Full wwPDB NMR Structure Validation Report (i)

Oct 21, 2023 – 01:46 PM EDT

PDB ID	:	8FTX
BMRB ID	:	31070
Title	:	FlgN-FliJ fusion complex
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Deposited on	:	2023-01-13

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

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

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

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

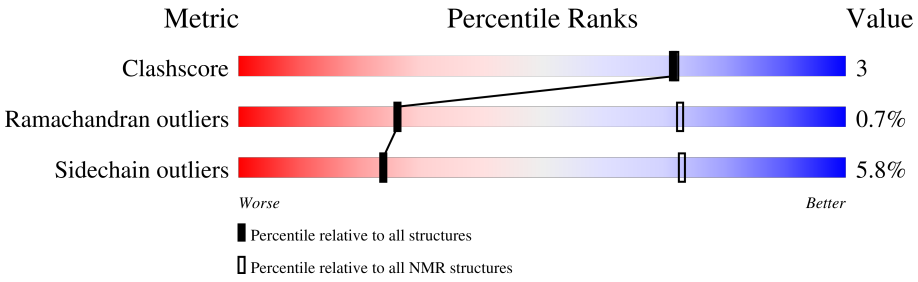
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 47%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	214	63% · 34%

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3-A:108, A:173-A:207 (141)	0.75	11

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

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

The models can be grouped into 3 clusters and 14 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3362 atoms, of which 1674 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	214	3362	1028	1674	312	341	7	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	VAL	-	linker	UNP A0A5K1US31
A	142	LEU	-	linker	UNP A0A5K1US31
A	143	PHE	-	linker	UNP A0A5K1US31
A	144	GLN	-	linker	UNP A0A5K1US31
A	145	GLY	-	linker	UNP A0A5K1US31
A	146	PRO	-	linker	UNP A0A5K1US31
A	147	SER	-	linker	UNP A0A5K1US31
A	148	ALA	-	linker	UNP A0A5K1US31
A	149	GLY	-	linker	UNP A0A5K1US31
A	150	LEU	-	linker	UNP A0A5K1US31
A	151	VAL	-	linker	UNP A0A5K1US31
A	152	PRO	-	linker	UNP A0A5K1US31
A	153	ARG	-	linker	UNP A0A5K1US31
A	154	GLY	-	linker	UNP A0A5K1US31
A	155	SER	-	linker	UNP A0A5K1US31
A	156	GLY	-	linker	UNP A0A5K1US31
A	157	GLY	-	linker	UNP A0A5K1US31
A	158	ILE	-	linker	UNP A0A5K1US31
A	159	GLU	-	linker	UNP A0A5K1US31
A	160	GLY	-	linker	UNP A0A5K1US31

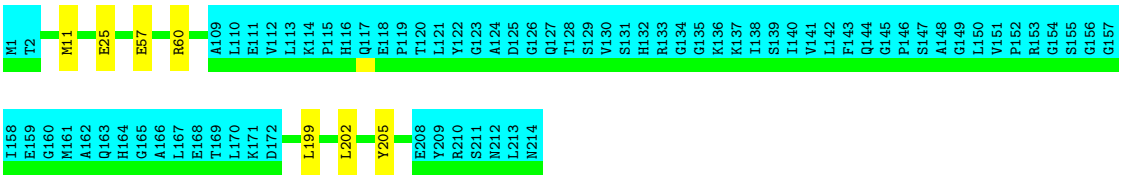
4 Residue-property plots

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: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

Chain A:



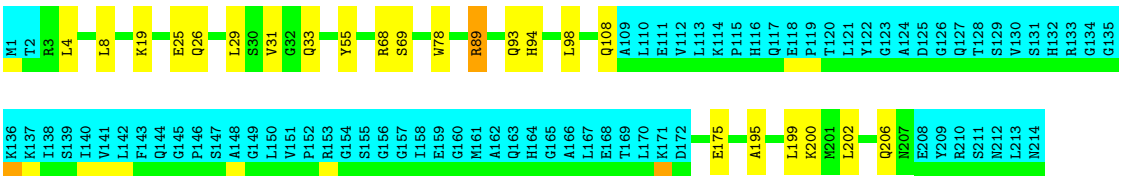
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

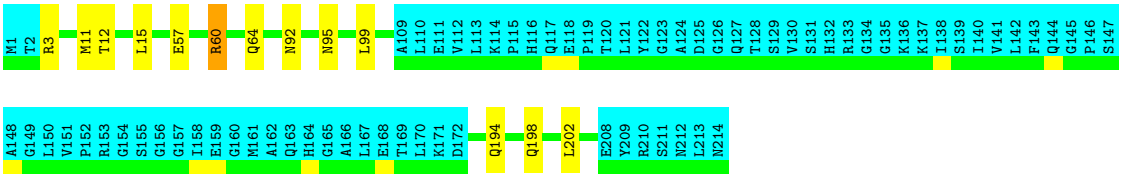
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

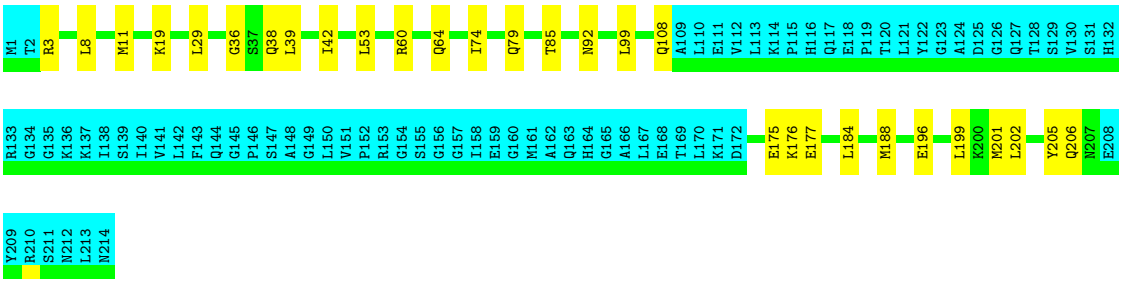
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

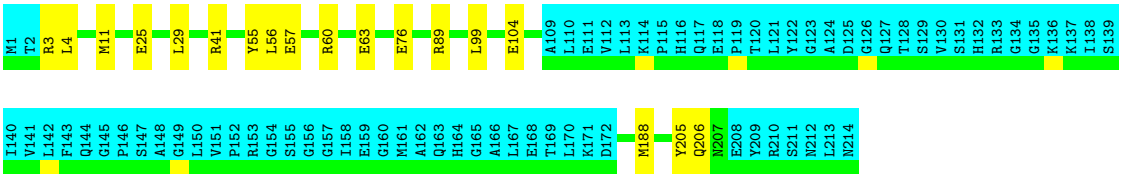
Chain A: 52% 14% 34%



4.2.4 Score per residue for model 4

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

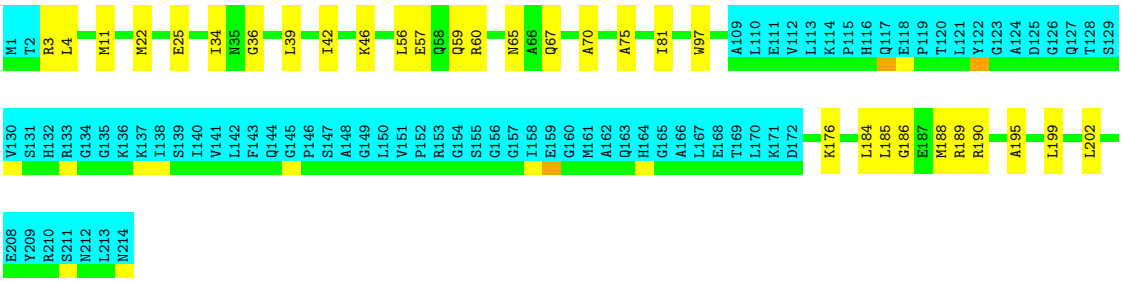
Chain A: 57% 8% 34%



4.2.5 Score per residue for model 5

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

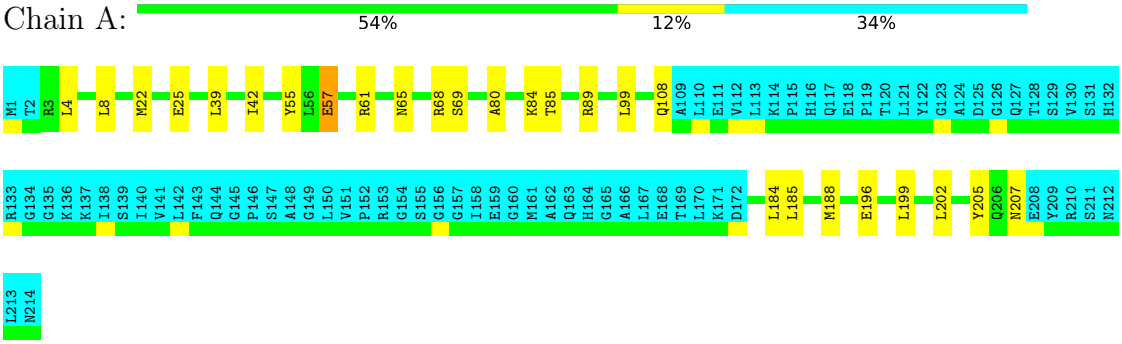
Chain A: 52% 14% 34%



4.2.6 Score per residue for model 6

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

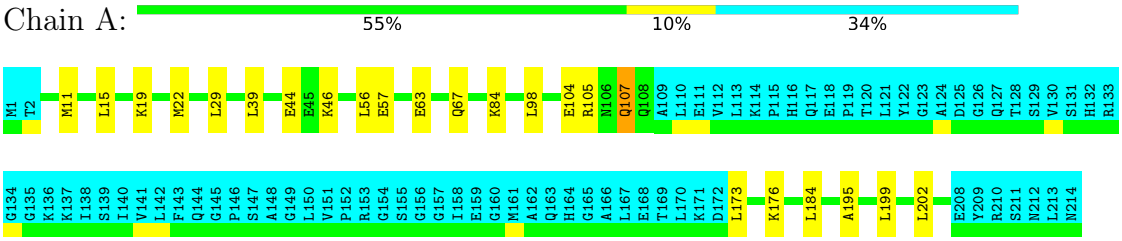
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

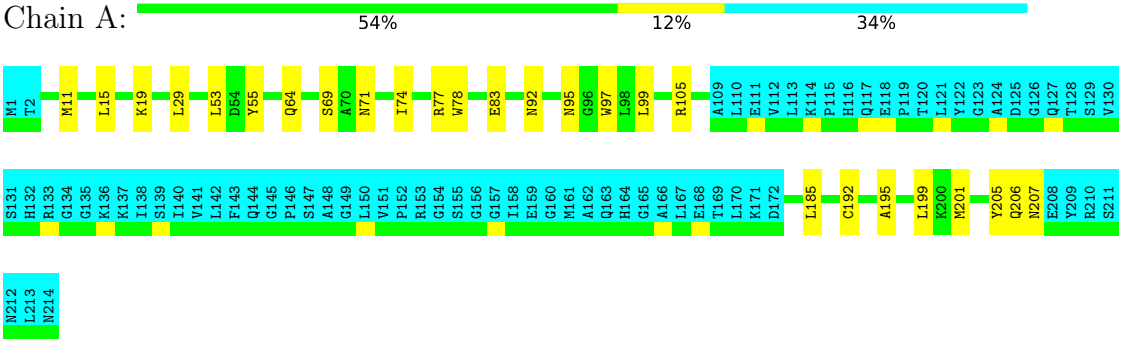
Chain A:



4.2.8 Score per residue for model 8

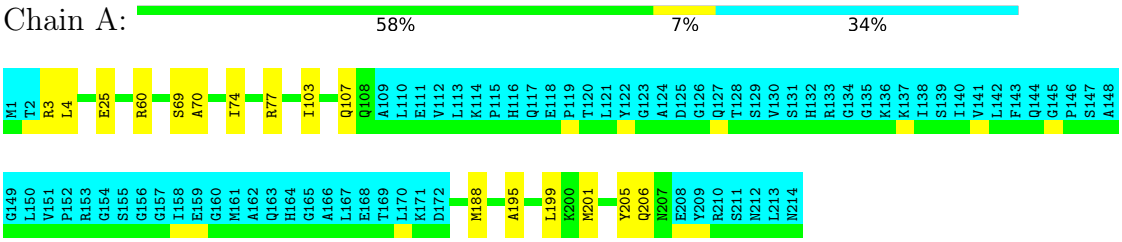
• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

Chain A:



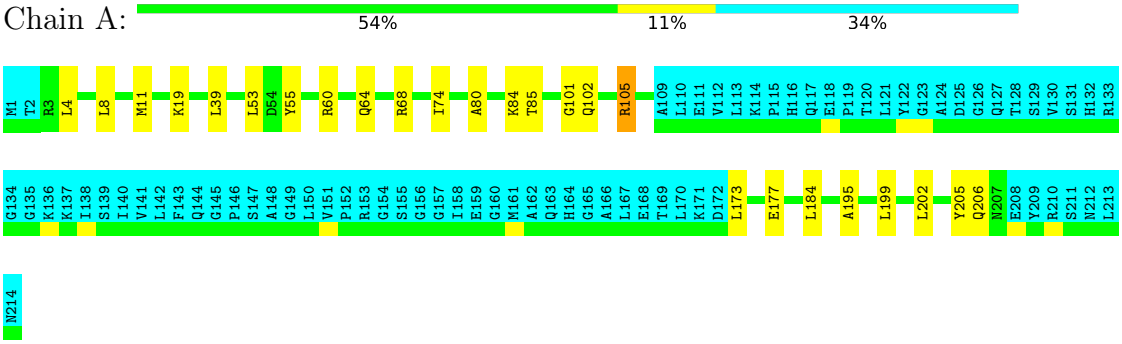
4.2.9 Score per residue for model 9

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



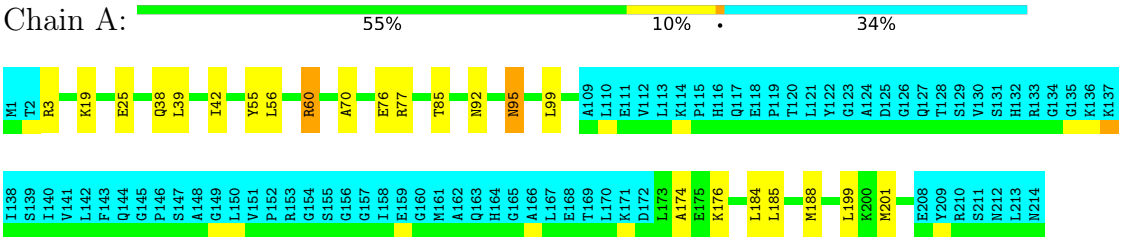
4.2.10 Score per residue for model 10

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



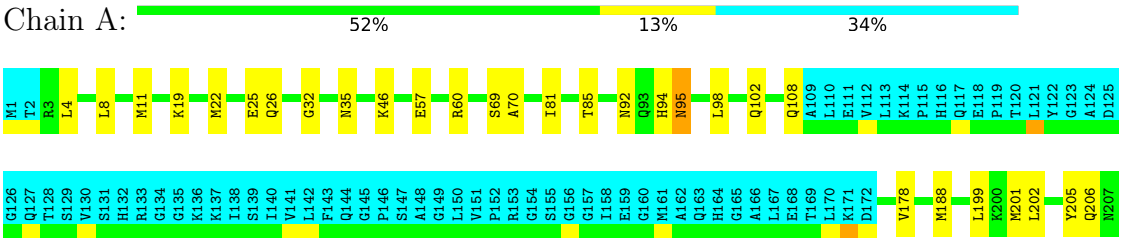
4.2.11 Score per residue for model 11 (medoid)

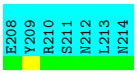
• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



4.2.12 Score per residue for model 12

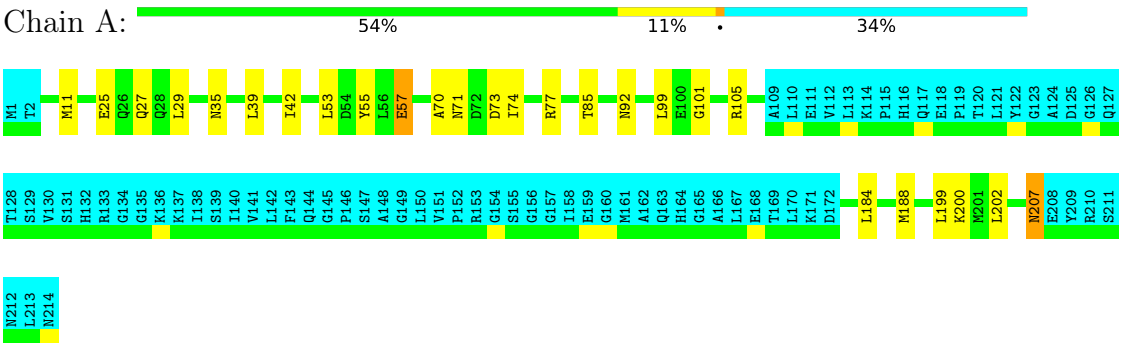
• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion





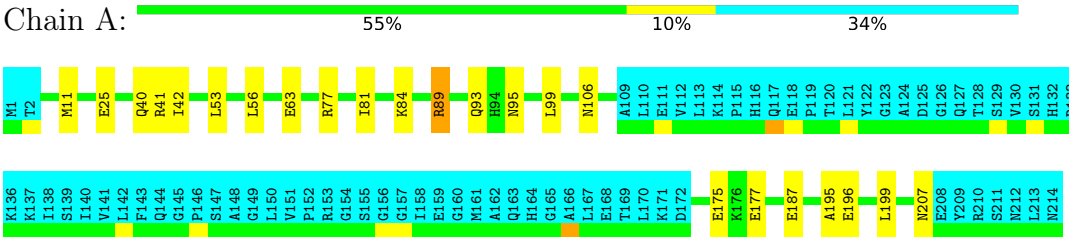
4.2.13 Score per residue for model 13

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



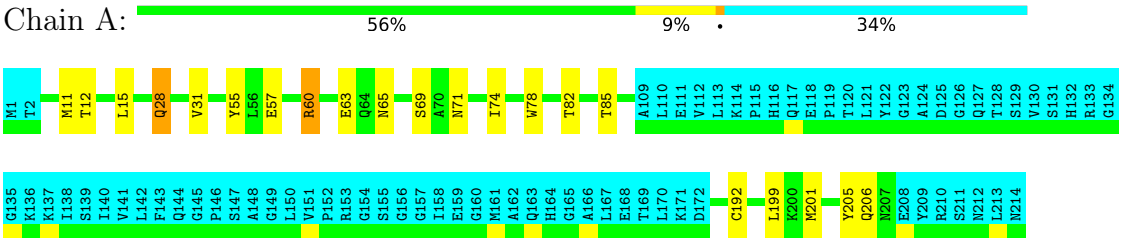
4.2.14 Score per residue for model 14

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



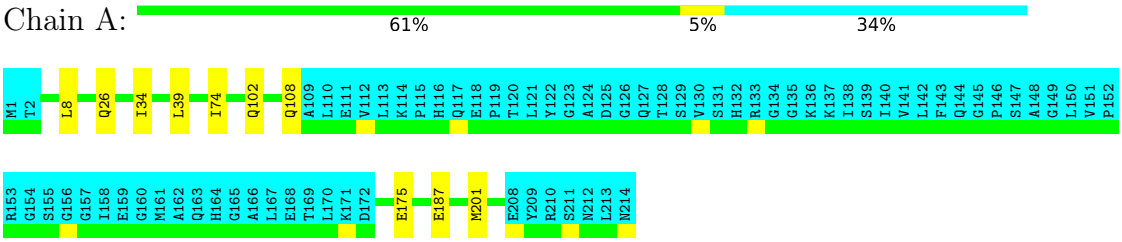
4.2.15 Score per residue for model 15

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



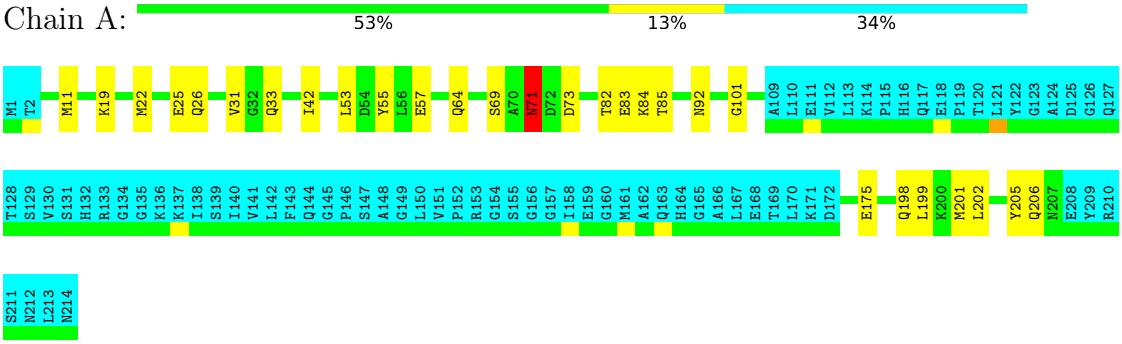
4.2.16 Score per residue for model 16

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



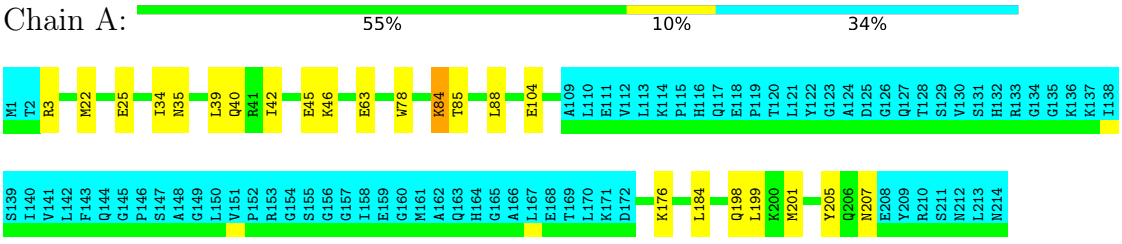
4.2.17 Score per residue for model 17

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



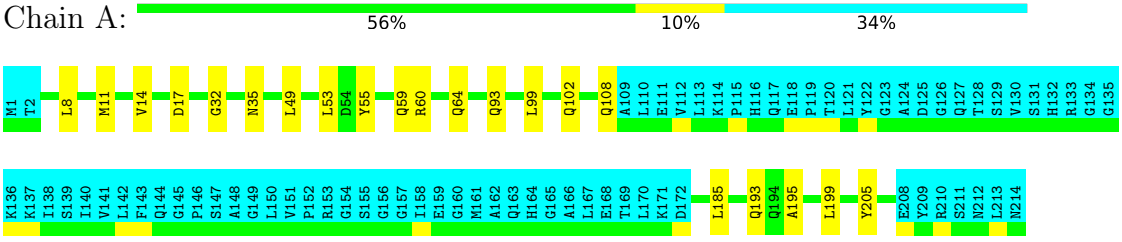
4.2.18 Score per residue for model 18

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



4.2.19 Score per residue for model 19

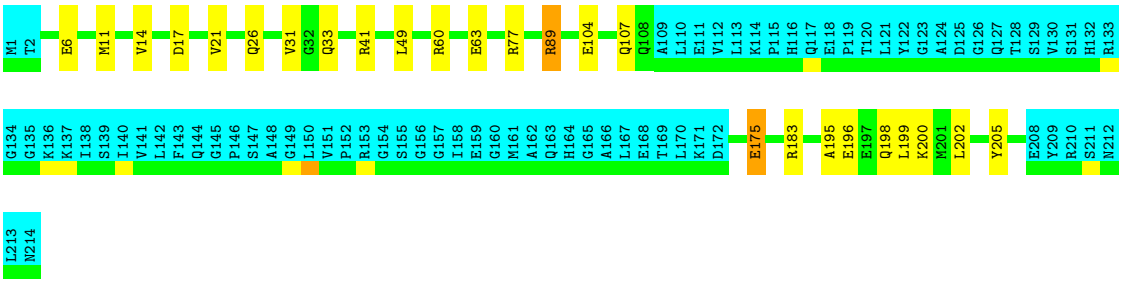
• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion



4.2.20 Score per residue for model 20

• Molecule 1: Flagella biosynthesis chaperone FlgN, Flagellar FliJ protein fusion

Chain A: 



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	
TALOS	geometry optimization	

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	1258
Number of shifts mapped to atoms	1258
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

6 Model quality

6.1 Standard geometry

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

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	1147	1129	1127	8±3
All	All	22940	22580	22540	158

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:MET:SD	1:A:53:LEU:HD22	0.67	2.29	13	7
1:A:99:LEU:HD21	1:A:188:MET:SD	0.60	2.35	6	4
1:A:11:MET:SD	1:A:60:ARG:HG2	0.59	2.38	15	1
1:A:60:ARG:HH12	1:A:81:ILE:HG21	0.58	1.58	5	2
1:A:85:THR:HB	1:A:199:LEU:HB3	0.57	1.75	11	3
1:A:57:GLU:HG2	1:A:202:LEU:HD21	0.55	1.79	5	5
1:A:25:GLU:HB3	1:A:42:ILE:HG21	0.54	1.78	18	3
1:A:36:GLY:HA2	1:A:184:LEU:HD11	0.54	1.78	5	2
1:A:46:LYS:NZ	1:A:188:MET:HB2	0.54	2.17	5	1
1:A:11:MET:SD	1:A:60:ARG:NH1	0.54	2.81	5	3
1:A:78:TRP:NE1	1:A:206:GLN:HG3	0.53	2.19	1	1
1:A:25:GLU:HB2	1:A:42:ILE:HG21	0.53	1.80	5	3
1:A:29:LEU:HD11	1:A:188:MET:SD	0.52	2.44	13	2
1:A:71:ASN:HD22	1:A:74:ILE:HG13	0.52	1.65	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HG	1:A:63:GLU:HG2	0.51	1.81	4	1
1:A:82:THR:HG23	1:A:206:GLN:HG2	0.51	1.81	17	1
1:A:39:LEU:HB2	1:A:184:LEU:HD13	0.50	1.84	11	7
1:A:11:MET:HA	1:A:56:LEU:HD13	0.50	1.83	7	3
1:A:60:ARG:NH2	1:A:202:LEU:HD22	0.50	2.21	2	4
1:A:89:ARG:HG3	1:A:196:GLU:HG3	0.49	1.83	6	1
1:A:89:ARG:HG2	1:A:196:GLU:HG3	0.49	1.83	20	2
1:A:25:GLU:HG3	1:A:188:MET:SD	0.49	2.47	12	3
1:A:29:LEU:HB3	1:A:98:LEU:HB3	0.49	1.84	7	1
1:A:102:GLN:HA	1:A:105:ARG:HB3	0.49	1.84	10	1
1:A:34:ILE:HG23	1:A:39:LEU:HD12	0.48	1.83	5	3
1:A:11:MET:SD	1:A:60:ARG:HD3	0.48	2.49	20	1
1:A:31:VAL:HG23	1:A:33:GLN:H	0.48	1.68	17	3
1:A:22:MET:SD	1:A:46:LYS:HE3	0.48	2.48	18	2
1:A:4:LEU:HB2	1:A:74:ILE:HD13	0.48	1.86	9	1
1:A:92:ASN:HB3	1:A:192:CYS:SG	0.48	2.49	8	1
1:A:195:ALA:O	1:A:199:LEU:HG	0.47	2.09	5	9
1:A:71:ASN:HD21	1:A:73:ASP:HB2	0.47	1.68	13	1
1:A:89:ARG:NH2	1:A:93:GLN:HE21	0.47	2.06	14	1
1:A:29:LEU:HD12	1:A:95:ASN:HB2	0.47	1.87	8	1
1:A:71:ASN:ND2	1:A:73:ASP:HB3	0.47	2.24	17	1
1:A:99:LEU:HD22	1:A:185:LEU:HB3	0.47	1.86	19	4
1:A:57:GLU:HG3	1:A:202:LEU:HD21	0.47	1.85	17	1
1:A:25:GLU:O	1:A:29:LEU:HG	0.47	2.10	1	2
1:A:11:MET:SD	1:A:60:ARG:HD2	0.47	2.50	12	1
1:A:22:MET:HG2	1:A:46:LYS:HD3	0.46	1.87	5	1
1:A:60:ARG:NH1	1:A:202:LEU:HD22	0.46	2.25	5	1
1:A:8:LEU:HD21	1:A:60:ARG:HD3	0.46	1.86	19	1
1:A:12:THR:HA	1:A:15:LEU:HD12	0.46	1.88	2	2
1:A:95:ASN:O	1:A:99:LEU:HG	0.46	2.11	2	2
1:A:8:LEU:HD11	1:A:74:ILE:HG23	0.46	1.88	3	3
1:A:46:LYS:HZ1	1:A:188:MET:HB2	0.45	1.71	5	1
1:A:78:TRP:HB3	1:A:206:GLN:HG2	0.45	1.87	8	1
1:A:92:ASN:HA	1:A:95:ASN:OD1	0.44	2.13	11	2
1:A:22:MET:HA	1:A:25:GLU:HG2	0.44	1.89	17	2
1:A:80:ALA:O	1:A:84:LYS:HD3	0.44	2.12	10	2
1:A:32:GLY:HA2	1:A:102:GLN:NE2	0.44	2.28	19	1
1:A:85:THR:HG22	1:A:199:LEU:HD22	0.44	1.87	17	6
1:A:78:TRP:HE1	1:A:206:GLN:HB2	0.44	1.72	15	1
1:A:101:GLY:O	1:A:105:ARG:HG2	0.44	2.12	13	1
1:A:94:HIS:O	1:A:98:LEU:HG	0.44	2.13	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:LEU:HA	1:A:188:MET:HG2	0.44	1.89	5	1
1:A:34:ILE:HD11	1:A:102:GLN:HG2	0.43	1.90	16	1
1:A:56:LEU:O	1:A:60:ARG:HB2	0.43	2.14	11	1
1:A:28:GLN:O	1:A:31:VAL:HG22	0.43	2.13	15	1
1:A:14:VAL:HG13	1:A:49:LEU:HB3	0.43	1.90	20	2
1:A:84:LYS:O	1:A:88:LEU:HG	0.42	2.14	18	1
1:A:17:ASP:O	1:A:21:VAL:HG23	0.42	2.15	20	1
1:A:22:MET:SD	1:A:46:LYS:NZ	0.42	2.91	12	1
1:A:4:LEU:O	1:A:8:LEU:HG	0.42	2.14	6	4
1:A:89:ARG:NH1	1:A:93:GLN:HB2	0.42	2.29	1	1
1:A:92:ASN:ND2	1:A:196:GLU:HB2	0.42	2.30	3	1
1:A:198:GLN:O	1:A:202:LEU:HG	0.42	2.14	20	1
1:A:103:ILE:O	1:A:107:GLN:HB2	0.42	2.15	9	1
1:A:77:ARG:O	1:A:81:ILE:HG13	0.41	2.15	14	1
1:A:4:LEU:HD12	1:A:67:GLN:NE2	0.41	2.30	5	1
1:A:63:GLU:O	1:A:67:GLN:HB2	0.41	2.15	7	1
1:A:106:ASN:HD21	1:A:177:GLU:HB3	0.41	1.73	14	1
1:A:78:TRP:O	1:A:82:THR:HG23	0.41	2.15	15	1
1:A:39:LEU:HD23	1:A:42:ILE:HD12	0.41	1.91	18	1
1:A:38:GLN:HE21	1:A:42:ILE:HD11	0.41	1.75	11	1
1:A:38:GLN:O	1:A:42:ILE:HG13	0.41	2.15	3	1
1:A:15:LEU:HB3	1:A:84:LYS:HB3	0.41	1.93	7	1
1:A:194:GLN:O	1:A:198:GLN:HB2	0.41	2.16	2	1
1:A:11:MET:O	1:A:15:LEU:HG	0.41	2.16	8	1
1:A:202:LEU:O	1:A:206:GLN:HB2	0.41	2.16	1	1
1:A:55:TYR:O	1:A:59:GLN:HG2	0.41	2.16	19	1
1:A:175:GLU:HG3	1:A:176:LYS:H	0.40	1.76	3	1
1:A:56:LEU:HD23	1:A:59:GLN:NE2	0.40	2.32	5	1
1:A:186:GLY:O	1:A:190:ARG:HG2	0.40	2.15	5	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	141/214 (66%)	135±2 (96±1%)	5±2 (3±1%)	1±1 (1±1%)	26 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2820/4280 (66%)	2706 (96%)	94 (3%)	20 (1%)	26 73

All 6 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	69	SER	6
1	A	70	ALA	4
1	A	207	ASN	4
1	A	3	ARG	3
1	A	175	GLU	2
1	A	71	ASN	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	125/182 (69%)	118±2 (94±2%)	7±2 (6±2%)	24 73
All	All	2500/3640 (69%)	2356 (94%)	144 (6%)	24 73

All 47 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	205	TYR	12
1	A	55	TYR	9
1	A	201	MET	9
1	A	19	LYS	8
1	A	64	GLN	6
1	A	26	GLN	5
1	A	57	GLU	5
1	A	60	ARG	5
1	A	206	GLN	5
1	A	77	ARG	5
1	A	89	ARG	4
1	A	176	LYS	4
1	A	35	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	63	GLU	4
1	A	68	ARG	3
1	A	200	LYS	3
1	A	92	ASN	3
1	A	3	ARG	3
1	A	41	ARG	3
1	A	104	GLU	3
1	A	65	ASN	3
1	A	84	LYS	3
1	A	177	GLU	2
1	A	76	GLU	2
1	A	97	TRP	2
1	A	107	GLN	2
1	A	83	GLU	2
1	A	95	ASN	2
1	A	207	ASN	2
1	A	40	GLN	2
1	A	187	GLU	2
1	A	198	GLN	2
1	A	108	GLN	1
1	A	61	ARG	1
1	A	44	GLU	1
1	A	105	ARG	1
1	A	27	GLN	1
1	A	175	GLU	1
1	A	28	GLN	1
1	A	71	ASN	1
1	A	45	GLU	1
1	A	78	TRP	1
1	A	17	ASP	1
1	A	93	GLN	1
1	A	193	GLN	1
1	A	6	GLU	1
1	A	183	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 47% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1258
Number of shifts mapped to atoms	1258
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	185	-0.95 ± 0.06	Should be checked
$^{13}C_{\beta}$	173	0.42 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	172	-0.65 ± 0.09	Should be applied
^{15}N	168	-0.16 ± 0.10	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 47%, i.e. 942 atoms were assigned a chemical shift out of a possible 1995. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	523/711 (74%)	128/288 (44%)	267/282 (95%)	128/141 (91%)
Sidechain	399/1226 (33%)	210/782 (27%)	189/377 (50%)	0/67 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	20/58 (34%)	10/28 (36%)	8/24 (33%)	2/6 (33%)
Overall	942/1995 (47%)	348/1098 (32%)	464/683 (68%)	130/214 (61%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 1258 atoms were assigned a chemical shift out of a possible 2937. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	693/1079 (64%)	168/441 (38%)	357/428 (83%)	168/210 (80%)
Sidechain	527/1748 (30%)	276/1123 (25%)	251/539 (47%)	0/86 (0%)
Aromatic	38/110 (35%)	19/53 (36%)	17/45 (38%)	2/12 (17%)
Overall	1258/2937 (43%)	463/1617 (29%)	625/1012 (62%)	170/308 (55%)

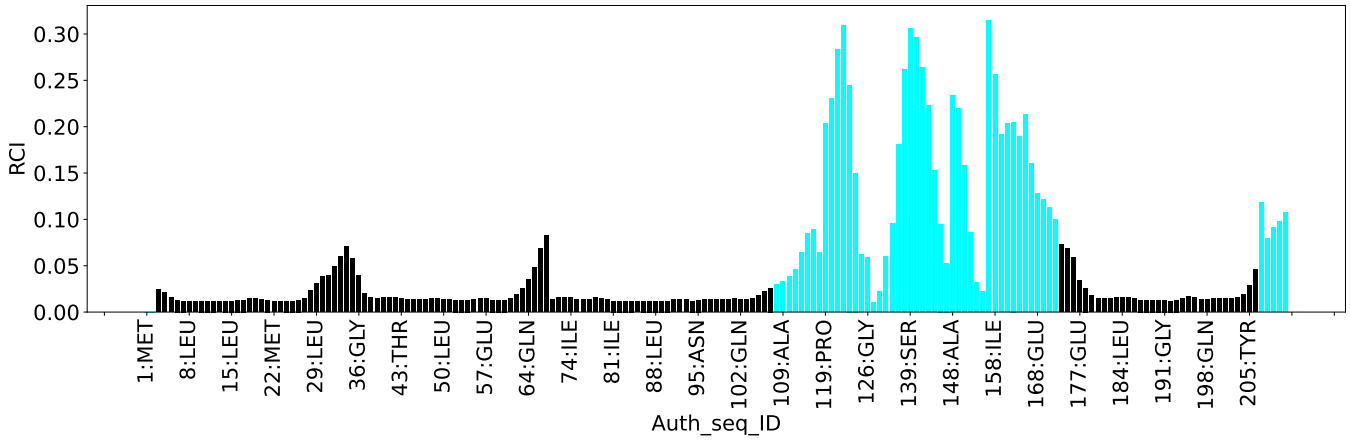
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1498
Intra-residue (|i-j|=0)	67
Sequential (|i-j|=1)	334
Medium range (|i-j|>1 and |i-j|<5)	466
Long range (|i-j|≥5)	357
Inter-chain	0
Hydrogen bond restraints	274
Disulfide bond restraints	0
Total dihedral-angle restraints	282
Number of unmapped restraints	0
Number of restraints per residue	8.3
Number of long range restraints per residue[1]	1.7

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	15.8	0.2
0.2-0.5 (Medium)	4.8	0.47
>0.5 (Large)	0.1	3.5

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)	11.2	9.26
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

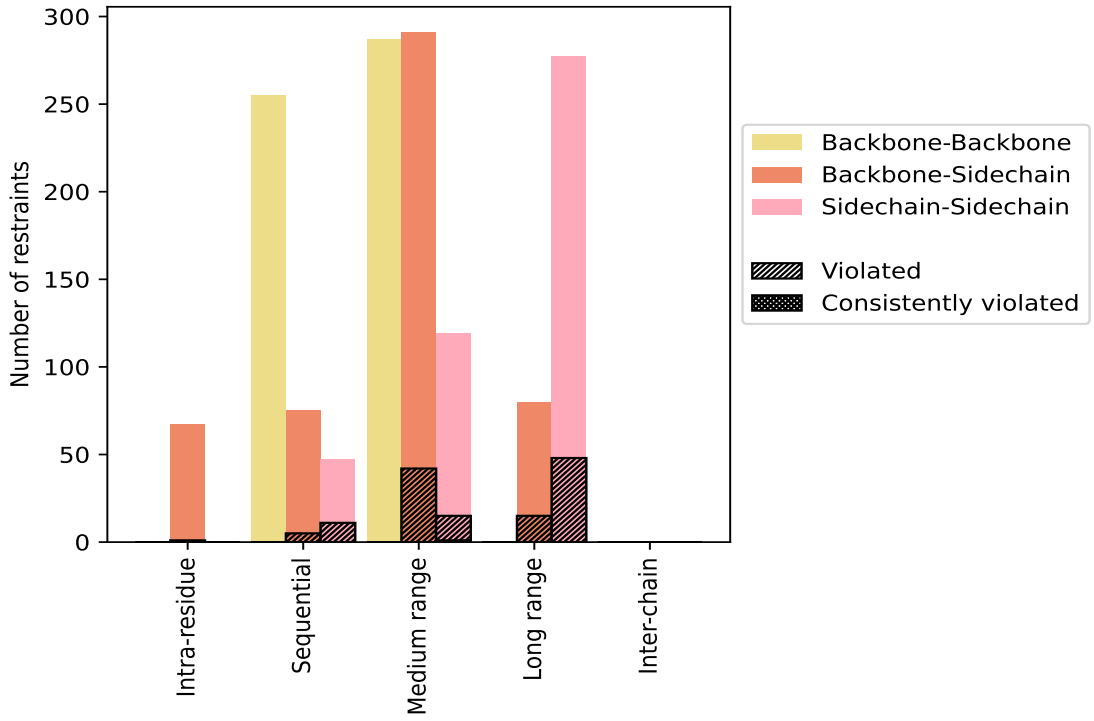
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	67	4.5	1	1.5	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	67	4.5	1	1.5	0.1	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	334	22.3	16	4.8	1.1	0	0.0	0.0
Backbone-Backbone	212	14.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	75	5.0	5	6.7	0.3	0	0.0	0.0
Sidechain-Sidechain	47	3.1	11	23.4	0.7	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	466	31.1	24	5.2	1.6	1	0.2	0.1
Backbone-Backbone	286	19.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	61	4.1	9	14.8	0.6	0	0.0	0.0
Sidechain-Sidechain	119	7.9	15	12.6	1.0	1	0.8	0.1
Long range (|i-j|≥5)	357	23.8	63	17.6	4.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	80	5.3	15	18.8	1.0	0	0.0	0.0
Sidechain-Sidechain	277	18.5	48	17.3	3.2	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	274	18.3	33	12.0	2.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1498	100.0	137	9.1	9.1	1	0.1	0.1
Backbone-Backbone	542	36.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	513	34.2	63	12.3	4.2	0	0.0	0.0
Sidechain-Sidechain	443	29.6	74	16.7	4.9	1	0.2	0.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	3	10	15	0	28	0.16	0.42	0.07	0.14
2	0	3	12	9	0	24	0.16	0.34	0.06	0.14
3	0	1	10	10	0	21	0.15	0.29	0.05	0.14
4	0	2	13	12	0	27	0.15	0.25	0.04	0.15
5	0	1	8	8	0	17	0.15	0.27	0.04	0.13
6	0	7	15	14	0	36	0.25	3.5	0.55	0.13
7	0	2	11	15	0	28	0.2	0.65	0.13	0.15
8	0	1	10	4	0	15	0.17	0.28	0.05	0.16
9	0	1	11	9	0	21	0.18	0.28	0.05	0.17
10	0	1	12	7	0	20	0.18	0.38	0.08	0.14
11	0	2	10	8	0	20	0.18	0.47	0.1	0.14

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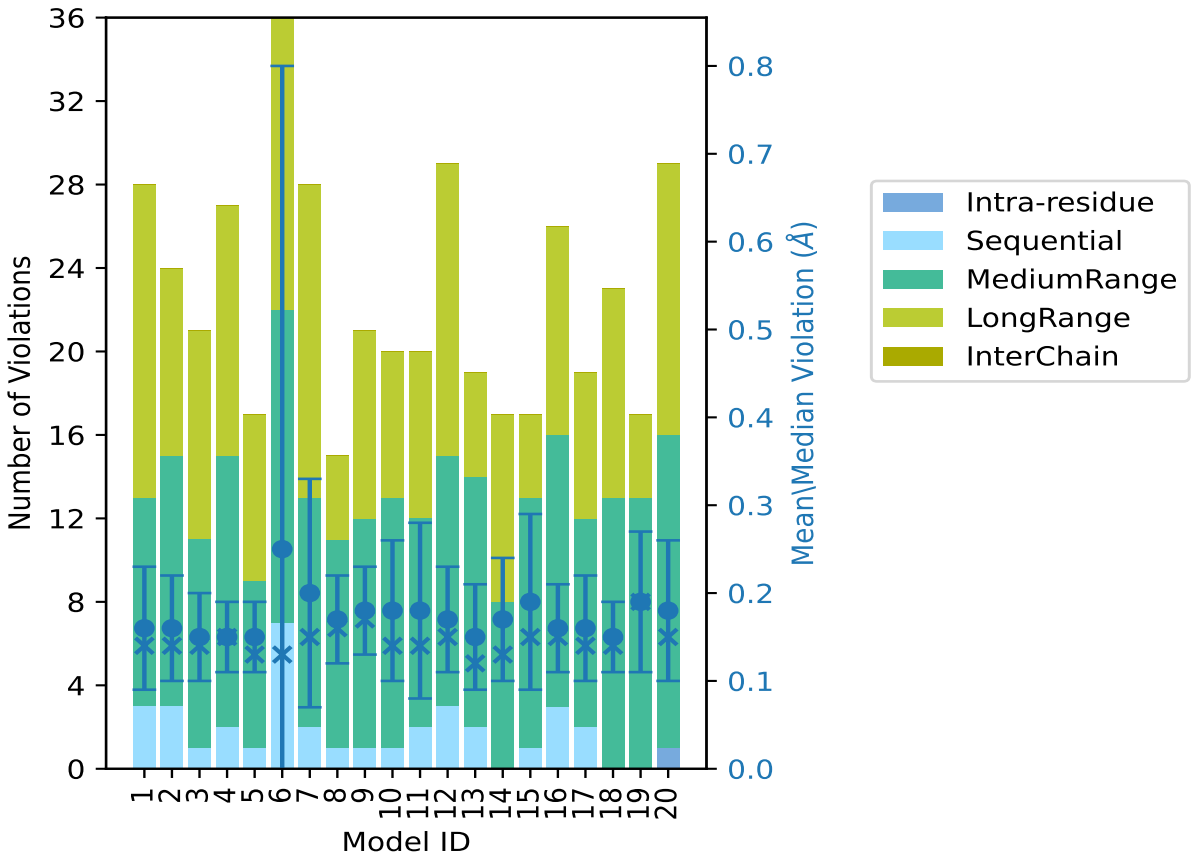
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	3	12	14	0	29	0.17	0.34	0.06	0.15
13	0	2	12	5	0	19	0.15	0.29	0.06	0.12
14	0	0	8	9	0	17	0.17	0.37	0.07	0.13
15	0	1	12	4	0	17	0.19	0.45	0.1	0.15
16	0	3	13	10	0	26	0.16	0.31	0.05	0.15
17	0	2	10	7	0	19	0.16	0.34	0.06	0.14
18	0	0	13	10	0	23	0.15	0.25	0.04	0.14
19	0	0	13	4	0	17	0.19	0.36	0.08	0.19
20	1	0	15	13	0	29	0.18	0.38	0.08	0.15

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

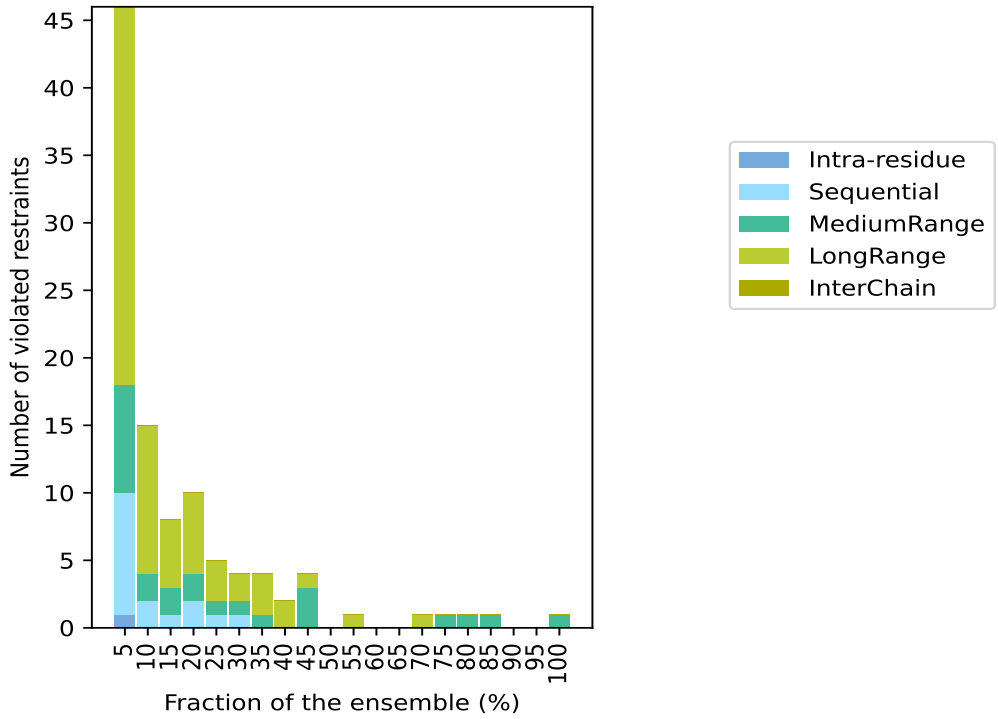
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1120(IR:66, SQ:318, MR:442, LR:294, 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]	%
1	9	8	28	0	46	1	5.0
0	2	2	11	0	15	2	10.0
0	1	2	5	0	8	3	15.0
0	2	2	6	0	10	4	20.0
0	1	1	3	0	5	5	25.0
0	1	1	2	0	4	6	30.0
0	0	1	3	0	4	7	35.0
0	0	0	2	0	2	8	40.0
0	0	3	1	0	4	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	1	0	1	14	70.0
0	0	1	0	0	1	15	75.0
0	0	1	0	0	1	16	80.0
0	0	1	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	1	0	0	1	20	100.0

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

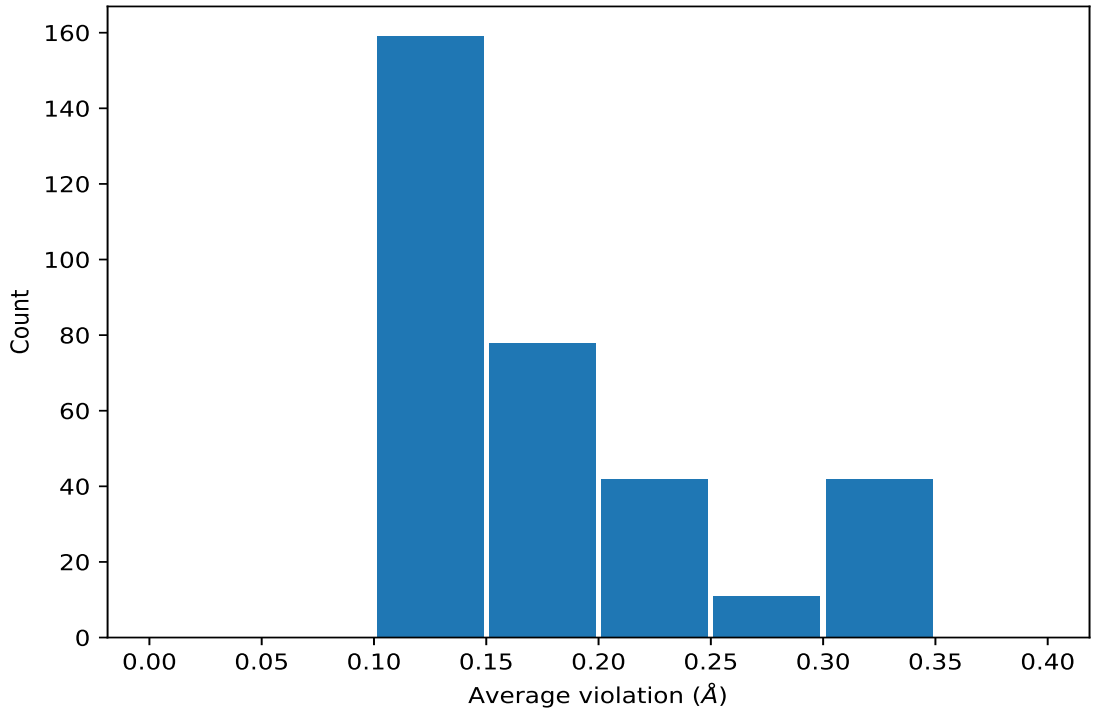
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of 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)
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	20	0.25	0.08	0.24
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	20	0.25	0.08	0.24
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	20	0.25	0.08	0.24
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	17	0.18	0.09	0.15
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	17	0.18	0.09	0.15
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	17	0.18	0.09	0.15
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	17	0.15	0.03	0.14
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	16	0.22	0.04	0.22
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	16	0.22	0.04	0.22
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	16	0.22	0.04	0.22
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	15	0.17	0.04	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	15	0.17	0.04	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	15	0.17	0.04	0.18
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	14	0.16	0.06	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	14	0.16	0.06	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	14	0.16	0.06	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	14	0.16	0.06	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	14	0.16	0.06	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	14	0.16	0.06	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	14	0.16	0.06	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	14	0.16	0.06	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	14	0.16	0.06	0.13
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	11	0.15	0.04	0.15
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	11	0.15	0.04	0.15
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	11	0.15	0.04	0.15
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	11	0.15	0.04	0.15
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	11	0.15	0.04	0.15
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	11	0.15	0.04	0.15
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	11	0.15	0.04	0.15
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	11	0.15	0.04	0.15
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	11	0.15	0.04	0.15
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	10	0.13	0.02	0.13
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	9	0.25	0.08	0.25
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	9	0.25	0.08	0.25
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	9	0.25	0.08	0.25
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	9	0.2	0.03	0.19
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	9	0.2	0.03	0.19
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	9	0.2	0.03	0.19
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	9	0.2	0.03	0.19
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	9	0.2	0.03	0.19
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	9	0.2	0.03	0.19
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	9	0.2	0.03	0.19
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	9	0.2	0.03	0.19
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	9	0.2	0.03	0.19
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	9	0.16	0.03	0.17
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	9	0.16	0.03	0.17
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	9	0.16	0.03	0.17
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	9	0.14	0.02	0.14
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	9	0.14	0.02	0.14
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	9	0.14	0.02	0.14
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	8	0.31	0.13	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	8	0.31	0.13	0.26
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	8	0.31	0.13	0.26
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	8	0.15	0.06	0.13
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	8	0.15	0.06	0.13
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	8	0.15	0.06	0.13
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD21	7	0.19	0.05	0.22
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD22	7	0.19	0.05	0.22
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD23	7	0.19	0.05	0.22
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD11	7	0.18	0.04	0.17
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD12	7	0.18	0.04	0.17
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD13	7	0.18	0.04	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD11	7	0.18	0.04	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD12	7	0.18	0.04	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD13	7	0.18	0.04	0.17
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD11	7	0.18	0.04	0.17
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD12	7	0.18	0.04	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD13	7	0.18	0.04	0.17
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD21	7	0.14	0.04	0.13
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD22	7	0.14	0.04	0.13
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD23	7	0.14	0.04	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD21	7	0.14	0.04	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD22	7	0.14	0.04	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD23	7	0.14	0.04	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD21	7	0.14	0.04	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD22	7	0.14	0.04	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD23	7	0.14	0.04	0.13
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD11	7	0.13	0.02	0.12
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD12	7	0.13	0.02	0.12
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD13	7	0.13	0.02	0.12
(1,188)	1:8:A:LEU:HD11	1:74:A:ILE:CD1	6	0.19	0.06	0.18
(1,188)	1:8:A:LEU:HD12	1:74:A:ILE:CD1	6	0.19	0.06	0.18
(1,188)	1:8:A:LEU:HD13	1:74:A:ILE:CD1	6	0.19	0.06	0.18
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG21	6	0.18	0.06	0.18
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG22	6	0.18	0.06	0.18
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG23	6	0.18	0.06	0.18
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD11	6	0.16	0.01	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD12	6	0.16	0.01	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD13	6	0.16	0.01	0.15
(4,183)	1:179:A:ASP:O	1:183:A:ARG:H	6	0.14	0.02	0.14
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD21	6	0.13	0.02	0.12
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD22	6	0.13	0.02	0.12
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD23	6	0.13	0.02	0.12
(4,25)	1:16:A:ASN:O	1:20:A:THR:H	6	0.11	0.01	0.11
(1,32)	1:202:A:LEU:HD21	1:205:A:TYR:CE2	5	0.19	0.06	0.22
(1,32)	1:202:A:LEU:HD22	1:205:A:TYR:CE2	5	0.19	0.06	0.22
(1,32)	1:202:A:LEU:HD23	1:205:A:TYR:CE2	5	0.19	0.06	0.22
(1,546)	1:201:A:MET:HE1	1:202:A:LEU:H	5	0.18	0.05	0.19
(1,546)	1:201:A:MET:HE2	1:202:A:LEU:H	5	0.18	0.05	0.19
(1,546)	1:201:A:MET:HE3	1:202:A:LEU:H	5	0.18	0.05	0.19
(1,961)	1:110:A:LEU:HD11	1:143:A:PHE:HE1	5	0.16	0.04	0.18
(1,961)	1:110:A:LEU:HD12	1:143:A:PHE:HE1	5	0.16	0.04	0.18
(1,961)	1:110:A:LEU:HD13	1:143:A:PHE:HE1	5	0.16	0.04	0.18
(1,961)	1:110:A:LEU:HD21	1:143:A:PHE:HE1	5	0.16	0.04	0.18
(1,961)	1:110:A:LEU:HD22	1:143:A:PHE:HE1	5	0.16	0.04	0.18
(1,961)	1:110:A:LEU:HD23	1:143:A:PHE:HE1	5	0.16	0.04	0.18
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD11	5	0.15	0.06	0.12
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD12	5	0.15	0.06	0.12
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD13	5	0.15	0.06	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,167)	1:107:A:GLN:O	1:111:A:GLU:H	5	0.14	0.03	0.14
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB1	5	0.12	0.01	0.12
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB2	5	0.12	0.01	0.12
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB3	5	0.12	0.01	0.12
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB1	5	0.12	0.01	0.12
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB2	5	0.12	0.01	0.12
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB3	5	0.12	0.01	0.12
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB1	5	0.12	0.01	0.12
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB2	5	0.12	0.01	0.12
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB3	5	0.12	0.01	0.12
(4,49)	1:40:A:GLN:O	1:44:A:GLU:H	5	0.12	0.01	0.11
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD11	4	0.23	0.03	0.23
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD12	4	0.23	0.03	0.23
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD13	4	0.23	0.03	0.23
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD21	4	0.23	0.03	0.23
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD22	4	0.23	0.03	0.23
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD23	4	0.23	0.03	0.23
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD1	4	0.18	0.04	0.18
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD2	4	0.18	0.04	0.18
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD1	4	0.18	0.04	0.18
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD2	4	0.18	0.04	0.18
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD1	4	0.18	0.04	0.18
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD2	4	0.18	0.04	0.18
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD21	4	0.17	0.02	0.16
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD22	4	0.17	0.02	0.16
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD23	4	0.17	0.02	0.16
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG21	4	0.16	0.06	0.16
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG22	4	0.16	0.06	0.16
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG23	4	0.16	0.06	0.16
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD21	4	0.15	0.02	0.15
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD22	4	0.15	0.02	0.15
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD23	4	0.15	0.02	0.15
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD21	4	0.15	0.02	0.15
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD22	4	0.15	0.02	0.15
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD23	4	0.15	0.02	0.15
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD21	4	0.15	0.02	0.15
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD22	4	0.15	0.02	0.15
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD23	4	0.15	0.02	0.15
(1,87)	1:22:A:MET:HE1	1:91:A:LEU:CD1	4	0.14	0.01	0.14
(1,87)	1:22:A:MET:HE2	1:91:A:LEU:CD1	4	0.14	0.01	0.14
(1,87)	1:22:A:MET:HE3	1:91:A:LEU:CD1	4	0.14	0.01	0.14
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD11	4	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD12	4	0.13	0.02	0.12
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD13	4	0.13	0.02	0.12
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD11	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD12	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD13	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD21	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD22	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD23	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD11	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD12	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD13	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD21	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD22	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD23	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD11	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD12	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD13	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD21	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD22	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD23	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD11	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD12	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD13	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD21	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD22	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD23	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD11	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD12	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD13	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD21	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD22	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD23	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD11	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD12	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD13	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD21	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD22	4	0.12	0.02	0.13
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD23	4	0.12	0.02	0.13
(1,389)	1:21:A:VAL:HG11	1:45:A:GLU:H	4	0.12	0.01	0.12
(1,389)	1:21:A:VAL:HG12	1:45:A:GLU:H	4	0.12	0.01	0.12
(1,389)	1:21:A:VAL:HG13	1:45:A:GLU:H	4	0.12	0.01	0.12
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD11	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD12	4	0.12	0.01	0.12
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD13	4	0.12	0.01	0.12
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD11	4	0.12	0.01	0.12
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD12	4	0.12	0.01	0.12
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD13	4	0.12	0.01	0.12
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD11	4	0.12	0.01	0.12
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD12	4	0.12	0.01	0.12
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD13	4	0.12	0.01	0.12
(4,191)	1:183:A:ARG:O	1:187:A:GLU:H	4	0.11	0.01	0.11
(1,960)	1:110:A:LEU:HD11	1:143:A:PHE:CE1	3	0.35	0.23	0.29
(1,960)	1:110:A:LEU:HD12	1:143:A:PHE:CE1	3	0.35	0.23	0.29
(1,960)	1:110:A:LEU:HD13	1:143:A:PHE:CE1	3	0.35	0.23	0.29
(1,960)	1:110:A:LEU:HD21	1:143:A:PHE:CE1	3	0.35	0.23	0.29
(1,960)	1:110:A:LEU:HD22	1:143:A:PHE:CE1	3	0.35	0.23	0.29
(1,960)	1:110:A:LEU:HD23	1:143:A:PHE:CE1	3	0.35	0.23	0.29
(1,13)	1:141:A:VAL:HG21	1:143:A:PHE:CD1	3	0.3	0.14	0.33
(1,13)	1:141:A:VAL:HG22	1:143:A:PHE:CD1	3	0.3	0.14	0.33
(1,13)	1:141:A:VAL:HG23	1:143:A:PHE:CD1	3	0.3	0.14	0.33
(1,547)	1:201:A:MET:HE1	1:205:A:TYR:H	3	0.2	0.11	0.14
(1,547)	1:201:A:MET:HE2	1:205:A:TYR:H	3	0.2	0.11	0.14
(1,547)	1:201:A:MET:HE3	1:205:A:TYR:H	3	0.2	0.11	0.14
(1,3)	1:74:A:ILE:HD11	1:209:A:TYR:CD1	3	0.16	0.02	0.16
(1,3)	1:74:A:ILE:HD12	1:209:A:TYR:CD1	3	0.16	0.02	0.16
(1,3)	1:74:A:ILE:HD13	1:209:A:TYR:CD1	3	0.16	0.02	0.16
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD11	3	0.13	0.02	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD12	3	0.13	0.02	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD13	3	0.13	0.02	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD21	3	0.13	0.02	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD22	3	0.13	0.02	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD23	3	0.13	0.02	0.12
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE1	3	0.12	0.01	0.12
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE2	3	0.12	0.01	0.12
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE3	3	0.12	0.01	0.12
(1,414)	1:188:A:MET:HE1	1:189:A:ARG:H	3	0.12	0.0	0.12
(1,414)	1:188:A:MET:HE2	1:189:A:ARG:H	3	0.12	0.0	0.12
(1,414)	1:188:A:MET:HE3	1:189:A:ARG:H	3	0.12	0.0	0.12
(4,91)	1:61:A:ARG:O	1:65:A:ASN:H	3	0.11	0.01	0.12
(1,277)	1:8:A:LEU:HD21	1:78:A:TRP:H	3	0.11	0.01	0.11
(1,277)	1:8:A:LEU:HD22	1:78:A:TRP:H	3	0.11	0.01	0.11
(1,277)	1:8:A:LEU:HD23	1:78:A:TRP:H	3	0.11	0.01	0.11
(1,518)	1:53:A:LEU:H	1:55:A:TYR:HD1	2	0.26	0.02	0.26
(1,518)	1:53:A:LEU:H	1:55:A:TYR:HD2	2	0.26	0.02	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,5)	1:74:A:ILE:HD11	1:209:A:TYR:CE1	2	0.24	0.05	0.24
(1,5)	1:74:A:ILE:HD12	1:209:A:TYR:CE1	2	0.24	0.05	0.24
(1,5)	1:74:A:ILE:HD13	1:209:A:TYR:CE1	2	0.24	0.05	0.24
(1,525)	1:14:A:VAL:HG21	1:55:A:TYR:HD1	2	0.24	0.05	0.24
(1,525)	1:14:A:VAL:HG21	1:55:A:TYR:HD2	2	0.24	0.05	0.24
(1,525)	1:14:A:VAL:HG22	1:55:A:TYR:HD1	2	0.24	0.05	0.24
(1,525)	1:14:A:VAL:HG22	1:55:A:TYR:HD2	2	0.24	0.05	0.24
(1,525)	1:14:A:VAL:HG23	1:55:A:TYR:HD1	2	0.24	0.05	0.24
(1,525)	1:14:A:VAL:HG23	1:55:A:TYR:HD2	2	0.24	0.05	0.24
(1,183)	1:112:A:VAL:HG21	1:158:A:ILE:CD1	2	0.22	0.01	0.22
(1,183)	1:112:A:VAL:HG22	1:158:A:ILE:CD1	2	0.22	0.01	0.22
(1,183)	1:112:A:VAL:HG23	1:158:A:ILE:CD1	2	0.22	0.01	0.22
(1,18)	1:141:A:VAL:HG11	1:143:A:PHE:CD1	2	0.21	0.07	0.21
(1,18)	1:141:A:VAL:HG12	1:143:A:PHE:CD1	2	0.21	0.07	0.21
(1,18)	1:141:A:VAL:HG13	1:143:A:PHE:CD1	2	0.21	0.07	0.21
(1,963)	1:110:A:LEU:HD11	1:143:A:PHE:HE2	2	0.21	0.05	0.21
(1,963)	1:110:A:LEU:HD12	1:143:A:PHE:HE2	2	0.21	0.05	0.21
(1,963)	1:110:A:LEU:HD13	1:143:A:PHE:HE2	2	0.21	0.05	0.21
(1,963)	1:110:A:LEU:HD21	1:143:A:PHE:HE2	2	0.21	0.05	0.21
(1,963)	1:110:A:LEU:HD22	1:143:A:PHE:HE2	2	0.21	0.05	0.21
(1,963)	1:110:A:LEU:HD23	1:143:A:PHE:HE2	2	0.21	0.05	0.21
(1,455)	1:8:A:LEU:HD11	1:74:A:ILE:H	2	0.18	0.06	0.18
(1,455)	1:8:A:LEU:HD12	1:74:A:ILE:H	2	0.18	0.06	0.18
(1,455)	1:8:A:LEU:HD13	1:74:A:ILE:H	2	0.18	0.06	0.18
(1,984)	1:142:A:LEU:HD11	1:143:A:PHE:CE1	2	0.16	0.06	0.16
(1,984)	1:142:A:LEU:HD12	1:143:A:PHE:CE1	2	0.16	0.06	0.16
(1,984)	1:142:A:LEU:HD13	1:143:A:PHE:CE1	2	0.16	0.06	0.16
(1,984)	1:142:A:LEU:HD21	1:143:A:PHE:CE1	2	0.16	0.06	0.16
(1,984)	1:142:A:LEU:HD22	1:143:A:PHE:CE1	2	0.16	0.06	0.16
(1,984)	1:142:A:LEU:HD23	1:143:A:PHE:CE1	2	0.16	0.06	0.16
(1,247)	1:21:A:VAL:HG11	1:42:A:ILE:CD1	2	0.16	0.01	0.16
(1,247)	1:21:A:VAL:HG12	1:42:A:ILE:CD1	2	0.16	0.01	0.16
(1,247)	1:21:A:VAL:HG13	1:42:A:ILE:CD1	2	0.16	0.01	0.16
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD11	2	0.14	0.0	0.14
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD12	2	0.14	0.0	0.14
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD13	2	0.14	0.0	0.14
(4,31)	1:19:A:LYS:O	1:23:A:ASP:H	2	0.14	0.02	0.14
(1,94)	1:34:A:ILE:HD11	1:39:A:LEU:CD2	2	0.13	0.02	0.13
(1,94)	1:34:A:ILE:HD12	1:39:A:LEU:CD2	2	0.13	0.02	0.13
(1,94)	1:34:A:ILE:HD13	1:39:A:LEU:CD2	2	0.13	0.02	0.13
(1,6)	1:74:A:ILE:HD11	1:209:A:TYR:CE2	2	0.12	0.01	0.12
(1,6)	1:74:A:ILE:HD12	1:209:A:TYR:CE2	2	0.12	0.01	0.12

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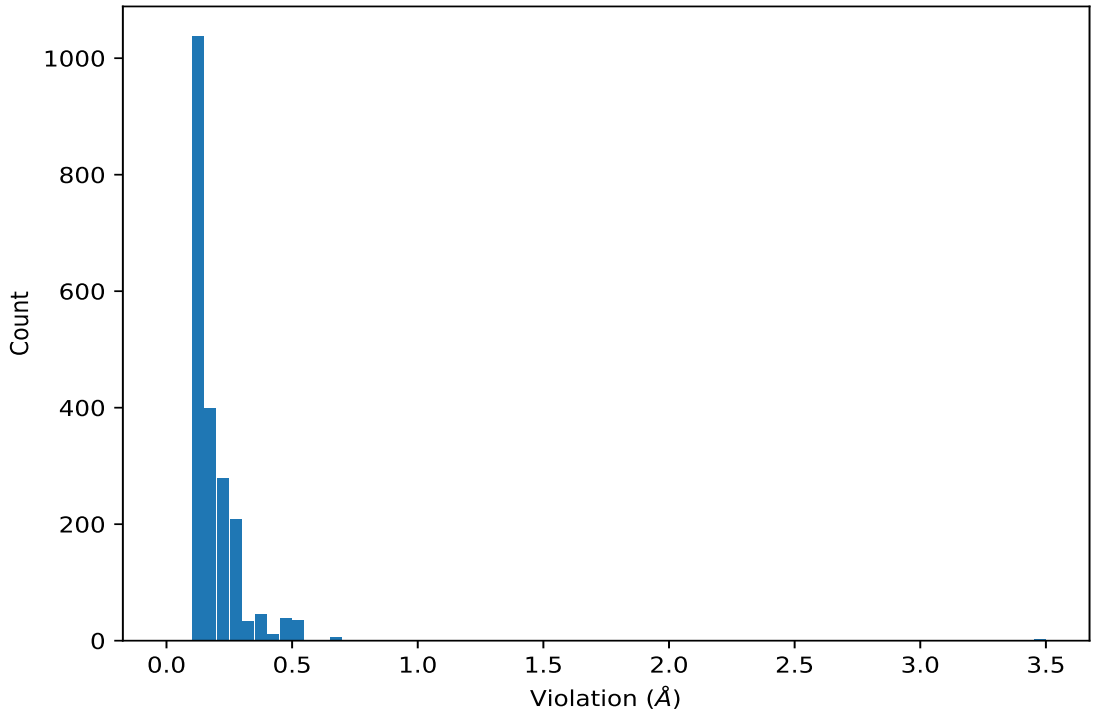
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,6)	1:74:A:ILE:HD13	1:209:A:TYR:CE2	2	0.12	0.01	0.12
(1,72)	1:11:A:MET:HE1	1:199:A:LEU:CD2	2	0.12	0.01	0.12
(1,72)	1:11:A:MET:HE2	1:199:A:LEU:CD2	2	0.12	0.01	0.12
(1,72)	1:11:A:MET:HE3	1:199:A:LEU:CD2	2	0.12	0.01	0.12
(4,93)	1:62:A:LEU:O	1:66:A:ALA:H	2	0.12	0.01	0.12
(4,229)	1:202:A:LEU:O	1:206:A:GLN:H	2	0.12	0.01	0.12
(4,175)	1:175:A:GLU:O	1:179:A:ASP:H	2	0.12	0.0	0.12
(4,211)	1:193:A:GLN:O	1:197:A:GLU:H	2	0.12	0.01	0.12
(4,217)	1:196:A:GLU:O	1:200:A:LYS:H	2	0.12	0.01	0.12
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD11	2	0.12	0.0	0.12
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD12	2	0.12	0.0	0.12
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD13	2	0.12	0.0	0.12
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD11	2	0.12	0.0	0.12
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD12	2	0.12	0.0	0.12
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD13	2	0.12	0.0	0.12
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB1	2	0.11	0.0	0.11
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB2	2	0.11	0.0	0.11
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB3	2	0.11	0.0	0.11
(4,13)	1:10:A:GLN:O	1:14:A:VAL:H	2	0.11	0.0	0.11
(4,17)	1:12:A:THR:O	1:16:A:ASN:H	2	0.11	0.0	0.11
(4,223)	1:199:A:LEU:O	1:203:A:ILE:H	2	0.11	0.0	0.11
(4,131)	1:89:A:ARG:O	1:93:A:GLN:H	2	0.1	0.0	0.1

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,528)	1:143:A:PHE:HE1	1:174:A:ALA:HB1	6	3.5
(1,528)	1:143:A:PHE:HE1	1:174:A:ALA:HB2	6	3.5
(1,528)	1:143:A:PHE:HE1	1:174:A:ALA:HB3	6	3.5
(1,960)	1:110:A:LEU:HD11	1:143:A:PHE:CE1	7	0.65
(1,960)	1:110:A:LEU:HD12	1:143:A:PHE:CE1	7	0.65
(1,960)	1:110:A:LEU:HD13	1:143:A:PHE:CE1	7	0.65
(1,960)	1:110:A:LEU:HD21	1:143:A:PHE:CE1	7	0.65
(1,960)	1:110:A:LEU:HD22	1:143:A:PHE:CE1	7	0.65
(1,960)	1:110:A:LEU:HD23	1:143:A:PHE:CE1	7	0.65
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	7	0.54
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	7	0.54
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	7	0.54
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	7	0.54
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	7	0.54
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	7	0.54
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	7	0.54
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	7	0.54
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	7	0.54
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	7	0.54
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	7	0.54
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	7	0.54
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	7	0.54
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	7	0.54
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	7	0.54
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	7	0.54
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	7	0.54
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	7	0.54
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	7	0.54
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	7	0.54
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	7	0.54
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	7	0.54
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	7	0.54
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	7	0.54
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	7	0.54
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	7	0.54
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	7	0.54
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	7	0.54
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	7	0.54
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	7	0.54
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	7	0.54
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	7	0.54
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	7	0.54
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	7	0.54
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	7	0.54
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	11	0.47
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	11	0.47
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	11	0.47
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	11	0.47
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	11	0.47
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	11	0.47
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	11	0.47
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	11	0.47
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	11	0.47
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	11	0.47
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	11	0.47
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	11	0.47
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	11	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	11	0.47
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	11	0.47
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	11	0.47
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	11	0.47
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	11	0.47
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	11	0.47
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	11	0.47
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	11	0.47
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	11	0.47
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	11	0.47
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	11	0.47
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	11	0.47
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	11	0.47
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	11	0.47
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	11	0.47
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	11	0.47
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	11	0.47
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	11	0.47
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	11	0.47
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	11	0.47
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	11	0.47
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	11	0.47
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	11	0.47
(1,13)	1:141:A:VAL:HG21	1:143:A:PHE:CD1	15	0.45
(1,13)	1:141:A:VAL:HG22	1:143:A:PHE:CD1	15	0.45
(1,13)	1:141:A:VAL:HG23	1:143:A:PHE:CD1	15	0.45
(1,985)	1:142:A:LEU:HD11	1:143:A:PHE:HE1	6	0.44
(1,985)	1:142:A:LEU:HD12	1:143:A:PHE:HE1	6	0.44
(1,985)	1:142:A:LEU:HD13	1:143:A:PHE:HE1	6	0.44
(1,985)	1:142:A:LEU:HD21	1:143:A:PHE:HE1	6	0.44
(1,985)	1:142:A:LEU:HD22	1:143:A:PHE:HE1	6	0.44
(1,985)	1:142:A:LEU:HD23	1:143:A:PHE:HE1	6	0.44
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	1	0.42
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	1	0.42
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	1	0.42
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	15	0.4
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	15	0.4
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	15	0.4
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	10	0.38
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	10	0.38
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	10	0.38
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	10	0.38
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	10	0.38
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	10	0.38
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	10	0.38
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	10	0.38
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	10	0.38
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	10	0.38
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	10	0.38
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	10	0.38
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	10	0.38
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	10	0.38
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	10	0.38
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	10	0.38
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	10	0.38
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	10	0.38
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	10	0.38
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	10	0.38
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	10	0.38
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	10	0.38
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	10	0.38
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	10	0.38
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	10	0.38
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	10	0.38
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	10	0.38
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	10	0.38
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	10	0.38
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	10	0.38
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	10	0.38
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	10	0.38
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	10	0.38
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	10	0.38
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	10	0.38
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	20	0.38
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	20	0.38
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	20	0.38
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	14	0.37
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	14	0.37
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	14	0.37
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	19	0.36
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	19	0.36
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	19	0.36
(1,547)	1:201:A:MET:HE1	1:205:A:TYR:H	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:201:A:MET:HE2	1:205:A:TYR:H	11	0.35
(1,547)	1:201:A:MET:HE3	1:205:A:TYR:H	11	0.35
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	2	0.34
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	2	0.34
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	2	0.34
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	7	0.34
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	7	0.34
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	7	0.34
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	12	0.34
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	12	0.34
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	12	0.34
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	17	0.34
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	17	0.34
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	17	0.34
(1,340)	1:151:A:VAL:H	1:151:A:VAL:HG21	20	0.33
(1,340)	1:151:A:VAL:H	1:151:A:VAL:HG22	20	0.33
(1,340)	1:151:A:VAL:H	1:151:A:VAL:HG23	20	0.33
(1,24)	1:142:A:LEU:HD21	1:143:A:PHE:CE1	6	0.33
(1,24)	1:142:A:LEU:HD22	1:143:A:PHE:CE1	6	0.33
(1,24)	1:142:A:LEU:HD23	1:143:A:PHE:CE1	6	0.33
(1,13)	1:141:A:VAL:HG21	1:143:A:PHE:CD1	10	0.33
(1,13)	1:141:A:VAL:HG22	1:143:A:PHE:CD1	10	0.33
(1,13)	1:141:A:VAL:HG23	1:143:A:PHE:CD1	10	0.33
(1,426)	1:169:A:THR:HG21	1:171:A:LYS:H	19	0.31
(1,426)	1:169:A:THR:HG22	1:171:A:LYS:H	19	0.31
(1,426)	1:169:A:THR:HG23	1:171:A:LYS:H	19	0.31
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	10	0.31
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	10	0.31
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	10	0.31
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	16	0.31
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	16	0.31
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	16	0.31
(1,188)	1:8:A:LEU:HD11	1:74:A:ILE:CD1	1	0.3
(1,188)	1:8:A:LEU:HD12	1:74:A:ILE:CD1	1	0.3
(1,188)	1:8:A:LEU:HD13	1:74:A:ILE:CD1	1	0.3
(1,960)	1:110:A:LEU:HD11	1:143:A:PHE:CE1	20	0.29
(1,960)	1:110:A:LEU:HD12	1:143:A:PHE:CE1	20	0.29
(1,960)	1:110:A:LEU:HD13	1:143:A:PHE:CE1	20	0.29
(1,960)	1:110:A:LEU:HD21	1:143:A:PHE:CE1	20	0.29
(1,960)	1:110:A:LEU:HD22	1:143:A:PHE:CE1	20	0.29
(1,960)	1:110:A:LEU:HD23	1:143:A:PHE:CE1	20	0.29
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	7	0.29
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	7	0.29
(1,525)	1:14:A:VAL:HG21	1:55:A:TYR:HD1	13	0.29
(1,525)	1:14:A:VAL:HG21	1:55:A:TYR:HD2	13	0.29
(1,525)	1:14:A:VAL:HG22	1:55:A:TYR:HD1	13	0.29
(1,525)	1:14:A:VAL:HG22	1:55:A:TYR:HD2	13	0.29
(1,525)	1:14:A:VAL:HG23	1:55:A:TYR:HD1	13	0.29
(1,525)	1:14:A:VAL:HG23	1:55:A:TYR:HD2	13	0.29
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	11	0.29
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	11	0.29
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	11	0.29
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	3	0.29
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	3	0.29
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	3	0.29
(1,5)	1:74:A:ILE:HD11	1:209:A:TYR:CE1	11	0.29
(1,5)	1:74:A:ILE:HD12	1:209:A:TYR:CE1	11	0.29
(1,5)	1:74:A:ILE:HD13	1:209:A:TYR:CE1	11	0.29
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	12	0.28
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	12	0.28
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	12	0.28
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	12	0.28
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	12	0.28
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	12	0.28
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	12	0.28
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	12	0.28
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	12	0.28
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	12	0.28
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	12	0.28
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	12	0.28
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	12	0.28
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	12	0.28
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	12	0.28
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	12	0.28
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	12	0.28
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	12	0.28
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	12	0.28
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	12	0.28
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	12	0.28
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	12	0.28
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	12	0.28
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	12	0.28
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	12	0.28
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	12	0.28
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	12	0.28
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	12	0.28
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	12	0.28
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	12	0.28
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	12	0.28
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	12	0.28
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	12	0.28
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	12	0.28
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	12	0.28
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	7	0.28
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	7	0.28
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	7	0.28
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	7	0.28
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	7	0.28
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	7	0.28
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	7	0.28
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	7	0.28
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	7	0.28
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD11	10	0.28
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD12	10	0.28
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD13	10	0.28
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD11	10	0.28
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD12	10	0.28
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD13	10	0.28
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD11	10	0.28
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD12	10	0.28
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD13	10	0.28
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	8	0.28
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	8	0.28
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	8	0.28
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	19	0.28
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	19	0.28
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	19	0.28
(1,18)	1:141:A:VAL:HG11	1:143:A:PHE:CD1	20	0.28
(1,18)	1:141:A:VAL:HG12	1:143:A:PHE:CD1	20	0.28
(1,18)	1:141:A:VAL:HG13	1:143:A:PHE:CD1	20	0.28
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	9	0.28
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	9	0.28
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	9	0.28
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD11	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD12	5	0.27
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD13	5	0.27
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD21	5	0.27
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD22	5	0.27
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD23	5	0.27
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	14	0.27
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	14	0.27
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	14	0.27
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	14	0.27
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	14	0.27
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	14	0.27
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	14	0.27
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	14	0.27
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	14	0.27
(1,518)	1:53:A:LEU:H	1:55:A:TYR:HD1	13	0.27
(1,518)	1:53:A:LEU:H	1:55:A:TYR:HD2	13	0.27
(1,32)	1:202:A:LEU:HD21	1:205:A:TYR:CE2	16	0.27
(1,32)	1:202:A:LEU:HD22	1:205:A:TYR:CE2	16	0.27
(1,32)	1:202:A:LEU:HD23	1:205:A:TYR:CE2	16	0.27
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	19	0.27
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	19	0.27
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	19	0.27
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	10	0.27
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	10	0.27
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	10	0.27
(1,963)	1:110:A:LEU:HD11	1:143:A:PHE:HE2	12	0.26
(1,963)	1:110:A:LEU:HD12	1:143:A:PHE:HE2	12	0.26
(1,963)	1:110:A:LEU:HD13	1:143:A:PHE:HE2	12	0.26
(1,963)	1:110:A:LEU:HD21	1:143:A:PHE:HE2	12	0.26
(1,963)	1:110:A:LEU:HD22	1:143:A:PHE:HE2	12	0.26
(1,963)	1:110:A:LEU:HD23	1:143:A:PHE:HE2	12	0.26
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG21	19	0.26
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG22	19	0.26
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG23	19	0.26
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD11	12	0.26
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD12	12	0.26
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD13	12	0.26
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	17	0.26
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	17	0.26
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	17	0.26
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	8	0.26
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	8	0.26
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	12	0.26
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	12	0.26
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	12	0.26
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	9	0.25
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	9	0.25
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	9	0.25
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	9	0.25
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	9	0.25
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	9	0.25
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	9	0.25
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	9	0.25
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	9	0.25
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	9	0.25
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	9	0.25
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	9	0.25
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	9	0.25
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	9	0.25
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	9	0.25
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	9	0.25
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	9	0.25
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	9	0.25
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	9	0.25
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	9	0.25
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	9	0.25
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	9	0.25
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	9	0.25
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	9	0.25
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	9	0.25
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	9	0.25
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	9	0.25
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	9	0.25
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	9	0.25
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	9	0.25
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	9	0.25
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	9	0.25
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	9	0.25
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	9	0.25
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	9	0.25
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	9	0.25
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD11	4	0.25
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD12	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD13	4	0.25
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD21	4	0.25
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD22	4	0.25
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD23	4	0.25
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	2	0.25
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	2	0.25
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	2	0.25
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	2	0.25
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	2	0.25
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	2	0.25
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	2	0.25
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	2	0.25
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	2	0.25
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	20	0.25
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	20	0.25
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	20	0.25
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	20	0.25
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	20	0.25
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	20	0.25
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	20	0.25
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	20	0.25
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	20	0.25
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	18	0.25
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	18	0.25
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	18	0.25
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	18	0.25
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	18	0.25
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	18	0.25
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	4	0.25
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	4	0.25
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	4	0.25
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	2	0.24
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	14	0.24
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	14	0.24
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	14	0.24
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	14	0.24
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	14	0.24
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	14	0.24
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	14	0.24
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	14	0.24
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	14	0.24
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	14	0.24
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	14	0.24
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	14	0.24
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	14	0.24
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	14	0.24
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	14	0.24
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	14	0.24
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	14	0.24
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	14	0.24
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	14	0.24
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	14	0.24
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	14	0.24
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	14	0.24
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	14	0.24
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	14	0.24
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	14	0.24
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	14	0.24
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	14	0.24
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	14	0.24
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	14	0.24
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	14	0.24
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	14	0.24
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	14	0.24
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	14	0.24
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	14	0.24
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	14	0.24
(1,546)	1:201:A:MET:HE1	1:202:A:LEU:H	9	0.24
(1,546)	1:201:A:MET:HE2	1:202:A:LEU:H	9	0.24
(1,546)	1:201:A:MET:HE3	1:202:A:LEU:H	9	0.24
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD1	3	0.24
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD2	3	0.24
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD1	3	0.24
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD2	3	0.24
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD1	3	0.24
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD2	3	0.24
(1,518)	1:53:A:LEU:H	1:55:A:TYR:HD1	15	0.24
(1,518)	1:53:A:LEU:H	1:55:A:TYR:HD2	15	0.24
(1,455)	1:8:A:LEU:HD11	1:74:A:ILE:H	9	0.24
(1,455)	1:8:A:LEU:HD12	1:74:A:ILE:H	9	0.24
(1,455)	1:8:A:LEU:HD13	1:74:A:ILE:H	9	0.24
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD21	13	0.24
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD22	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD23	13	0.24
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG21	20	0.24
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG22	20	0.24
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG23	20	0.24
(1,188)	1:8:A:LEU:HD11	1:74:A:ILE:CD1	15	0.24
(1,188)	1:8:A:LEU:HD12	1:74:A:ILE:CD1	15	0.24
(1,188)	1:8:A:LEU:HD13	1:74:A:ILE:CD1	15	0.24
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	14	0.24
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	14	0.24
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	14	0.24
(1,984)	1:142:A:LEU:HD11	1:143:A:PHE:CE1	6	0.23
(1,984)	1:142:A:LEU:HD12	1:143:A:PHE:CE1	6	0.23
(1,984)	1:142:A:LEU:HD13	1:143:A:PHE:CE1	6	0.23
(1,984)	1:142:A:LEU:HD21	1:143:A:PHE:CE1	6	0.23
(1,984)	1:142:A:LEU:HD22	1:143:A:PHE:CE1	6	0.23
(1,984)	1:142:A:LEU:HD23	1:143:A:PHE:CE1	6	0.23
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	6	0.23
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	6	0.23
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	6	0.23
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	6	0.23
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	6	0.23
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	6	0.23
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	6	0.23
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	6	0.23
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	6	0.23
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	6	0.23
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	6	0.23
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	6	0.23
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	6	0.23
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	6	0.23
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	6	0.23
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	6	0.23
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	6	0.23
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	6	0.23
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	6	0.23
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	6	0.23
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	6	0.23
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	6	0.23
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	6	0.23
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	6	0.23
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	6	0.23
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	6	0.23
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	6	0.23
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	6	0.23
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	6	0.23
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	6	0.23
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	6	0.23
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	6	0.23
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	6	0.23
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	6	0.23
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	6	0.23
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD21	1	0.23
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD22	1	0.23
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD23	1	0.23
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD21	1	0.23
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD22	1	0.23
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD23	1	0.23
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD21	1	0.23
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD22	1	0.23
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD23	1	0.23
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	7	0.23
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	7	0.23
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	7	0.23
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	7	0.23
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	7	0.23
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	7	0.23
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	7	0.23
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	7	0.23
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	7	0.23
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	12	0.23
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	12	0.23
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	12	0.23
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	12	0.23
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	12	0.23
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	12	0.23
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	12	0.23
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	12	0.23
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	12	0.23
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	7	0.23
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	7	0.23
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	7	0.23
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD21	14	0.23
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD22	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD23	14	0.23
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD21	20	0.23
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD22	20	0.23
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD23	20	0.23
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	19	0.23
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	19	0.23
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	19	0.23
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG21	2	0.23
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG22	2	0.23
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG23	2	0.23
(1,183)	1:112:A:VAL:HG21	1:158:A:ILE:CD1	12	0.23
(1,183)	1:112:A:VAL:HG22	1:158:A:ILE:CD1	12	0.23
(1,183)	1:112:A:VAL:HG23	1:158:A:ILE:CD1	12	0.23
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	9	0.23
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	9	0.23
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	9	0.23
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	20	0.23
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	20	0.23
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	20	0.23
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	20	0.23
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	20	0.23
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	20	0.23
(1,977)	1:141:A:VAL:HG11	1:143:A:PHE:HZ	7	0.22
(1,977)	1:141:A:VAL:HG12	1:143:A:PHE:HZ	7	0.22
(1,977)	1:141:A:VAL:HG13	1:143:A:PHE:HZ	7	0.22
(1,977)	1:141:A:VAL:HG21	1:143:A:PHE:HZ	7	0.22
(1,977)	1:141:A:VAL:HG22	1:143:A:PHE:HZ	7	0.22
(1,977)	1:141:A:VAL:HG23	1:143:A:PHE:HZ	7	0.22
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	9	0.22
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	9	0.22
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	9	0.22
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	9	0.22
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	9	0.22
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	9	0.22
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	9	0.22
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	9	0.22
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	9	0.22
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	20	0.22
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	20	0.22
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	20	0.22
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	20	0.22
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	20	0.22
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	20	0.22
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	20	0.22
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	20	0.22
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD21	7	0.22
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD22	7	0.22
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD23	7	0.22
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	13	0.22
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	13	0.22
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	13	0.22
(1,32)	1:202:A:LEU:HD21	1:205:A:TYR:CE2	18	0.22
(1,32)	1:202:A:LEU:HD22	1:205:A:TYR:CE2	18	0.22
(1,32)	1:202:A:LEU:HD23	1:205:A:TYR:CE2	18	0.22
(1,32)	1:202:A:LEU:HD21	1:205:A:TYR:CE2	19	0.22
(1,32)	1:202:A:LEU:HD22	1:205:A:TYR:CE2	19	0.22
(1,32)	1:202:A:LEU:HD23	1:205:A:TYR:CE2	19	0.22
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	5	0.22
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	5	0.22
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	5	0.22
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	6	0.22
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	6	0.22
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	6	0.22
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	7	0.22
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	7	0.22
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	7	0.22
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	6	0.22
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	6	0.22
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	6	0.22
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	8	0.22
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	8	0.22
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	8	0.22
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD11	6	0.21
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD12	6	0.21
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD13	6	0.21
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD21	6	0.21
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD22	6	0.21
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD23	6	0.21
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	20	0.21
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	20	0.21
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	20	0.21
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	20	0.21
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	20	0.21
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	20	0.21
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	20	0.21
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	20	0.21
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	1	0.21
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	1	0.21
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	1	0.21
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	1	0.21
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	1	0.21
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	1	0.21
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	1	0.21
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	1	0.21
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	1	0.21
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG21	12	0.21
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG22	12	0.21
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG23	12	0.21
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG21	7	0.21
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG22	7	0.21
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG23	7	0.21
(1,183)	1:112:A:VAL:HG21	1:158:A:ILE:CD1	3	0.21
(1,183)	1:112:A:VAL:HG22	1:158:A:ILE:CD1	3	0.21
(1,183)	1:112:A:VAL:HG23	1:158:A:ILE:CD1	3	0.21
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD21	15	0.21
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD22	15	0.21
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD23	15	0.21
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	2	0.21
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	2	0.21
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	2	0.21
(1,961)	1:110:A:LEU:HD11	1:143:A:PHE:HE1	18	0.2
(1,961)	1:110:A:LEU:HD12	1:143:A:PHE:HE1	18	0.2
(1,961)	1:110:A:LEU:HD13	1:143:A:PHE:HE1	18	0.2
(1,961)	1:110:A:LEU:HD21	1:143:A:PHE:HE1	18	0.2
(1,961)	1:110:A:LEU:HD22	1:143:A:PHE:HE1	18	0.2
(1,961)	1:110:A:LEU:HD23	1:143:A:PHE:HE1	18	0.2
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD11	17	0.2
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD12	17	0.2
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD13	17	0.2
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD21	17	0.2
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD22	17	0.2
(1,952)	1:90:A:ASP:H	1:91:A:LEU:HD23	17	0.2
(1,546)	1:201:A:MET:HE1	1:202:A:LEU:H	3	0.2
(1,546)	1:201:A:MET:HE2	1:202:A:LEU:H	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:201:A:MET:HE3	1:202:A:LEU:H	3	0.2
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	19	0.2
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	19	0.2
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	19	0.2
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	1	0.2
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	1	0.2
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	1	0.2
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	11	0.2
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	11	0.2
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	11	0.2
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	16	0.2
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	16	0.2
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	16	0.2
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	11	0.2
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	11	0.2
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	11	0.2
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD21	17	0.19
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD22	17	0.19
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD23	17	0.19
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD21	17	0.19
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD22	17	0.19
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD23	17	0.19
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD21	17	0.19
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD22	17	0.19
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD23	17	0.19
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	4	0.19
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	4	0.19
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	4	0.19
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	4	0.19
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	4	0.19
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	4	0.19
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	4	0.19
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	4	0.19
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	4	0.19
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	5	0.19
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	5	0.19
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	5	0.19
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	5	0.19
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	5	0.19
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	5	0.19
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	5	0.19
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	5	0.19
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD11	1	0.19
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD12	1	0.19
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD13	1	0.19
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD11	1	0.19
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD12	1	0.19
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD13	1	0.19
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD11	1	0.19
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD12	1	0.19
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD13	1	0.19
(1,553)	1:202:A:LEU:HD21	1:205:A:TYR:HE1	16	0.19
(1,553)	1:202:A:LEU:HD21	1:205:A:TYR:HE2	16	0.19
(1,553)	1:202:A:LEU:HD22	1:205:A:TYR:HE1	16	0.19
(1,553)	1:202:A:LEU:HD22	1:205:A:TYR:HE2	16	0.19
(1,553)	1:202:A:LEU:HD23	1:205:A:TYR:HE1	16	0.19
(1,553)	1:202:A:LEU:HD23	1:205:A:TYR:HE2	16	0.19
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	8	0.19
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	8	0.19
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	8	0.19
(1,546)	1:201:A:MET:HE1	1:202:A:LEU:H	8	0.19
(1,546)	1:201:A:MET:HE2	1:202:A:LEU:H	8	0.19
(1,546)	1:201:A:MET:HE3	1:202:A:LEU:H	8	0.19
(1,525)	1:14:A:VAL:HG21	1:55:A:TYR:HD1	15	0.19
(1,525)	1:14:A:VAL:HG21	1:55:A:TYR:HD2	15	0.19
(1,525)	1:14:A:VAL:HG22	1:55:A:TYR:HD1	15	0.19
(1,525)	1:14:A:VAL:HG22	1:55:A:TYR:HD2	15	0.19
(1,525)	1:14:A:VAL:HG23	1:55:A:TYR:HD1	15	0.19
(1,525)	1:14:A:VAL:HG23	1:55:A:TYR:HD2	15	0.19
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD1	19	0.19
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD2	19	0.19
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD1	19	0.19
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD2	19	0.19
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD1	19	0.19
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD2	19	0.19
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	4	0.19
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	4	0.19
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	4	0.19
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	16	0.19
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	16	0.19
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	16	0.19
(1,188)	1:8:A:LEU:HD11	1:74:A:ILE:CD1	12	0.19
(1,188)	1:8:A:LEU:HD12	1:74:A:ILE:CD1	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:8:A:LEU:HD13	1:74:A:ILE:CD1	12	0.19
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	15	0.19
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	15	0.19
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	15	0.19
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	17	0.19
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	17	0.19
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	17	0.19
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	3	0.19
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	3	0.19
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	3	0.19
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	12	0.19
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	12	0.19
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	12	0.19
(1,27)	1:4:A:LEU:HD11	1:209:A:TYR:CE1	4	0.19
(1,27)	1:4:A:LEU:HD12	1:209:A:TYR:CE1	4	0.19
(1,27)	1:4:A:LEU:HD13	1:209:A:TYR:CE1	4	0.19
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	9	0.19
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	9	0.19
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	9	0.19
(1,5)	1:74:A:ILE:HD11	1:209:A:TYR:CE1	1	0.19
(1,5)	1:74:A:ILE:HD12	1:209:A:TYR:CE1	1	0.19
(1,5)	1:74:A:ILE:HD13	1:209:A:TYR:CE1	1	0.19
(1,961)	1:110:A:LEU:HD11	1:143:A:PHE:HE1	4	0.18
(1,961)	1:110:A:LEU:HD12	1:143:A:PHE:HE1	4	0.18
(1,961)	1:110:A:LEU:HD13	1:143:A:PHE:HE1	4	0.18
(1,961)	1:110:A:LEU:HD21	1:143:A:PHE:HE1	4	0.18
(1,961)	1:110:A:LEU:HD22	1:143:A:PHE:HE1	4	0.18
(1,961)	1:110:A:LEU:HD23	1:143:A:PHE:HE1	4	0.18
(1,961)	1:110:A:LEU:HD11	1:143:A:PHE:HE1	7	0.18
(1,961)	1:110:A:LEU:HD12	1:143:A:PHE:HE1	7	0.18
(1,961)	1:110:A:LEU:HD13	1:143:A:PHE:HE1	7	0.18
(1,961)	1:110:A:LEU:HD21	1:143:A:PHE:HE1	7	0.18
(1,961)	1:110:A:LEU:HD22	1:143:A:PHE:HE1	7	0.18
(1,961)	1:110:A:LEU:HD23	1:143:A:PHE:HE1	7	0.18
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	9	0.18
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	9	0.18
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	9	0.18
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	9	0.18
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	9	0.18
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	9	0.18
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	9	0.18
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	9	0.18
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD11	16	0.18
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD12	16	0.18
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD13	16	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	6	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	6	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	6	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	9	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	9	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	9	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	13	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	13	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	13	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	17	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	17	0.18
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	17	0.18
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	6	0.18
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	6	0.18
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	6	0.18
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	9	0.18
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	9	0.18
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	9	0.18
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	6	0.18
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	6	0.18
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	6	0.18
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	5	0.18
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	5	0.18
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	5	0.18
(1,3)	1:74:A:ILE:HD11	1:209:A:TYR:CD1	1	0.18
(1,3)	1:74:A:ILE:HD12	1:209:A:TYR:CD1	1	0.18
(1,3)	1:74:A:ILE:HD13	1:209:A:TYR:CD1	1	0.18
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	10	0.17
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	11	0.17
(4,167)	1:107:A:GLN:O	1:111:A:GLU:H	9	0.17
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD21	17	0.17
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD22	17	0.17
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD23	17	0.17
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD21	17	0.17
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD22	17	0.17
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD23	17	0.17
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD21	17	0.17
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD22	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD23	17	0.17
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	4	0.17
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	4	0.17
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	4	0.17
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	4	0.17
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	4	0.17
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	4	0.17
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	4	0.17
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	4	0.17
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	4	0.17
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD11	2	0.17
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD12	2	0.17
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD13	2	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD11	2	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD12	2	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD13	2	0.17
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD11	2	0.17
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD12	2	0.17
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD13	2	0.17
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD11	17	0.17
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD12	17	0.17
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD13	17	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD11	17	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD12	17	0.17
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD13	17	0.17
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD11	17	0.17
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD12	17	0.17
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD13	17	0.17
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD11	20	0.17
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD12	20	0.17
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD13	20	0.17
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD1	10	0.17
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD2	10	0.17
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD1	10	0.17
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD2	10	0.17
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD1	10	0.17
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD2	10	0.17
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	8	0.17
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	8	0.17
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	8	0.17
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	18	0.17
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	18	0.17
(1,251)	1:124:A:ALA:HB1	1:158:A:ILE:CD1	20	0.17
(1,251)	1:124:A:ALA:HB2	1:158:A:ILE:CD1	20	0.17
(1,251)	1:124:A:ALA:HB3	1:158:A:ILE:CD1	20	0.17
(1,247)	1:21:A:VAL:HG11	1:42:A:ILE:CD1	3	0.17
(1,247)	1:21:A:VAL:HG12	1:42:A:ILE:CD1	3	0.17
(1,247)	1:21:A:VAL:HG13	1:42:A:ILE:CD1	3	0.17
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD21	16	0.17
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD22	16	0.17
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD23	16	0.17
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	1	0.17
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	1	0.17
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	1	0.17
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	4	0.17
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	4	0.17
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	4	0.17
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD11	18	0.17
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD12	18	0.17
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD13	18	0.17
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD21	6	0.17
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD22	6	0.17
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD23	6	0.17
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	9	0.17
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	9	0.17
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	9	0.17
(1,30)	1:142:A:LEU:HD11	1:143:A:PHE:CE1	12	0.17
(1,30)	1:142:A:LEU:HD12	1:143:A:PHE:CE1	12	0.17
(1,30)	1:142:A:LEU:HD13	1:143:A:PHE:CE1	12	0.17
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	18	0.17
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	18	0.17
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	18	0.17
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	8	0.16
(4,183)	1:179:A:ASP:O	1:183:A:ARG:H	20	0.16
(4,167)	1:107:A:GLN:O	1:111:A:GLU:H	16	0.16
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	11	0.16
(1,972)	1:141:A:VAL:HG11	1:142:A:LEU:CD1	2	0.16
(1,972)	1:141:A:VAL:HG12	1:142:A:LEU:CD1	2	0.16
(1,972)	1:141:A:VAL:HG13	1:142:A:LEU:CD1	2	0.16
(1,972)	1:141:A:VAL:HG21	1:142:A:LEU:CD1	2	0.16
(1,972)	1:141:A:VAL:HG22	1:142:A:LEU:CD1	2	0.16
(1,972)	1:141:A:VAL:HG23	1:142:A:LEU:CD1	2	0.16
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD11	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD12	12	0.16
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD13	12	0.16
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD21	12	0.16
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD22	12	0.16
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD23	12	0.16
(1,963)	1:110:A:LEU:HD11	1:143:A:PHE:HE2	7	0.16
(1,963)	1:110:A:LEU:HD12	1:143:A:PHE:HE2	7	0.16
(1,963)	1:110:A:LEU:HD13	1:143:A:PHE:HE2	7	0.16
(1,963)	1:110:A:LEU:HD21	1:143:A:PHE:HE2	7	0.16
(1,963)	1:110:A:LEU:HD22	1:143:A:PHE:HE2	7	0.16
(1,963)	1:110:A:LEU:HD23	1:143:A:PHE:HE2	7	0.16
(1,959)	1:110:A:LEU:HD11	1:142:A:LEU:HD11	6	0.16
(1,959)	1:110:A:LEU:HD11	1:142:A:LEU:HD12	6	0.16
(1,959)	1:110:A:LEU:HD11	1:142:A:LEU:HD13	6	0.16
(1,959)	1:110:A:LEU:HD11	1:142:A:LEU:HD21	6	0.16
(1,959)	1:110:A:LEU:HD11	1:142:A:LEU:HD22	6	0.16
(1,959)	1:110:A:LEU:HD11	1:142:A:LEU:HD23	6	0.16
(1,959)	1:110:A:LEU:HD12	1:142:A:LEU:HD11	6	0.16
(1,959)	1:110:A:LEU:HD12	1:142:A:LEU:HD12	6	0.16
(1,959)	1:110:A:LEU:HD12	1:142:A:LEU:HD13	6	0.16
(1,959)	1:110:A:LEU:HD12	1:142:A:LEU:HD21	6	0.16
(1,959)	1:110:A:LEU:HD12	1:142:A:LEU:HD22	6	0.16
(1,959)	1:110:A:LEU:HD12	1:142:A:LEU:HD23	6	0.16
(1,959)	1:110:A:LEU:HD13	1:142:A:LEU:HD11	6	0.16
(1,959)	1:110:A:LEU:HD13	1:142:A:LEU:HD12	6	0.16
(1,959)	1:110:A:LEU:HD13	1:142:A:LEU:HD13	6	0.16
(1,959)	1:110:A:LEU:HD13	1:142:A:LEU:HD21	6	0.16
(1,959)	1:110:A:LEU:HD13	1:142:A:LEU:HD22	6	0.16
(1,959)	1:110:A:LEU:HD13	1:142:A:LEU:HD23	6	0.16
(1,959)	1:110:A:LEU:HD21	1:142:A:LEU:HD11	6	0.16
(1,959)	1:110:A:LEU:HD21	1:142:A:LEU:HD12	6	0.16
(1,959)	1:110:A:LEU:HD21	1:142:A:LEU:HD13	6	0.16
(1,959)	1:110:A:LEU:HD21	1:142:A:LEU:HD21	6	0.16
(1,959)	1:110:A:LEU:HD21	1:142:A:LEU:HD22	6	0.16
(1,959)	1:110:A:LEU:HD21	1:142:A:LEU:HD23	6	0.16
(1,959)	1:110:A:LEU:HD22	1:142:A:LEU:HD11	6	0.16
(1,959)	1:110:A:LEU:HD22	1:142:A:LEU:HD12	6	0.16
(1,959)	1:110:A:LEU:HD22	1:142:A:LEU:HD13	6	0.16
(1,959)	1:110:A:LEU:HD22	1:142:A:LEU:HD21	6	0.16
(1,959)	1:110:A:LEU:HD22	1:142:A:LEU:HD22	6	0.16
(1,959)	1:110:A:LEU:HD22	1:142:A:LEU:HD23	6	0.16
(1,959)	1:110:A:LEU:HD23	1:142:A:LEU:HD11	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:110:A:LEU:HD23	1:142:A:LEU:HD12	6	0.16
(1,959)	1:110:A:LEU:HD23	1:142:A:LEU:HD13	6	0.16
(1,959)	1:110:A:LEU:HD23	1:142:A:LEU:HD21	6	0.16
(1,959)	1:110:A:LEU:HD23	1:142:A:LEU:HD22	6	0.16
(1,959)	1:110:A:LEU:HD23	1:142:A:LEU:HD23	6	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	1	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	1	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	1	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	1	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	1	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	1	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	1	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	1	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	1	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	6	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	6	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	6	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	6	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	6	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	6	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	6	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	6	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	6	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	14	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	14	0.16
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	14	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	14	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	14	0.16
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	14	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	14	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	14	0.16
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	14	0.16
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	3	0.16
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	3	0.16
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	3	0.16
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	3	0.16
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	3	0.16
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	3	0.16
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	3	0.16
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	3	0.16
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	3	0.16
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	6	0.16
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	6	0.16
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	6	0.16
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	6	0.16
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	6	0.16
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	6	0.16
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	6	0.16
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	6	0.16
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB1	16	0.16
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB2	16	0.16
(1,615)	1:99:A:LEU:HD21	1:181:A:ALA:HB3	16	0.16
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB1	16	0.16
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB2	16	0.16
(1,615)	1:99:A:LEU:HD22	1:181:A:ALA:HB3	16	0.16
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB1	16	0.16
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB2	16	0.16
(1,615)	1:99:A:LEU:HD23	1:181:A:ALA:HB3	16	0.16
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD11	14	0.16
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD12	14	0.16
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD13	14	0.16
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD11	14	0.16
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD12	14	0.16
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD13	14	0.16
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD11	14	0.16
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD12	14	0.16
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD13	14	0.16
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD11	16	0.16
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD12	16	0.16
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD13	16	0.16
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD11	16	0.16
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD12	16	0.16
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD13	16	0.16
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD11	16	0.16
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD12	16	0.16
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD13	16	0.16
(1,517)	1:4:A:LEU:HD11	1:209:A:TYR:HD1	16	0.16
(1,517)	1:4:A:LEU:HD11	1:209:A:TYR:HD2	16	0.16
(1,517)	1:4:A:LEU:HD12	1:209:A:TYR:HD1	16	0.16
(1,517)	1:4:A:LEU:HD12	1:209:A:TYR:HD2	16	0.16
(1,517)	1:4:A:LEU:HD13	1:209:A:TYR:HD1	16	0.16
(1,517)	1:4:A:LEU:HD13	1:209:A:TYR:HD2	16	0.16
(1,506)	1:205:A:TYR:HE1	1:206:A:GLN:H	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:205:A:TYR:HE2	1:206:A:GLN:H	16	0.16
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	9	0.16
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	9	0.16
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	9	0.16
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	10	0.16
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	10	0.16
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	10	0.16
(1,188)	1:8:A:LEU:HD11	1:74:A:ILE:CD1	5	0.16
(1,188)	1:8:A:LEU:HD12	1:74:A:ILE:CD1	5	0.16
(1,188)	1:8:A:LEU:HD13	1:74:A:ILE:CD1	5	0.16
(1,148)	1:15:A:LEU:HD11	1:202:A:LEU:CD1	18	0.16
(1,148)	1:15:A:LEU:HD12	1:202:A:LEU:CD1	18	0.16
(1,148)	1:15:A:LEU:HD13	1:202:A:LEU:CD1	18	0.16
(1,145)	1:29:A:LEU:CD1	1:34:A:ILE:HD11	11	0.16
(1,145)	1:29:A:LEU:CD1	1:34:A:ILE:HD12	11	0.16
(1,145)	1:29:A:LEU:CD1	1:34:A:ILE:HD13	11	0.16
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD11	12	0.16
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD12	12	0.16
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD13	12	0.16
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD11	15	0.16
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD12	15	0.16
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD13	15	0.16
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD21	18	0.16
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD22	18	0.16
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD23	18	0.16
(1,31)	1:202:A:LEU:HD21	1:205:A:TYR:CD2	8	0.16
(1,31)	1:202:A:LEU:HD22	1:205:A:TYR:CD2	8	0.16
(1,31)	1:202:A:LEU:HD23	1:205:A:TYR:CD2	8	0.16
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	4	0.16
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	4	0.16
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	4	0.16
(1,11)	1:52:A:THR:HG21	1:55:A:TYR:CE1	10	0.16
(1,11)	1:52:A:THR:HG22	1:55:A:TYR:CE1	10	0.16
(1,11)	1:52:A:THR:HG23	1:55:A:TYR:CE1	10	0.16
(1,3)	1:74:A:ILE:HD11	1:209:A:TYR:CD1	12	0.16
(1,3)	1:74:A:ILE:HD12	1:209:A:TYR:CD1	12	0.16
(1,3)	1:74:A:ILE:HD13	1:209:A:TYR:CD1	12	0.16
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	3	0.15
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	12	0.15
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	18	0.15
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	19	0.15
(4,183)	1:179:A:ASP:O	1:183:A:ARG:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,31)	1:19:A:LYS:O	1:23:A:ASP:H	1	0.15
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	4	0.15
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	12	0.15
(1,680)	1:142:A:LEU:HD11	1:174:A:ALA:HB1	8	0.15
(1,680)	1:142:A:LEU:HD11	1:174:A:ALA:HB2	8	0.15
(1,680)	1:142:A:LEU:HD11	1:174:A:ALA:HB3	8	0.15
(1,680)	1:142:A:LEU:HD12	1:174:A:ALA:HB1	8	0.15
(1,680)	1:142:A:LEU:HD12	1:174:A:ALA:HB2	8	0.15
(1,680)	1:142:A:LEU:HD12	1:174:A:ALA:HB3	8	0.15
(1,680)	1:142:A:LEU:HD13	1:174:A:ALA:HB1	8	0.15
(1,680)	1:142:A:LEU:HD13	1:174:A:ALA:HB2	8	0.15
(1,680)	1:142:A:LEU:HD13	1:174:A:ALA:HB3	8	0.15
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	16	0.15
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	16	0.15
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	16	0.15
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	16	0.15
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	16	0.15
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	16	0.15
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	16	0.15
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	16	0.15
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	16	0.15
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD21	4	0.15
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD22	4	0.15
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD23	4	0.15
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD21	4	0.15
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD22	4	0.15
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD23	4	0.15
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD21	4	0.15
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD22	4	0.15
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD23	4	0.15
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB1	7	0.15
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB2	7	0.15
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB3	7	0.15
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB1	7	0.15
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB2	7	0.15
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB3	7	0.15
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB1	7	0.15
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB2	7	0.15
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB3	7	0.15
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD11	8	0.15
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD12	8	0.15
(1,582)	1:99:A:LEU:HD11	1:185:A:LEU:HD13	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD11	8	0.15
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD12	8	0.15
(1,582)	1:99:A:LEU:HD12	1:185:A:LEU:HD13	8	0.15
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD11	8	0.15
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD12	8	0.15
(1,582)	1:99:A:LEU:HD13	1:185:A:LEU:HD13	8	0.15
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	20	0.15
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	20	0.15
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	20	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD11	4	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD12	4	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD13	4	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD11	14	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD12	14	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD13	14	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD11	15	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD12	15	0.15
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD13	15	0.15
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	2	0.15
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	2	0.15
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	2	0.15
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	10	0.15
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	10	0.15
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	10	0.15
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	16	0.15
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	16	0.15
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	16	0.15
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG21	18	0.15
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG22	18	0.15
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG23	18	0.15
(1,247)	1:21:A:VAL:HG11	1:42:A:ILE:CD1	4	0.15
(1,247)	1:21:A:VAL:HG12	1:42:A:ILE:CD1	4	0.15
(1,247)	1:21:A:VAL:HG13	1:42:A:ILE:CD1	4	0.15
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	15	0.15
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	15	0.15
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	15	0.15
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	5	0.15
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	5	0.15
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	5	0.15
(1,94)	1:34:A:ILE:HD11	1:39:A:LEU:CD2	1	0.15
(1,94)	1:34:A:ILE:HD12	1:39:A:LEU:CD2	1	0.15
(1,94)	1:34:A:ILE:HD13	1:39:A:LEU:CD2	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:22:A:MET:HE1	1:91:A:LEU:CD1	4	0.15
(1,87)	1:22:A:MET:HE2	1:91:A:LEU:CD1	4	0.15
(1,87)	1:22:A:MET:HE3	1:91:A:LEU:CD1	4	0.15
(1,83)	1:43:A:THR:CG2	1:188:A:MET:HE1	20	0.15
(1,83)	1:43:A:THR:CG2	1:188:A:MET:HE2	20	0.15
(1,83)	1:43:A:THR:CG2	1:188:A:MET:HE3	20	0.15
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD21	16	0.15
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD22	16	0.15
(1,49)	1:34:A:ILE:CD1	1:99:A:LEU:HD23	16	0.15
(1,22)	1:141:A:VAL:HG11	1:143:A:PHE:HE1	17	0.15
(1,22)	1:141:A:VAL:HG11	1:143:A:PHE:HE2	17	0.15
(1,22)	1:141:A:VAL:HG12	1:143:A:PHE:HE1	17	0.15
(1,22)	1:141:A:VAL:HG12	1:143:A:PHE:HE2	17	0.15
(1,22)	1:141:A:VAL:HG13	1:143:A:PHE:HE1	17	0.15
(1,22)	1:141:A:VAL:HG13	1:143:A:PHE:HE2	17	0.15
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	12	0.15
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	12	0.15
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	12	0.15
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	6	0.14
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	15	0.14
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	16	0.14
(4,183)	1:179:A:ASP:O	1:183:A:ARG:H	1	0.14
(4,167)	1:107:A:GLN:O	1:111:A:GLU:H	19	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD11	1	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD12	1	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD13	1	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD21	1	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD22	1	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD23	1	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD11	1	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD12	1	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD13	1	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD21	1	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD22	1	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD23	1	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD11	1	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD12	1	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD13	1	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD21	1	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD22	1	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD23	1	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD11	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD12	1	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD13	1	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD21	1	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD22	1	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD23	1	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD11	1	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD12	1	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD13	1	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD21	1	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD22	1	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD23	1	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD11	1	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD12	1	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD13	1	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD21	1	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD22	1	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD23	1	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD11	2	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD12	2	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD13	2	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD21	2	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD22	2	0.14
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD23	2	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD11	2	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD12	2	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD13	2	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD21	2	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD22	2	0.14
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD23	2	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD11	2	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD12	2	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD13	2	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD21	2	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD22	2	0.14
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD23	2	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD11	2	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD12	2	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD13	2	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD21	2	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD22	2	0.14
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD23	2	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD11	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD12	2	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD13	2	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD21	2	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD22	2	0.14
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD23	2	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD11	2	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD12	2	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD13	2	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD21	2	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD22	2	0.14
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD23	2	0.14
(1,961)	1:110:A:LEU:HD11	1:143:A:PHE:HE1	17	0.14
(1,961)	1:110:A:LEU:HD12	1:143:A:PHE:HE1	17	0.14
(1,961)	1:110:A:LEU:HD13	1:143:A:PHE:HE1	17	0.14
(1,961)	1:110:A:LEU:HD21	1:143:A:PHE:HE1	17	0.14
(1,961)	1:110:A:LEU:HD22	1:143:A:PHE:HE1	17	0.14
(1,961)	1:110:A:LEU:HD23	1:143:A:PHE:HE1	17	0.14
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD21	5	0.14
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD22	5	0.14
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD23	5	0.14
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD21	5	0.14
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD22	5	0.14
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD23	5	0.14
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD21	5	0.14
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD22	5	0.14
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD23	5	0.14
(1,547)	1:201:A:MET:HE1	1:205:A:TYR:H	2	0.14
(1,547)	1:201:A:MET:HE2	1:205:A:TYR:H	2	0.14
(1,547)	1:201:A:MET:HE3	1:205:A:TYR:H	2	0.14
(1,546)	1:201:A:MET:HE1	1:202:A:LEU:H	16	0.14
(1,546)	1:201:A:MET:HE2	1:202:A:LEU:H	16	0.14
(1,546)	1:201:A:MET:HE3	1:202:A:LEU:H	16	0.14
(1,543)	1:11:A:MET:HE1	1:57:A:GLU:H	9	0.14
(1,543)	1:11:A:MET:HE2	1:57:A:GLU:H	9	0.14
(1,543)	1:11:A:MET:HE3	1:57:A:GLU:H	9	0.14
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD11	3	0.14
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD12	3	0.14
(1,529)	1:83:A:GLU:H	1:203:A:ILE:HD13	3	0.14
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	15	0.14
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	15	0.14
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	15	0.14
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD21	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD22	2	0.14
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD23	2	0.14
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	11	0.14
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	11	0.14
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	11	0.14
(1,261)	1:81:A:ILE:CD1	1:202:A:LEU:HD21	3	0.14
(1,261)	1:81:A:ILE:CD1	1:202:A:LEU:HD22	3	0.14
(1,261)	1:81:A:ILE:CD1	1:202:A:LEU:HD23	3	0.14
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD21	6	0.14
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD22	6	0.14
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD23	6	0.14
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	2	0.14
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	2	0.14
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	2	0.14
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	18	0.14
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	18	0.14
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	18	0.14
(1,188)	1:8:A:LEU:HD11	1:74:A:ILE:CD1	2	0.14
(1,188)	1:8:A:LEU:HD12	1:74:A:ILE:CD1	2	0.14
(1,188)	1:8:A:LEU:HD13	1:74:A:ILE:CD1	2	0.14
(1,188)	1:8:A:LEU:HD11	1:74:A:ILE:CD1	18	0.14
(1,188)	1:8:A:LEU:HD12	1:74:A:ILE:CD1	18	0.14
(1,188)	1:8:A:LEU:HD13	1:74:A:ILE:CD1	18	0.14
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	3	0.14
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	3	0.14
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	3	0.14
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD11	1	0.14
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD12	1	0.14
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD13	1	0.14
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD11	7	0.14
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD12	7	0.14
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD13	7	0.14
(1,87)	1:22:A:MET:HE1	1:91:A:LEU:CD1	5	0.14
(1,87)	1:22:A:MET:HE2	1:91:A:LEU:CD1	5	0.14
(1,87)	1:22:A:MET:HE3	1:91:A:LEU:CD1	5	0.14
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD11	1	0.14
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD12	1	0.14
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD13	1	0.14
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD11	9	0.14
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD12	9	0.14
(1,50)	1:53:A:LEU:CD1	1:88:A:LEU:HD13	9	0.14
(1,18)	1:141:A:VAL:HG11	1:143:A:PHE:CD1	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:141:A:VAL:HG12	1:143:A:PHE:CD1	2	0.14
(1,18)	1:141:A:VAL:HG13	1:143:A:PHE:CD1	2	0.14
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	20	0.14
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	20	0.14
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	20	0.14
(1,3)	1:74:A:ILE:HD11	1:209:A:TYR:CD1	7	0.14
(1,3)	1:74:A:ILE:HD12	1:209:A:TYR:CD1	7	0.14
(1,3)	1:74:A:ILE:HD13	1:209:A:TYR:CD1	7	0.14
(4,229)	1:202:A:LEU:O	1:206:A:GLN:H	10	0.13
(4,217)	1:196:A:GLU:O	1:200:A:LYS:H	18	0.13
(4,211)	1:193:A:GLN:O	1:197:A:GLU:H	1	0.13
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	1	0.13
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	4	0.13
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	7	0.13
(4,183)	1:179:A:ASP:O	1:183:A:ARG:H	5	0.13
(4,93)	1:62:A:LEU:O	1:66:A:ALA:H	12	0.13
(4,49)	1:40:A:GLN:O	1:44:A:GLU:H	4	0.13
(4,25)	1:16:A:ASN:O	1:20:A:THR:H	13	0.13
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	5	0.13
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	7	0.13
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	14	0.13
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD21	7	0.13
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD22	7	0.13
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD23	7	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD21	7	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD22	7	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD23	7	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD21	7	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD22	7	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD23	7	0.13
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD21	16	0.13
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD22	16	0.13
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD23	16	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD21	16	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD22	16	0.13
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD23	16	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD21	16	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD22	16	0.13
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD23	16	0.13
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD21	6	0.13
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD22	6	0.13
(1,646)	1:88:A:LEU:HD21	1:91:A:LEU:HD23	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD21	6	0.13
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD22	6	0.13
(1,646)	1:88:A:LEU:HD22	1:91:A:LEU:HD23	6	0.13
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD21	6	0.13
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD22	6	0.13
(1,646)	1:88:A:LEU:HD23	1:91:A:LEU:HD23	6	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	10	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	10	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	10	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	10	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	10	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	10	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	10	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	10	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	10	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	16	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	16	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	16	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	16	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	16	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	16	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	16	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	16	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	16	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	18	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	18	0.13
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	18	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	18	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	18	0.13
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	18	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	18	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	18	0.13
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	18	0.13
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB1	4	0.13
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB2	4	0.13
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB3	4	0.13
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB1	4	0.13
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB2	4	0.13
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB3	4	0.13
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB1	4	0.13
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB2	4	0.13
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD11	18	0.13
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD12	18	0.13
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD13	18	0.13
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD11	18	0.13
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD12	18	0.13
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD13	18	0.13
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD11	18	0.13
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD12	18	0.13
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD13	18	0.13
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	14	0.13
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	14	0.13
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	14	0.13
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	16	0.13
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	16	0.13
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	16	0.13
(1,537)	1:75:A:ALA:HB1	1:209:A:TYR:HD1	6	0.13
(1,537)	1:75:A:ALA:HB1	1:209:A:TYR:HD2	6	0.13
(1,537)	1:75:A:ALA:HB2	1:209:A:TYR:HD1	6	0.13
(1,537)	1:75:A:ALA:HB2	1:209:A:TYR:HD2	6	0.13
(1,537)	1:75:A:ALA:HB3	1:209:A:TYR:HD1	6	0.13
(1,537)	1:75:A:ALA:HB3	1:209:A:TYR:HD2	6	0.13
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD1	7	0.13
(1,523)	1:74:A:ILE:HD11	1:209:A:TYR:HD2	7	0.13
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD1	7	0.13
(1,523)	1:74:A:ILE:HD12	1:209:A:TYR:HD2	7	0.13
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD1	7	0.13
(1,523)	1:74:A:ILE:HD13	1:209:A:TYR:HD2	7	0.13
(1,496)	1:21:A:VAL:HG21	1:46:A:LYS:H	11	0.13
(1,496)	1:21:A:VAL:HG22	1:46:A:LYS:H	11	0.13
(1,496)	1:21:A:VAL:HG23	1:46:A:LYS:H	11	0.13
(1,478)	1:90:A:ASP:H	1:199:A:LEU:HD11	13	0.13
(1,478)	1:90:A:ASP:H	1:199:A:LEU:HD12	13	0.13
(1,478)	1:90:A:ASP:H	1:199:A:LEU:HD13	13	0.13
(1,429)	1:6:A:GLU:H	1:8:A:LEU:HD11	4	0.13
(1,429)	1:6:A:GLU:H	1:8:A:LEU:HD12	4	0.13
(1,429)	1:6:A:GLU:H	1:8:A:LEU:HD13	4	0.13
(1,389)	1:21:A:VAL:HG11	1:45:A:GLU:H	20	0.13
(1,389)	1:21:A:VAL:HG12	1:45:A:GLU:H	20	0.13
(1,389)	1:21:A:VAL:HG13	1:45:A:GLU:H	20	0.13
(1,371)	1:22:A:MET:HE1	1:89:A:ARG:H	7	0.13
(1,371)	1:22:A:MET:HE2	1:89:A:ARG:H	7	0.13
(1,371)	1:22:A:MET:HE3	1:89:A:ARG:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD21	2	0.13
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD22	2	0.13
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD23	2	0.13
(1,87)	1:22:A:MET:HE1	1:91:A:LEU:CD1	6	0.13
(1,87)	1:22:A:MET:HE2	1:91:A:LEU:CD1	6	0.13
(1,87)	1:22:A:MET:HE3	1:91:A:LEU:CD1	6	0.13
(1,87)	1:22:A:MET:HE1	1:91:A:LEU:CD1	17	0.13
(1,87)	1:22:A:MET:HE2	1:91:A:LEU:CD1	17	0.13
(1,87)	1:22:A:MET:HE3	1:91:A:LEU:CD1	17	0.13
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE1	4	0.13
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE2	4	0.13
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE3	4	0.13
(1,72)	1:11:A:MET:HE1	1:199:A:LEU:CD2	14	0.13
(1,72)	1:11:A:MET:HE2	1:199:A:LEU:CD2	14	0.13
(1,72)	1:11:A:MET:HE3	1:199:A:LEU:CD2	14	0.13
(1,34)	1:55:A:TYR:CE2	1:56:A:LEU:HD21	15	0.13
(1,34)	1:55:A:TYR:CE2	1:56:A:LEU:HD22	15	0.13
(1,34)	1:55:A:TYR:CE2	1:56:A:LEU:HD23	15	0.13
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	2	0.13
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	2	0.13
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	2	0.13
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	14	0.13
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	14	0.13
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	14	0.13
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	19	0.13
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	19	0.13
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	19	0.13
(1,6)	1:74:A:ILE:HD11	1:209:A:TYR:CE2	6	0.13
(1,6)	1:74:A:ILE:HD12	1:209:A:TYR:CE2	6	0.13
(1,6)	1:74:A:ILE:HD13	1:209:A:TYR:CE2	6	0.13
(4,229)	1:202:A:LEU:O	1:206:A:GLN:H	7	0.12
(4,213)	1:194:A:GLN:O	1:198:A:GLN:H	20	0.12
(4,191)	1:183:A:ARG:O	1:187:A:GLU:H	10	0.12
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	13	0.12
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	14	0.12
(4,183)	1:179:A:ASP:O	1:183:A:ARG:H	15	0.12
(4,175)	1:175:A:GLU:O	1:179:A:ASP:H	3	0.12
(4,175)	1:175:A:GLU:O	1:179:A:ASP:H	8	0.12
(4,169)	1:108:A:GLN:O	1:112:A:VAL:H	9	0.12
(4,153)	1:100:A:GLU:O	1:104:A:GLU:H	6	0.12
(4,93)	1:62:A:LEU:O	1:66:A:ALA:H	17	0.12
(4,91)	1:61:A:ARG:O	1:65:A:ASN:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,91)	1:61:A:ARG:O	1:65:A:ASN:H	8	0.12
(4,49)	1:40:A:GLN:O	1:44:A:GLU:H	8	0.12
(4,31)	1:19:A:LYS:O	1:23:A:ASP:H	10	0.12
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	1	0.12
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	15	0.12
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD11	6	0.12
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD12	6	0.12
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD13	6	0.12
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD21	6	0.12
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD22	6	0.12
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD23	6	0.12
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD11	6	0.12
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD12	6	0.12
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD13	6	0.12
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD21	6	0.12
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD22	6	0.12
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD23	6	0.12
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD11	6	0.12
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD12	6	0.12
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD13	6	0.12
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD21	6	0.12
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD22	6	0.12
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD23	6	0.12
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD11	6	0.12
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD12	6	0.12
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD13	6	0.12
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD21	6	0.12
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD22	6	0.12
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD23	6	0.12
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD11	6	0.12
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD12	6	0.12
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD13	6	0.12
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD21	6	0.12
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD22	6	0.12
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD23	6	0.12
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD11	6	0.12
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD12	6	0.12
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD13	6	0.12
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD21	6	0.12
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD22	6	0.12
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD23	6	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD11	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD12	18	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD13	18	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD21	18	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD22	18	0.12
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD23	18	0.12
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG11	2	0.12
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG12	2	0.12
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG13	2	0.12
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG21	2	0.12
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG22	2	0.12
(1,958)	1:110:A:LEU:HD11	1:141:A:VAL:HG23	2	0.12
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG11	2	0.12
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG12	2	0.12
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG13	2	0.12
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG21	2	0.12
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG22	2	0.12
(1,958)	1:110:A:LEU:HD12	1:141:A:VAL:HG23	2	0.12
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG11	2	0.12
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG12	2	0.12
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG13	2	0.12
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG21	2	0.12
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG22	2	0.12
(1,958)	1:110:A:LEU:HD13	1:141:A:VAL:HG23	2	0.12
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG11	2	0.12
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG12	2	0.12
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG13	2	0.12
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG21	2	0.12
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG22	2	0.12
(1,958)	1:110:A:LEU:HD21	1:141:A:VAL:HG23	2	0.12
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG11	2	0.12
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG12	2	0.12
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG13	2	0.12
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG21	2	0.12
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG22	2	0.12
(1,958)	1:110:A:LEU:HD22	1:141:A:VAL:HG23	2	0.12
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG11	2	0.12
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG12	2	0.12
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG13	2	0.12
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG21	2	0.12
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG22	2	0.12
(1,958)	1:110:A:LEU:HD23	1:141:A:VAL:HG23	2	0.12
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD21	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD22	12	0.12
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD23	12	0.12
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD21	12	0.12
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD22	12	0.12
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD23	12	0.12
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD21	12	0.12
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD22	12	0.12
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD23	12	0.12
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	5	0.12
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	5	0.12
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	5	0.12
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	5	0.12
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	5	0.12
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	5	0.12
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	5	0.12
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	5	0.12
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	5	0.12
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	7	0.12
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	7	0.12
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	7	0.12
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	7	0.12
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	7	0.12
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	7	0.12
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	7	0.12
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	7	0.12
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	7	0.12
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	1	0.12
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	1	0.12
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	1	0.12
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	1	0.12
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	1	0.12
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	1	0.12
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	1	0.12
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	1	0.12
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	1	0.12
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	12	0.12
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	12	0.12
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	12	0.12
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	12	0.12
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	12	0.12
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	12	0.12
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	12	0.12
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	12	0.12
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB1	8	0.12
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB2	8	0.12
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB3	8	0.12
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB1	8	0.12
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB2	8	0.12
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB3	8	0.12
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB1	8	0.12
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB2	8	0.12
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB3	8	0.12
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD11	19	0.12
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD12	19	0.12
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD13	19	0.12
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD11	19	0.12
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD12	19	0.12
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD13	19	0.12
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD11	19	0.12
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD12	19	0.12
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD13	19	0.12
(1,544)	1:11:A:MET:HE1	1:54:A:ASP:H	11	0.12
(1,544)	1:11:A:MET:HE2	1:54:A:ASP:H	11	0.12
(1,544)	1:11:A:MET:HE3	1:54:A:ASP:H	11	0.12
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD11	13	0.12
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD12	13	0.12
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD13	13	0.12
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD11	13	0.12
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD12	13	0.12
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD13	13	0.12
(1,464)	1:7:A:ILE:HD11	1:62:A:LEU:H	2	0.12
(1,464)	1:7:A:ILE:HD12	1:62:A:LEU:H	2	0.12
(1,464)	1:7:A:ILE:HD13	1:62:A:LEU:H	2	0.12
(1,452)	1:27:A:GLN:H	1:98:A:LEU:HD11	11	0.12
(1,452)	1:27:A:GLN:H	1:98:A:LEU:HD12	11	0.12
(1,452)	1:27:A:GLN:H	1:98:A:LEU:HD13	11	0.12
(1,414)	1:188:A:MET:HE1	1:189:A:ARG:H	4	0.12
(1,414)	1:188:A:MET:HE2	1:189:A:ARG:H	4	0.12
(1,414)	1:188:A:MET:HE3	1:189:A:ARG:H	4	0.12
(1,414)	1:188:A:MET:HE1	1:189:A:ARG:H	6	0.12
(1,414)	1:188:A:MET:HE2	1:189:A:ARG:H	6	0.12
(1,414)	1:188:A:MET:HE3	1:189:A:ARG:H	6	0.12
(1,414)	1:188:A:MET:HE1	1:189:A:ARG:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:188:A:MET:HE2	1:189:A:ARG:H	13	0.12
(1,414)	1:188:A:MET:HE3	1:189:A:ARG:H	13	0.12
(1,389)	1:21:A:VAL:HG11	1:45:A:GLU:H	5	0.12
(1,389)	1:21:A:VAL:HG12	1:45:A:GLU:H	5	0.12
(1,389)	1:21:A:VAL:HG13	1:45:A:GLU:H	5	0.12
(1,389)	1:21:A:VAL:HG11	1:45:A:GLU:H	13	0.12
(1,389)	1:21:A:VAL:HG12	1:45:A:GLU:H	13	0.12
(1,389)	1:21:A:VAL:HG13	1:45:A:GLU:H	13	0.12
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD21	6	0.12
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD22	6	0.12
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD23	6	0.12
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD21	16	0.12
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD22	16	0.12
(1,351)	1:57:A:GLU:H	1:202:A:LEU:HD23	16	0.12
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	2	0.12
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	2	0.12
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	2	0.12
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	3	0.12
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	3	0.12
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	3	0.12
(1,277)	1:8:A:LEU:HD21	1:78:A:TRP:H	1	0.12
(1,277)	1:8:A:LEU:HD22	1:78:A:TRP:H	1	0.12
(1,277)	1:8:A:LEU:HD23	1:78:A:TRP:H	1	0.12
(1,269)	1:109:A:ALA:HB1	1:158:A:ILE:CD1	12	0.12
(1,269)	1:109:A:ALA:HB2	1:158:A:ILE:CD1	12	0.12
(1,269)	1:109:A:ALA:HB3	1:158:A:ILE:CD1	12	0.12
(1,260)	1:201:A:MET:CE	1:202:A:LEU:HD21	1	0.12
(1,260)	1:201:A:MET:CE	1:202:A:LEU:HD22	1	0.12
(1,260)	1:201:A:MET:CE	1:202:A:LEU:HD23	1	0.12
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG21	16	0.12
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG22	16	0.12
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG23	16	0.12
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD21	10	0.12
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD22	10	0.12
(1,220)	1:4:A:LEU:CD1	1:8:A:LEU:HD23	10	0.12
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD11	1	0.12
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD12	1	0.12
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD13	1	0.12
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD11	4	0.12
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD12	4	0.12
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD13	4	0.12
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG21	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG22	4	0.12
(1,126)	1:39:A:LEU:CD1	1:43:A:THR:HG23	4	0.12
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD11	2	0.12
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD12	2	0.12
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD13	2	0.12
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD11	9	0.12
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD12	9	0.12
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD13	9	0.12
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD11	2	0.12
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD12	2	0.12
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD13	2	0.12
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD11	17	0.12
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD12	17	0.12
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD13	17	0.12
(1,88)	1:22:A:MET:HE1	1:91:A:LEU:CD2	10	0.12
(1,88)	1:22:A:MET:HE2	1:91:A:LEU:CD2	10	0.12
(1,88)	1:22:A:MET:HE3	1:91:A:LEU:CD2	10	0.12
(1,81)	1:29:A:LEU:CD2	1:188:A:MET:HE1	6	0.12
(1,81)	1:29:A:LEU:CD2	1:188:A:MET:HE2	6	0.12
(1,81)	1:29:A:LEU:CD2	1:188:A:MET:HE3	6	0.12
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE1	5	0.12
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE2	5	0.12
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE3	5	0.12
(1,72)	1:11:A:MET:HE1	1:199:A:LEU:CD2	19	0.12
(1,72)	1:11:A:MET:HE2	1:199:A:LEU:CD2	19	0.12
(1,72)	1:11:A:MET:HE3	1:199:A:LEU:CD2	19	0.12
(1,67)	1:11:A:MET:HE1	1:53:A:LEU:CD1	10	0.12
(1,67)	1:11:A:MET:HE2	1:53:A:LEU:CD1	10	0.12
(1,67)	1:11:A:MET:HE3	1:53:A:LEU:CD1	10	0.12
(1,32)	1:202:A:LEU:HD21	1:205:A:TYR:CE2	12	0.12
(1,32)	1:202:A:LEU:HD22	1:205:A:TYR:CE2	12	0.12
(1,32)	1:202:A:LEU:HD23	1:205:A:TYR:CE2	12	0.12
(1,13)	1:141:A:VAL:HG21	1:143:A:PHE:CD1	6	0.12
(1,13)	1:141:A:VAL:HG22	1:143:A:PHE:CD1	6	0.12
(1,13)	1:141:A:VAL:HG23	1:143:A:PHE:CD1	6	0.12
(1,6)	1:74:A:ILE:HD11	1:209:A:TYR:CE2	18	0.12
(1,6)	1:74:A:ILE:HD12	1:209:A:TYR:CE2	18	0.12
(1,6)	1:74:A:ILE:HD13	1:209:A:TYR:CE2	18	0.12
(4,223)	1:199:A:LEU:O	1:203:A:ILE:H	11	0.11
(4,219)	1:197:A:GLU:O	1:201:A:MET:H	1	0.11
(4,217)	1:196:A:GLU:O	1:200:A:LYS:H	13	0.11
(4,211)	1:193:A:GLN:O	1:197:A:GLU:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,205)	1:190:A:ARG:O	1:194:A:GLN:H	13	0.11
(4,191)	1:183:A:ARG:O	1:187:A:GLU:H	2	0.11
(4,191)	1:183:A:ARG:O	1:187:A:GLU:H	11	0.11
(4,189)	1:182:A:ALA:O	1:186:A:GLY:H	9	0.11
(4,185)	1:180:A:ASP:O	1:184:A:LEU:H	20	0.11
(4,183)	1:179:A:ASP:O	1:183:A:ARG:H	18	0.11
(4,173)	1:174:A:ALA:O	1:178:A:VAL:H	17	0.11
(4,167)	1:107:A:GLN:O	1:111:A:GLU:H	4	0.11
(4,133)	1:90:A:ASP:O	1:94:A:HIS:H	10	0.11
(4,85)	1:58:A:GLN:O	1:62:A:LEU:H	20	0.11
(4,49)	1:40:A:GLN:O	1:44:A:GLU:H	6	0.11
(4,49)	1:40:A:GLN:O	1:44:A:GLU:H	12	0.11
(4,49)	1:40:A:GLN:O	1:44:A:GLU:H	14	0.11
(4,39)	1:23:A:ASP:O	1:27:A:GLN:H	5	0.11
(4,26)	1:16:A:ASN:O	1:20:A:THR:N	13	0.11
(4,25)	1:16:A:ASN:O	1:20:A:THR:H	11	0.11
(4,25)	1:16:A:ASN:O	1:20:A:THR:H	20	0.11
(4,17)	1:12:A:THR:O	1:16:A:ASN:H	6	0.11
(4,13)	1:10:A:GLN:O	1:14:A:VAL:H	7	0.11
(1,988)	1:142:A:LEU:HD11	1:174:A:ALA:HB1	20	0.11
(1,988)	1:142:A:LEU:HD11	1:174:A:ALA:HB2	20	0.11
(1,988)	1:142:A:LEU:HD11	1:174:A:ALA:HB3	20	0.11
(1,988)	1:142:A:LEU:HD12	1:174:A:ALA:HB1	20	0.11
(1,988)	1:142:A:LEU:HD12	1:174:A:ALA:HB2	20	0.11
(1,988)	1:142:A:LEU:HD12	1:174:A:ALA:HB3	20	0.11
(1,988)	1:142:A:LEU:HD13	1:174:A:ALA:HB1	20	0.11
(1,988)	1:142:A:LEU:HD13	1:174:A:ALA:HB2	20	0.11
(1,988)	1:142:A:LEU:HD13	1:174:A:ALA:HB3	20	0.11
(1,988)	1:142:A:LEU:HD21	1:174:A:ALA:HB1	20	0.11
(1,988)	1:142:A:LEU:HD21	1:174:A:ALA:HB2	20	0.11
(1,988)	1:142:A:LEU:HD21	1:174:A:ALA:HB3	20	0.11
(1,988)	1:142:A:LEU:HD22	1:174:A:ALA:HB1	20	0.11
(1,988)	1:142:A:LEU:HD22	1:174:A:ALA:HB2	20	0.11
(1,988)	1:142:A:LEU:HD22	1:174:A:ALA:HB3	20	0.11
(1,988)	1:142:A:LEU:HD23	1:174:A:ALA:HB1	20	0.11
(1,988)	1:142:A:LEU:HD23	1:174:A:ALA:HB2	20	0.11
(1,988)	1:142:A:LEU:HD23	1:174:A:ALA:HB3	20	0.11
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD21	20	0.11
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD22	20	0.11
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD23	20	0.11
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD21	20	0.11
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD22	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD23	20	0.11
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD21	20	0.11
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD22	20	0.11
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD23	20	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	4	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	4	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	4	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	4	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	4	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	4	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	4	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	4	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	4	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	13	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	13	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	13	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	13	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	13	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	13	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	13	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	13	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	13	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD21	17	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD22	17	0.11
(1,667)	1:39:A:LEU:HD11	1:184:A:LEU:HD23	17	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD21	17	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD22	17	0.11
(1,667)	1:39:A:LEU:HD12	1:184:A:LEU:HD23	17	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD21	17	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD22	17	0.11
(1,667)	1:39:A:LEU:HD13	1:184:A:LEU:HD23	17	0.11
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	5	0.11
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	5	0.11
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	5	0.11
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	5	0.11
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	5	0.11
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	5	0.11
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	5	0.11
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	5	0.11
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	5	0.11
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	9	0.11
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	9	0.11
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	9	0.11
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	9	0.11
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	9	0.11
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	9	0.11
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	9	0.11
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	9	0.11
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB1	3	0.11
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB2	3	0.11
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB3	3	0.11
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB1	3	0.11
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB2	3	0.11
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB3	3	0.11
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB1	3	0.11
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB2	3	0.11
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB3	3	0.11
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB1	11	0.11
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB2	11	0.11
(1,610)	1:14:A:VAL:HG21	1:51:A:ALA:HB3	11	0.11
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB1	11	0.11
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB2	11	0.11
(1,610)	1:14:A:VAL:HG22	1:51:A:ALA:HB3	11	0.11
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB1	11	0.11
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB2	11	0.11
(1,610)	1:14:A:VAL:HG23	1:51:A:ALA:HB3	11	0.11
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD11	3	0.11
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD12	3	0.11
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD13	3	0.11
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD11	3	0.11
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD12	3	0.11
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD13	3	0.11
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD11	3	0.11
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD12	3	0.11
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD13	3	0.11
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	2	0.11
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	2	0.11
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	2	0.11
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	12	0.11
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	12	0.11
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	12	0.11
(1,551)	1:22:A:MET:HE1	1:92:A:ASN:H	19	0.11
(1,551)	1:22:A:MET:HE2	1:92:A:ASN:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:22:A:MET:HE3	1:92:A:ASN:H	19	0.11
(1,547)	1:201:A:MET:HE1	1:205:A:TYR:H	13	0.11
(1,547)	1:201:A:MET:HE2	1:205:A:TYR:H	13	0.11
(1,547)	1:201:A:MET:HE3	1:205:A:TYR:H	13	0.11
(1,546)	1:201:A:MET:HE1	1:202:A:LEU:H	17	0.11
(1,546)	1:201:A:MET:HE2	1:202:A:LEU:H	17	0.11
(1,546)	1:201:A:MET:HE3	1:202:A:LEU:H	17	0.11
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD11	1	0.11
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD12	1	0.11
(1,511)	1:55:A:TYR:HD1	1:56:A:LEU:HD13	1	0.11
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD11	1	0.11
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD12	1	0.11
(1,511)	1:55:A:TYR:HD2	1:56:A:LEU:HD13	1	0.11
(1,472)	1:87:A:HIS:H	1:88:A:LEU:HD21	10	0.11
(1,472)	1:87:A:HIS:H	1:88:A:LEU:HD22	10	0.11
(1,472)	1:87:A:HIS:H	1:88:A:LEU:HD23	10	0.11
(1,455)	1:8:A:LEU:HD11	1:74:A:ILE:H	1	0.11
(1,455)	1:8:A:LEU:HD12	1:74:A:ILE:H	1	0.11
(1,455)	1:8:A:LEU:HD13	1:74:A:ILE:H	1	0.11
(1,430)	1:98:A:LEU:HD21	1:102:A:GLN:H	8	0.11
(1,430)	1:98:A:LEU:HD22	1:102:A:GLN:H	8	0.11
(1,430)	1:98:A:LEU:HD23	1:102:A:GLN:H	8	0.11
(1,389)	1:21:A:VAL:HG11	1:45:A:GLU:H	1	0.11
(1,389)	1:21:A:VAL:HG12	1:45:A:GLU:H	1	0.11
(1,389)	1:21:A:VAL:HG13	1:45:A:GLU:H	1	0.11
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	3	0.11
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	3	0.11
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	3	0.11
(1,356)	1:181:A:ALA:HB1	1:185:A:LEU:H	20	0.11
(1,356)	1:181:A:ALA:HB2	1:185:A:LEU:H	20	0.11
(1,356)	1:181:A:ALA:HB3	1:185:A:LEU:H	20	0.11
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	6	0.11
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	6	0.11
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	6	0.11
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD11	19	0.11
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD12	19	0.11
(1,346)	1:53:A:LEU:H	1:56:A:LEU:HD13	19	0.11
(1,343)	1:14:A:VAL:HG21	1:53:A:LEU:H	14	0.11
(1,343)	1:14:A:VAL:HG22	1:53:A:LEU:H	14	0.11
(1,343)	1:14:A:VAL:HG23	1:53:A:LEU:H	14	0.11
(1,277)	1:8:A:LEU:HD21	1:78:A:TRP:H	9	0.11
(1,277)	1:8:A:LEU:HD22	1:78:A:TRP:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:8:A:LEU:HD23	1:78:A:TRP:H	9	0.11
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB1	12	0.11
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB2	12	0.11
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB3	12	0.11
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB1	20	0.11
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB2	20	0.11
(1,266)	1:99:A:LEU:CD2	1:181:A:ALA:HB3	20	0.11
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG21	13	0.11
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG22	13	0.11
(1,250)	1:109:A:ALA:CB	1:112:A:VAL:HG23	13	0.11
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD21	11	0.11
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD22	11	0.11
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD23	11	0.11
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD21	12	0.11
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD22	12	0.11
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD23	12	0.11
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG21	6	0.11
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG22	6	0.11
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG23	6	0.11
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD11	6	0.11
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD12	6	0.11
(1,185)	1:29:A:LEU:CD2	1:42:A:ILE:HD13	6	0.11
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD11	10	0.11
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD12	10	0.11
(1,104)	1:29:A:LEU:CD2	1:103:A:ILE:HD13	10	0.11
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD11	6	0.11
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD12	6	0.11
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD13	6	0.11
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD11	14	0.11
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD12	14	0.11
(1,97)	1:31:A:VAL:CG2	1:34:A:ILE:HD13	14	0.11
(1,94)	1:34:A:ILE:HD11	1:39:A:LEU:CD2	11	0.11
(1,94)	1:34:A:ILE:HD12	1:39:A:LEU:CD2	11	0.11
(1,94)	1:34:A:ILE:HD13	1:39:A:LEU:CD2	11	0.11
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE1	3	0.11
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE2	3	0.11
(1,78)	1:99:A:LEU:CD1	1:188:A:MET:HE3	3	0.11
(1,76)	1:29:A:LEU:CD1	1:188:A:MET:HE1	5	0.11
(1,76)	1:29:A:LEU:CD1	1:188:A:MET:HE2	5	0.11
(1,76)	1:29:A:LEU:CD1	1:188:A:MET:HE3	5	0.11
(1,69)	1:11:A:MET:HE1	1:202:A:LEU:CD2	3	0.11
(1,69)	1:11:A:MET:HE2	1:202:A:LEU:CD2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:11:A:MET:HE3	1:202:A:LEU:CD2	3	0.11
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	4	0.11
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	4	0.11
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	4	0.11
(4,223)	1:199:A:LEU:O	1:203:A:ILE:H	18	0.1
(4,191)	1:183:A:ARG:O	1:187:A:GLU:H	19	0.1
(4,167)	1:107:A:GLN:O	1:111:A:GLU:H	6	0.1
(4,139)	1:93:A:GLN:O	1:97:A:TRP:H	3	0.1
(4,131)	1:89:A:ARG:O	1:93:A:GLN:H	13	0.1
(4,131)	1:89:A:ARG:O	1:93:A:GLN:H	15	0.1
(4,117)	1:82:A:THR:O	1:86:A:GLN:H	16	0.1
(4,91)	1:61:A:ARG:O	1:65:A:ASN:H	14	0.1
(4,77)	1:54:A:ASP:O	1:58:A:GLN:H	18	0.1
(4,71)	1:51:A:ALA:O	1:55:A:TYR:H	13	0.1
(4,25)	1:16:A:ASN:O	1:20:A:THR:H	3	0.1
(4,25)	1:16:A:ASN:O	1:20:A:THR:H	16	0.1
(4,25)	1:16:A:ASN:O	1:20:A:THR:H	17	0.1
(4,17)	1:12:A:THR:O	1:16:A:ASN:H	20	0.1
(4,13)	1:10:A:GLN:O	1:14:A:VAL:H	15	0.1
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	16	0.1
(4,3)	1:5:A:SER:O	1:9:A:ASP:H	20	0.1
(1,984)	1:142:A:LEU:HD11	1:143:A:PHE:CE1	12	0.1
(1,984)	1:142:A:LEU:HD12	1:143:A:PHE:CE1	12	0.1
(1,984)	1:142:A:LEU:HD13	1:143:A:PHE:CE1	12	0.1
(1,984)	1:142:A:LEU:HD21	1:143:A:PHE:CE1	12	0.1
(1,984)	1:142:A:LEU:HD22	1:143:A:PHE:CE1	12	0.1
(1,984)	1:142:A:LEU:HD23	1:143:A:PHE:CE1	12	0.1
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD11	11	0.1
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD12	11	0.1
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD13	11	0.1
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD21	11	0.1
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD22	11	0.1
(1,971)	1:141:A:VAL:HG11	1:142:A:LEU:HD23	11	0.1
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD11	11	0.1
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD12	11	0.1
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD13	11	0.1
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD21	11	0.1
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD22	11	0.1
(1,971)	1:141:A:VAL:HG12	1:142:A:LEU:HD23	11	0.1
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD11	11	0.1
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD12	11	0.1
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD13	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD21	11	0.1
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD22	11	0.1
(1,971)	1:141:A:VAL:HG13	1:142:A:LEU:HD23	11	0.1
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD11	11	0.1
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD12	11	0.1
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD13	11	0.1
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD21	11	0.1
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD22	11	0.1
(1,971)	1:141:A:VAL:HG21	1:142:A:LEU:HD23	11	0.1
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD11	11	0.1
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD12	11	0.1
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD13	11	0.1
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD21	11	0.1
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD22	11	0.1
(1,971)	1:141:A:VAL:HG22	1:142:A:LEU:HD23	11	0.1
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD11	11	0.1
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD12	11	0.1
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD13	11	0.1
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD21	11	0.1
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD22	11	0.1
(1,971)	1:141:A:VAL:HG23	1:142:A:LEU:HD23	11	0.1
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD11	6	0.1
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD12	6	0.1
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD13	6	0.1
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD21	6	0.1
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD22	6	0.1
(1,968)	1:111:A:GLU:H	1:142:A:LEU:HD23	6	0.1
(1,961)	1:110:A:LEU:HD11	1:143:A:PHE:HE1	6	0.1
(1,961)	1:110:A:LEU:HD12	1:143:A:PHE:HE1	6	0.1
(1,961)	1:110:A:LEU:HD13	1:143:A:PHE:HE1	6	0.1
(1,961)	1:110:A:LEU:HD21	1:143:A:PHE:HE1	6	0.1
(1,961)	1:110:A:LEU:HD22	1:143:A:PHE:HE1	6	0.1
(1,961)	1:110:A:LEU:HD23	1:143:A:PHE:HE1	6	0.1
(1,960)	1:110:A:LEU:HD11	1:143:A:PHE:CE1	4	0.1
(1,960)	1:110:A:LEU:HD12	1:143:A:PHE:CE1	4	0.1
(1,960)	1:110:A:LEU:HD13	1:143:A:PHE:CE1	4	0.1
(1,960)	1:110:A:LEU:HD21	1:143:A:PHE:CE1	4	0.1
(1,960)	1:110:A:LEU:HD22	1:143:A:PHE:CE1	4	0.1
(1,960)	1:110:A:LEU:HD23	1:143:A:PHE:CE1	4	0.1
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD21	18	0.1
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD22	18	0.1
(1,674)	1:99:A:LEU:HD11	1:185:A:LEU:HD23	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD21	18	0.1
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD22	18	0.1
(1,674)	1:99:A:LEU:HD12	1:185:A:LEU:HD23	18	0.1
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD21	18	0.1
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD22	18	0.1
(1,674)	1:99:A:LEU:HD13	1:185:A:LEU:HD23	18	0.1
(1,643)	1:85:A:THR:HG21	1:199:A:LEU:HD21	17	0.1
(1,643)	1:85:A:THR:HG21	1:199:A:LEU:HD22	17	0.1
(1,643)	1:85:A:THR:HG21	1:199:A:LEU:HD23	17	0.1
(1,643)	1:85:A:THR:HG22	1:199:A:LEU:HD21	17	0.1
(1,643)	1:85:A:THR:HG22	1:199:A:LEU:HD22	17	0.1
(1,643)	1:85:A:THR:HG22	1:199:A:LEU:HD23	17	0.1
(1,643)	1:85:A:THR:HG23	1:199:A:LEU:HD21	17	0.1
(1,643)	1:85:A:THR:HG23	1:199:A:LEU:HD22	17	0.1
(1,643)	1:85:A:THR:HG23	1:199:A:LEU:HD23	17	0.1
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD21	17	0.1
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD22	17	0.1
(1,639)	1:13:A:THR:HG21	1:53:A:LEU:HD23	17	0.1
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD21	17	0.1
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD22	17	0.1
(1,639)	1:13:A:THR:HG22	1:53:A:LEU:HD23	17	0.1
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD21	17	0.1
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD22	17	0.1
(1,639)	1:13:A:THR:HG23	1:53:A:LEU:HD23	17	0.1
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD11	7	0.1
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD12	7	0.1
(1,569)	1:29:A:LEU:HD11	1:39:A:LEU:HD13	7	0.1
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD11	7	0.1
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD12	7	0.1
(1,569)	1:29:A:LEU:HD12	1:39:A:LEU:HD13	7	0.1
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD11	7	0.1
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD12	7	0.1
(1,569)	1:29:A:LEU:HD13	1:39:A:LEU:HD13	7	0.1
(1,397)	1:35:A:ASN:H	1:39:A:LEU:HD21	16	0.1
(1,397)	1:35:A:ASN:H	1:39:A:LEU:HD22	16	0.1
(1,397)	1:35:A:ASN:H	1:39:A:LEU:HD23	16	0.1
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG11	5	0.1
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG12	5	0.1
(1,385)	1:28:A:GLN:H	1:31:A:VAL:HG13	5	0.1
(1,277)	1:8:A:LEU:HD21	1:78:A:TRP:H	12	0.1
(1,277)	1:8:A:LEU:HD22	1:78:A:TRP:H	12	0.1
(1,277)	1:8:A:LEU:HD23	1:78:A:TRP:H	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD21	7	0.1
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD22	7	0.1
(1,230)	1:52:A:THR:CG2	1:53:A:LEU:HD23	7	0.1
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG21	4	0.1
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG22	4	0.1
(1,218)	1:11:A:MET:CE	1:14:A:VAL:HG23	4	0.1
(1,99)	1:124:A:ALA:CB	1:158:A:ILE:HD11	2	0.1
(1,99)	1:124:A:ALA:CB	1:158:A:ILE:HD12	2	0.1
(1,99)	1:124:A:ALA:CB	1:158:A:ILE:HD13	2	0.1
(1,73)	1:201:A:MET:HE1	1:202:A:LEU:CD1	7	0.1
(1,73)	1:201:A:MET:HE2	1:202:A:LEU:CD1	7	0.1
(1,73)	1:201:A:MET:HE3	1:202:A:LEU:CD1	7	0.1
(1,32)	1:202:A:LEU:HD21	1:205:A:TYR:CE2	20	0.1
(1,32)	1:202:A:LEU:HD22	1:205:A:TYR:CE2	20	0.1
(1,32)	1:202:A:LEU:HD23	1:205:A:TYR:CE2	20	0.1
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	3	0.1
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	3	0.1
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	3	0.1
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	7	0.1
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	7	0.1
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	7	0.1
(1,9)	1:52:A:THR:HG21	1:55:A:TYR:CD1	18	0.1
(1,9)	1:52:A:THR:HG22	1:55:A:TYR:CD1	18	0.1
(1,9)	1:52:A:THR:HG23	1:55:A:TYR:CD1	18	0.1

10 Dihedral-angle violation analysis

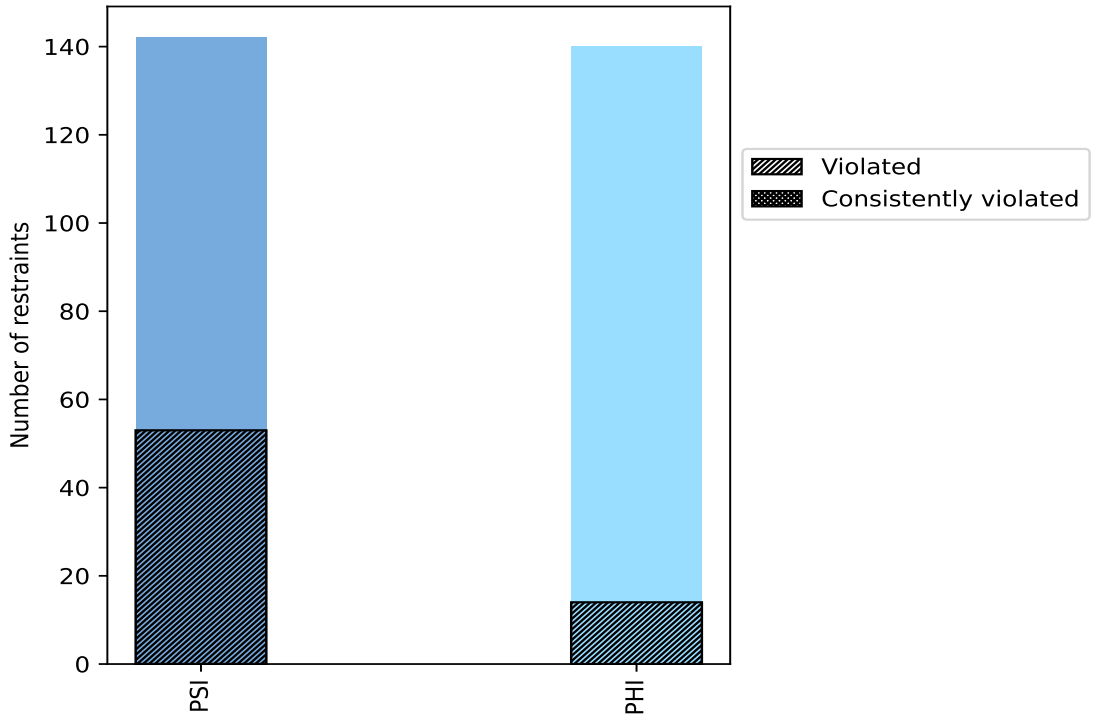
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	142	50.4	53	37.3	18.8	0	0.0	0.0
PHI	140	49.6	14	10.0	5.0	0	0.0	0.0
Total	282	100.0	67	23.8	23.8	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



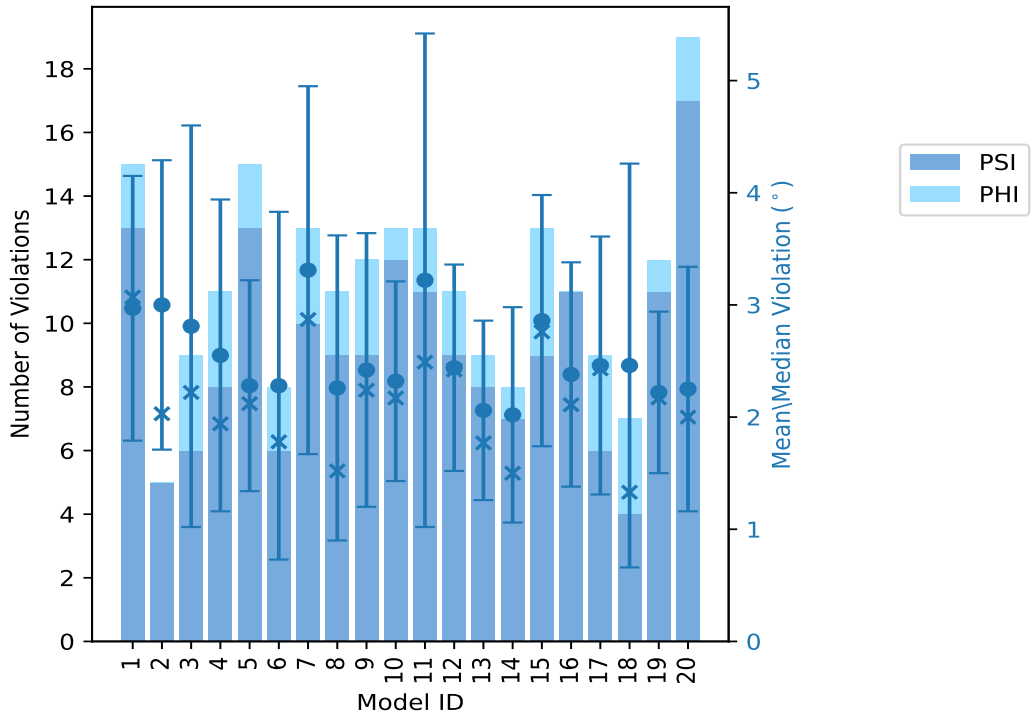
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	13	2	15	2.97	4.76	1.18	3.07
2	5	0	5	3.0	5.07	1.29	2.03
3	6	3	9	2.81	7.29	1.79	2.22
4	8	3	11	2.55	5.88	1.39	1.94
5	13	2	15	2.28	4.11	0.94	2.12
6	6	2	8	2.28	6.31	1.55	1.78
7	10	3	13	3.31	6.33	1.64	2.87
8	9	2	11	2.26	5.44	1.36	1.52
9	9	3	12	2.42	4.83	1.22	2.24
10	12	1	13	2.32	4.44	0.89	2.17
11	11	2	13	3.22	9.26	2.2	2.49
12	9	2	11	2.44	4.82	0.92	2.42
13	8	1	9	2.06	4.04	0.8	1.77
14	7	1	8	2.02	3.83	0.96	1.5
15	9	4	13	2.86	5.24	1.12	2.76
16	11	0	11	2.38	5.17	1.0	2.11
17	6	3	9	2.46	4.45	1.15	2.43
18	4	3	7	2.46	6.07	1.8	1.33
19	11	1	12	2.22	3.58	0.72	2.17
20	17	2	19	2.25	4.51	1.09	2.0

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
24	6	30	1	5.0
4	3	7	2	10.0
3	2	5	3	15.0
7	2	9	4	20.0
5	0	5	5	25.0
1	0	1	6	30.0
2	0	2	7	35.0
2	0	2	8	40.0
2	0	2	9	45.0
0	0	0	10	50.0
2	0	2	11	55.0

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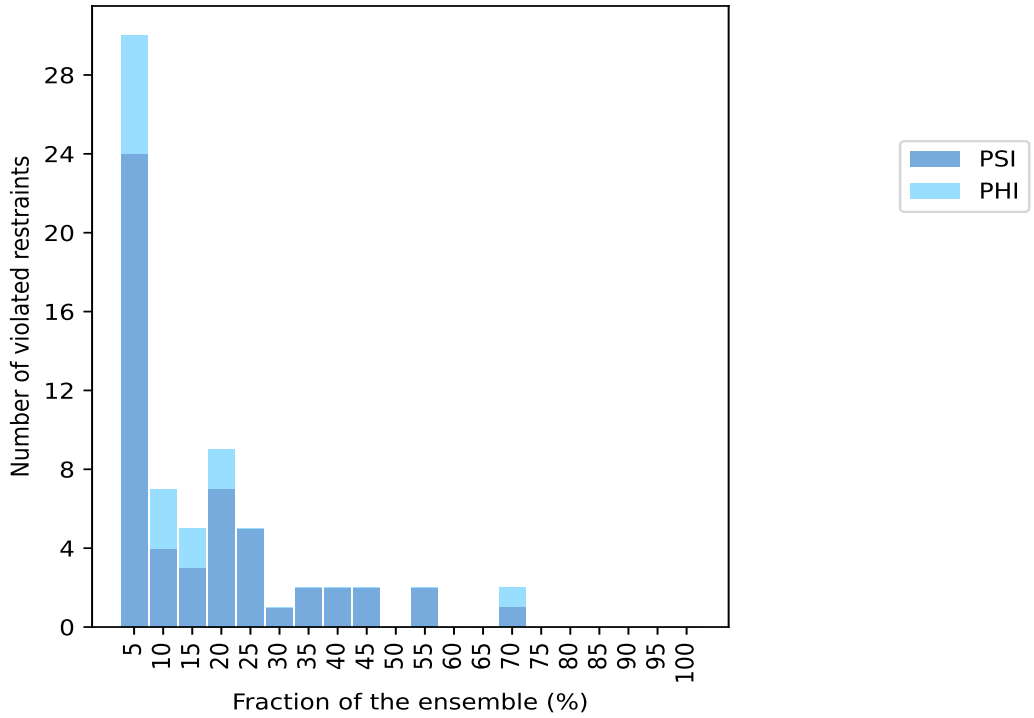
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
1	1	2	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

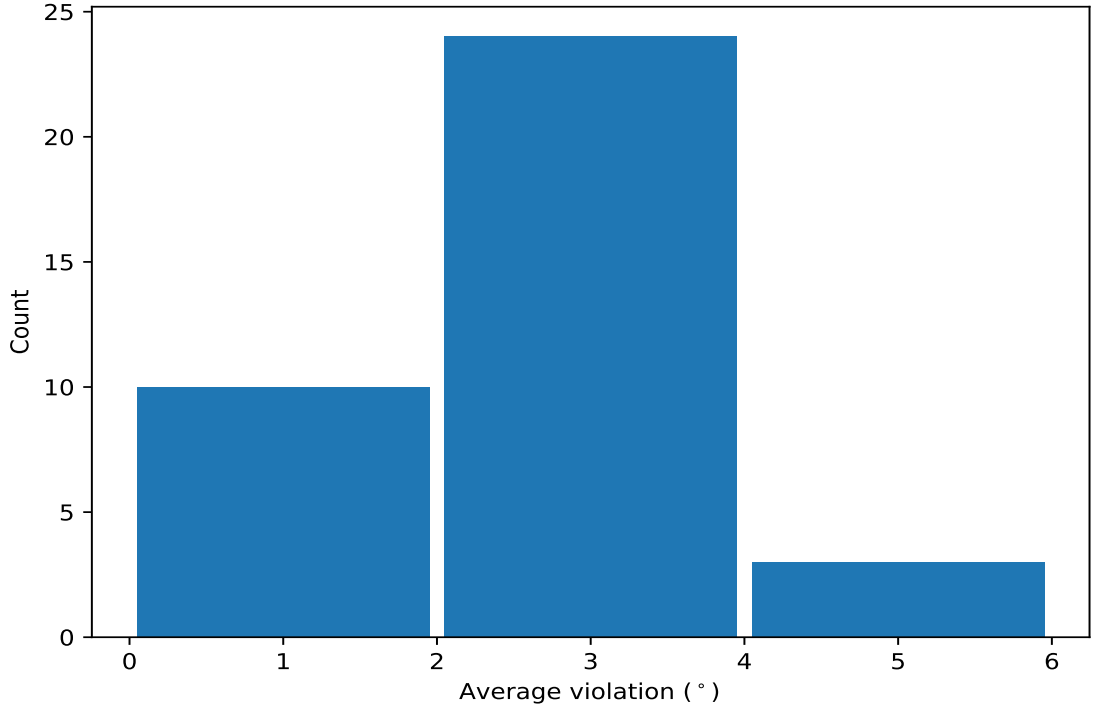


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	14	2.85	1.19	2.6
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	14	2.05	0.64	1.97
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	11	4.14	2.41	3.65
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	11	2.72	1.42	2.3
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	9	4.18	1.48	4.44
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	9	2.09	0.85	1.85
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	8	2.32	0.82	2.2
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	8	2.21	0.85	2.01
(1,211)	1:115:A:PRO:N	1:115:A:PRO:CA	1:115:A:PRO:C	1:116:A:HIS:N	7	3.06	1.5	3.45
(1,236)	1:183:A:ARG:N	1:183:A:ARG:CA	1:183:A:ARG:C	1:184:A:LEU:N	7	2.32	0.53	2.34
(1,216)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ARG:N	6	1.85	0.33	1.94
(1,52)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:SER:N	5	2.95	2.36	1.66
(1,120)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:GLN:N	5	2.4	1.16	2.57
(1,260)	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	1:196:A:GLU:N	5	2.21	1.28	1.69
(1,166)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:ASN:N	5	1.93	0.53	1.9
(1,278)	1:204:A:ASP:N	1:204:A:ASP:CA	1:204:A:ASP:C	1:205:A:TYR:N	5	1.68	0.43	1.89
(1,232)	1:181:A:ALA:N	1:181:A:ALA:CA	1:181:A:ALA:C	1:182:A:ALA:N	4	3.21	1.06	3.47
(1,228)	1:179:A:ASP:N	1:179:A:ASP:CA	1:179:A:ASP:C	1:180:A:ASP:N	4	3.06	1.31	2.83
(1,208)	1:112:A:VAL:N	1:112:A:VAL:CA	1:112:A:VAL:C	1:113:A:LEU:N	4	2.62	0.3	2.76
(1,279)	1:204:A:ASP:C	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	4	2.55	0.71	2.6

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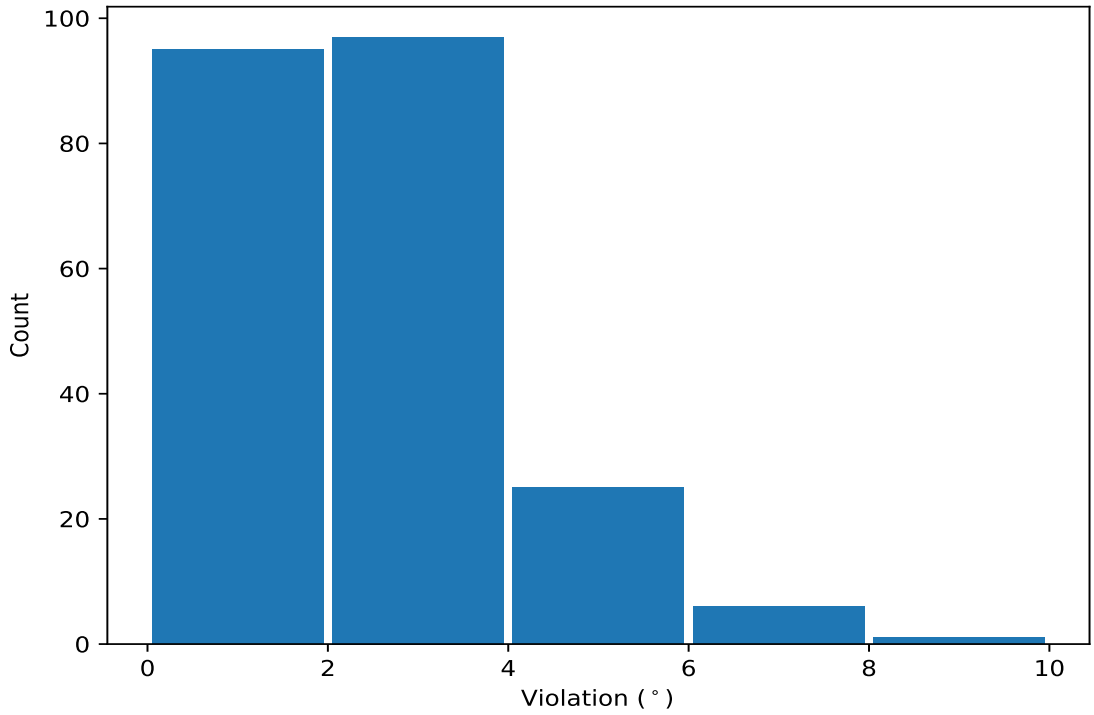
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,164)	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	1:91:A:LEU:N	4	2.36	0.57	2.46
(1,53)	1:29:A:LEU:C	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	4	1.88	1.17	1.32
(1,238)	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	1:185:A:LEU:N	4	1.84	0.28	1.8
(1,70)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:LEU:N	4	1.81	0.21	1.9
(1,215)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	4	1.39	0.22	1.48
(1,114)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:ARG:N	3	3.86	1.18	3.98
(1,126)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:GLN:N	3	3.27	0.64	2.96
(1,224)	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	1:178:A:VAL:N	3	3.0	0.08	3.02
(1,59)	1:32:A:GLY:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	3	2.05	0.95	1.79
(1,214)	1:150:A:LEU:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	3	1.64	0.39	1.73
(1,281)	1:205:A:TYR:C	1:206:A:GLN:N	1:206:A:GLN:CA	1:206:A:GLN:C	2	5.17	1.05	5.17
(1,218)	1:153:A:ARG:N	1:153:A:ARG:CA	1:153:A:ARG:C	1:154:A:GLY:N	2	3.46	0.95	3.46
(1,56)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:GLY:N	2	2.56	1.33	2.56
(1,182)	1:99:A:LEU:N	1:99:A:LEU:CA	1:99:A:LEU:C	1:100:A:GLU:N	2	2.46	0.59	2.46
(1,219)	1:172:A:ASP:C	1:173:A:LEU:N	1:173:A:LEU:CA	1:173:A:LEU:C	2	2.09	0.88	2.09
(1,51)	1:28:A:GLN:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	2	1.9	0.55	1.9
(1,198)	1:107:A:GLN:N	1:107:A:GLN:CA	1:107:A:GLN:C	1:108:A:GLN:N	2	1.4	0.38	1.4

[1] Number of violated models, [2]Standard 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 (°)
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	11	9.26
(1,52)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:SER:N	3	7.29
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	11	6.46
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	7	6.33
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	6	6.31
(1,281)	1:205:A:TYR:C	1:206:A:GLN:N	1:206:A:GLN:CA	1:206:A:GLN:C	7	6.22
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	18	6.07
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	4	5.88
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	7	5.59
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	8	5.44
(1,114)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:ARG:N	15	5.24
(1,211)	1:115:A:PRO:N	1:115:A:PRO:CA	1:115:A:PRO:C	1:116:A:HIS:N	16	5.17
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	2	5.07
(1,228)	1:179:A:ASP:N	1:179:A:ASP:CA	1:179:A:ASP:C	1:180:A:ASP:N	9	4.83
(1,210)	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	1:115:A:PRO:N	12	4.82
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	4	4.81
(1,260)	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	1:196:A:GLU:N	1	4.76
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	20	4.51
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	17	4.45
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	10	4.44
(1,218)	1:153:A:ARG:N	1:153:A:ARG:CA	1:153:A:ARG:C	1:154:A:GLY:N	15	4.4
(1,120)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:GLN:N	1	4.36
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	1	4.35
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	17	4.33
(1,211)	1:115:A:PRO:N	1:115:A:PRO:CA	1:115:A:PRO:C	1:116:A:HIS:N	18	4.27
(1,232)	1:181:A:ALA:N	1:181:A:ALA:CA	1:181:A:ALA:C	1:182:A:ALA:N	20	4.25
(1,211)	1:115:A:PRO:N	1:115:A:PRO:CA	1:115:A:PRO:C	1:116:A:HIS:N	9	4.17
(1,126)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:GLN:N	3	4.16
(1,281)	1:205:A:TYR:C	1:206:A:GLN:N	1:206:A:GLN:CA	1:206:A:GLN:C	11	4.12
(1,232)	1:181:A:ALA:N	1:181:A:ALA:CA	1:181:A:ALA:C	1:182:A:ALA:N	5	4.11
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	1	4.1
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	13	4.04
(1,114)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:ARG:N	2	3.98
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	9	3.92
(1,282)	1:206:A:GLN:N	1:206:A:GLN:CA	1:206:A:GLN:C	1:207:A:ASN:N	8	3.91
(1,56)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:GLY:N	20	3.89
(1,53)	1:29:A:LEU:C	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	20	3.89
(1,206)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:VAL:N	14	3.83
(1,228)	1:179:A:ASP:N	1:179:A:ASP:CA	1:179:A:ASP:C	1:180:A:ASP:N	15	3.81
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	5	3.65
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	5	3.61
(1,52)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:SER:N	1	3.61
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	19	3.58
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1	3.55
(1,279)	1:204:A:ASP:C	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	7	3.5
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	1	3.49
(1,211)	1:115:A:PRO:N	1:115:A:PRO:CA	1:115:A:PRO:C	1:116:A:HIS:N	5	3.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	15	3.39
(1,59)	1:32:A:GLY:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	7	3.33
(1,236)	1:183:A:ARG:N	1:183:A:ARG:CA	1:183:A:ARG:C	1:184:A:LEU:N	11	3.29
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	19	3.15
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	8	3.1
(1,224)	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	1:178:A:VAL:N	8	3.08
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	1	3.07
(1,182)	1:99:A:LEU:N	1:99:A:LEU:CA	1:99:A:LEU:C	1:100:A:GLU:N	10	3.05
(1,246)	1:188:A:MET:N	1:188:A:MET:CA	1:188:A:MET:C	1:189:A:ARG:N	15	3.04
(1,224)	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	1:178:A:VAL:N	10	3.02
(1,219)	1:172:A:ASP:C	1:173:A:LEU:N	1:173:A:LEU:CA	1:173:A:LEU:C	3	2.98
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	1	2.98
(1,126)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:GLN:N	20	2.96
(1,164)	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	1:91:A:LEU:N	12	2.94
(1,72)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:GLN:N	7	2.93
(1,188)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:ILE:N	10	2.92
(1,224)	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	1:178:A:VAL:N	15	2.89
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	14	2.89
(1,208)	1:112:A:VAL:N	1:112:A:VAL:CA	1:112:A:VAL:C	1:113:A:LEU:N	16	2.87
(1,166)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:ASN:N	7	2.87
(1,164)	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	1:91:A:LEU:N	14	2.86
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	12	2.86
(1,174)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:96:A:GLY:N	9	2.84
(1,50)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:LEU:N	11	2.84
(1,232)	1:181:A:ALA:N	1:181:A:ALA:CA	1:181:A:ALA:C	1:182:A:ALA:N	1	2.83
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	19	2.79
(1,279)	1:204:A:ASP:C	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	15	2.76
(1,208)	1:112:A:VAL:N	1:112:A:VAL:CA	1:112:A:VAL:C	1:113:A:LEU:N	12	2.76
(1,208)	1:112:A:VAL:N	1:112:A:VAL:CA	1:112:A:VAL:C	1:113:A:LEU:N	11	2.75
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	7	2.75
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	19	2.74
(1,236)	1:183:A:ARG:N	1:183:A:ARG:CA	1:183:A:ARG:C	1:184:A:LEU:N	7	2.7
(1,126)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:GLN:N	16	2.7
(1,217)	1:152:A:PRO:C	1:153:A:ARG:N	1:153:A:ARG:CA	1:153:A:ARG:C	15	2.67
(1,120)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:GLN:N	17	2.64
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	10	2.64
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	4	2.6
(1,220)	1:173:A:LEU:N	1:173:A:LEU:CA	1:173:A:LEU:C	1:174:A:ALA:N	4	2.59
(1,120)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:GLN:N	16	2.57
(1,218)	1:153:A:ARG:N	1:153:A:ARG:CA	1:153:A:ARG:C	1:154:A:GLY:N	20	2.51
(1,86)	1:46:A:LYS:N	1:46:A:LYS:CA	1:46:A:LYS:C	1:47:A:SER:N	11	2.49
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	11	2.49
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	12	2.49
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	17	2.49
(1,51)	1:28:A:GLN:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	15	2.46
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	13	2.44
(1,279)	1:204:A:ASP:C	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	17	2.43
(1,236)	1:183:A:ARG:N	1:183:A:ARG:CA	1:183:A:ARG:C	1:184:A:LEU:N	19	2.43
(1,234)	1:182:A:ALA:N	1:182:A:ALA:CA	1:182:A:ALA:C	1:183:A:ARG:N	5	2.43
(1,252)	1:191:A:GLY:N	1:191:A:GLY:CA	1:191:A:GLY:C	1:192:A:CYS:N	13	2.42
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	12	2.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,114)	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	1:61:A:ARG:N	9	2.36
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	9	2.35
(1,236)	1:183:A:ARG:N	1:183:A:ARG:CA	1:183:A:ARG:C	1:184:A:LEU:N	10	2.34
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	11	2.32
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	7	2.3
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	19	2.27
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	5	2.26
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	3	2.23
(1,54)	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	1:31:A:VAL:N	3	2.22
(1,238)	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	1:185:A:LEU:N	15	2.2
(1,216)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ARG:N	6	2.19
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	20	2.19
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	16	2.18
(1,216)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ARG:N	10	2.17
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	11	2.13
(1,278)	1:204:A:ASP:N	1:204:A:ASP:CA	1:204:A:ASP:C	1:205:A:TYR:N	5	2.12
(1,236)	1:183:A:ARG:N	1:183:A:ARG:CA	1:183:A:ARG:C	1:184:A:LEU:N	4	2.12
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	9	2.12
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	5	2.12
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	16	2.11
(1,216)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ARG:N	16	2.1
(1,208)	1:112:A:VAL:N	1:112:A:VAL:CA	1:112:A:VAL:C	1:113:A:LEU:N	20	2.1
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	16	2.07
(1,164)	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	1:91:A:LEU:N	19	2.07
(1,278)	1:204:A:ASP:N	1:204:A:ASP:CA	1:204:A:ASP:C	1:205:A:TYR:N	10	2.06
(1,214)	1:150:A:LEU:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	12	2.06
(1,211)	1:115:A:PRO:N	1:115:A:PRO:CA	1:115:A:PRO:C	1:116:A:HIS:N	2	2.03
(1,238)	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	1:185:A:LEU:N	2	2.02
(1,166)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:ASN:N	10	2.0
(1,70)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:LEU:N	20	2.0
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	20	2.0
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	4	1.94
(1,70)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:LEU:N	5	1.93
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	6	1.93
(1,166)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:ASN:N	19	1.9
(1,278)	1:204:A:ASP:N	1:204:A:ASP:CA	1:204:A:ASP:C	1:205:A:TYR:N	2	1.89
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	18	1.89
(1,236)	1:183:A:ARG:N	1:183:A:ARG:CA	1:183:A:ARG:C	1:184:A:LEU:N	12	1.86
(1,182)	1:99:A:LEU:N	1:99:A:LEU:CA	1:99:A:LEU:C	1:100:A:GLU:N	3	1.86
(1,70)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:LEU:N	13	1.86
(1,228)	1:179:A:ASP:N	1:179:A:ASP:CA	1:179:A:ASP:C	1:180:A:ASP:N	1	1.85
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	17	1.85
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	10	1.85
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	15	1.85
(1,230)	1:180:A:ASP:N	1:180:A:ASP:CA	1:180:A:ASP:C	1:181:A:ALA:N	20	1.84
(1,59)	1:32:A:GLY:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	6	1.79
(1,216)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ARG:N	4	1.78
(1,198)	1:107:A:GLN:N	1:107:A:GLN:CA	1:107:A:GLN:C	1:108:A:GLN:N	12	1.78
(1,260)	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	1:196:A:GLU:N	6	1.77
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	4	1.77
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	13	1.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	13	1.77
(1,228)	1:179:A:ASP:N	1:179:A:ASP:CA	1:179:A:ASP:C	1:180:A:ASP:N	20	1.75
(1,214)	1:150:A:LEU:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	3	1.73
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	4	1.71
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	5	1.71
(1,260)	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	1:196:A:GLU:N	14	1.69
(1,52)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:SER:N	7	1.66
(1,232)	1:181:A:ALA:N	1:181:A:ALA:CA	1:181:A:ALA:C	1:182:A:ALA:N	7	1.65
(1,178)	1:97:A:TRP:N	1:97:A:TRP:CA	1:97:A:TRP:C	1:98:A:LEU:N	5	1.63
(1,130)	1:73:A:ASP:N	1:73:A:ASP:CA	1:73:A:ASP:C	1:74:A:ILE:N	6	1.6
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	16	1.6
(1,61)	1:33:A:GLN:C	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	17	1.6
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	13	1.6
(1,166)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:ASN:N	1	1.59
(1,215)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	19	1.58
(1,238)	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	1:185:A:LEU:N	3	1.57
(1,238)	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	1:185:A:LEU:N	16	1.57
(1,164)	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	1:91:A:LEU:N	20	1.57
(1,216)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ARG:N	9	1.55
(1,209)	1:113:A:LEU:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	13	1.55
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	8	1.55
(1,200)	1:108:A:GLN:N	1:108:A:GLN:CA	1:108:A:GLN:C	1:109:A:ALA:N	5	1.54
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	19	1.53
(1,279)	1:204:A:ASP:C	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	4	1.52
(1,236)	1:183:A:ARG:N	1:183:A:ARG:CA	1:183:A:ARG:C	1:184:A:LEU:N	8	1.52
(1,215)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	1	1.51
(1,260)	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	1:196:A:GLU:N	19	1.5
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	20	1.5
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	12	1.49
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	5	1.49
(1,215)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	8	1.46
(1,70)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:LEU:N	10	1.45
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	6	1.42
(1,58)	1:32:A:GLY:N	1:32:A:GLY:CA	1:32:A:GLY:C	1:33:A:GLN:N	11	1.41
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	15	1.39
(1,53)	1:29:A:LEU:C	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	9	1.38
(1,51)	1:28:A:GLN:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	4	1.35
(1,260)	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	1:196:A:GLU:N	12	1.33
(1,121)	1:63:A:GLU:C	1:64:A:GLN:N	1:64:A:GLN:CA	1:64:A:GLN:C	18	1.33
(1,216)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ARG:N	14	1.32
(1,128)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:ASP:N	17	1.3
(1,120)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:GLN:N	8	1.3
(1,244)	1:187:A:GLU:N	1:187:A:GLU:CA	1:187:A:GLU:C	1:188:A:MET:N	9	1.29
(1,166)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:ASN:N	16	1.29
(1,46)	1:26:A:GLN:N	1:26:A:GLN:CA	1:26:A:GLN:C	1:27:A:GLN:N	20	1.29
(1,119)	1:62:A:LEU:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	8	1.28
(1,211)	1:115:A:PRO:N	1:115:A:PRO:CA	1:115:A:PRO:C	1:116:A:HIS:N	20	1.26
(1,53)	1:29:A:LEU:C	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	14	1.26
(1,38)	1:22:A:MET:N	1:22:A:MET:CA	1:22:A:MET:C	1:23:A:ASP:N	18	1.26
(1,278)	1:204:A:ASP:N	1:204:A:ASP:CA	1:204:A:ASP:C	1:205:A:TYR:N	6	1.25
(1,167)	1:91:A:LEU:C	1:92:A:ASN:N	1:92:A:ASN:CA	1:92:A:ASN:C	18	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,56)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:GLY:N	1	1.24
(1,213)	1:116:A:HIS:N	1:116:A:HIS:CA	1:116:A:HIS:C	1:117:A:GLN:N	14	1.23
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	11	1.23
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	3	1.22
(1,219)	1:172:A:ASP:C	1:173:A:LEU:N	1:173:A:LEU:CA	1:173:A:LEU:C	1	1.21
(1,110)	1:58:A:GLN:N	1:58:A:GLN:CA	1:58:A:GLN:C	1:59:A:GLN:N	7	1.19
(1,16)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:THR:N	9	1.19
(1,66)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:SER:N	20	1.18
(1,60)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:ILE:N	8	1.14
(1,52)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:SER:N	5	1.14
(1,214)	1:150:A:LEU:C	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	18	1.12
(1,120)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:GLN:N	11	1.12
(1,2)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:SER:N	10	1.11
(1,278)	1:204:A:ASP:N	1:204:A:ASP:CA	1:204:A:ASP:C	1:205:A:TYR:N	13	1.1
(1,132)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ALA:N	8	1.1
(1,62)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	14	1.1
(1,280)	1:205:A:TYR:N	1:205:A:TYR:CA	1:205:A:TYR:C	1:206:A:GLN:N	15	1.07
(1,55)	1:30:A:SER:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	10	1.06
(1,211)	1:115:A:PRO:N	1:115:A:PRO:CA	1:115:A:PRO:C	1:116:A:HIS:N	17	1.04
(1,59)	1:32:A:GLY:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	9	1.04
(1,52)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:SER:N	19	1.04
(1,198)	1:107:A:GLN:N	1:107:A:GLN:CA	1:107:A:GLN:C	1:108:A:GLN:N	20	1.03
(1,215)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:PRO:N	20	1.01
(1,53)	1:29:A:LEU:C	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	5	1.01