6	1.42
(1,69)	1:66:A:ASP:C	1:67:A:PRO:N	1:67:A:PRO:CA	1:67:A:PRO:C	3	1.42
(1,184)	1:178:A:GLU:N	1:178:A:GLU:CA	1:178:A:GLU:C	1:179:A:PRO:N	9	1.41
(1,153)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:HIS:N	7	1.4
(1,119)	1:117:A:ALA:C	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	8	1.39
(1,152)	1:152:A:THR:C	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1	1.37
(1,14)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:ILE:N	10	1.37
(1,157)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	7	1.35
(1,71)	1:67:A:PRO:C	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	9	1.34
(1,235)	1:236:A:GLU:N	1:236:A:GLU:CA	1:236:A:GLU:C	1:237:A:GLU:N	6	1.26
(1,187)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	10	1.26
(1,154)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	5	1.26
(1,83)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	5	1.23
(1,200)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	10	1.22
(1,90)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:ASP:N	10	1.22
(1,187)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	3	1.21
(1,185)	1:178:A:GLU:C	1:179:A:PRO:N	1:179:A:PRO:CA	1:179:A:PRO:C	9	1.21
(1,144)	1:148:A:VAL:C	1:149:A:THR:N	1:149:A:THR:CA	1:149:A:THR:C	5	1.19
(1,83)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	7	1.19
(1,175)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	10	1.18
(1,175)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	6	1.16
(1,15)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	4	1.12

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,194)	1:185:A:LYS:C	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	4	1.06
(1,157)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	10	1.05
(1,15)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	2	1.05
(1,15)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	10	1.04
(1,157)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	6	1.03
(1,114)	1:100:A:LYS:C	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	6	1.03
(1,186)	1:179:A:PRO:N	1:179:A:PRO:CA	1:179:A:PRO:C	1:180:A:MET:N	4	1.02
(1,134)	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	1:131:A:ILE:N	6	1.02
(1,133)	1:129:A:SER:C	1:130:A:MET:N	1:130:A:MET:CA	1:130:A:MET:C	2	1.02
(1,33)	1:40:A:ASN:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	6	1.01