Full wwPDB NMR Structure Validation Report (i)

Dec 25, 2024 – 08:22 PM EST

PDB ID	:	8V9U
BMRB ID	:	31134
Title	:	Solution NMR structure of human DNMT1 N-terminal alpha-helical domain
Authors	:	Hu, Q.; Botuyan, M.V.; Mer, G.
Deposited on	:	2023-12-09

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

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

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

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

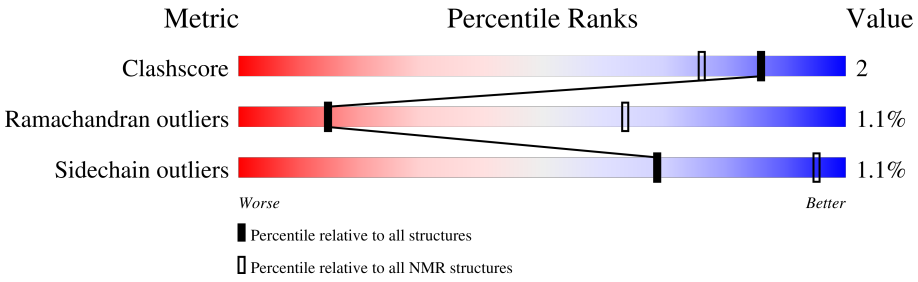
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 90%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	81	83% · 14%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 22 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:21-A:90 (70)	0.57	22

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

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

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

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 20, 21, 22, 24, 25, 26, 28, 29
2	19, 27, 30
Single-model clusters	23

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1353 atoms, of which 690 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	81	1353	413	690	115	132	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP P26358
A	14	HIS	-	expression tag	UNP P26358
A	15	MET	-	expression tag	UNP P26358

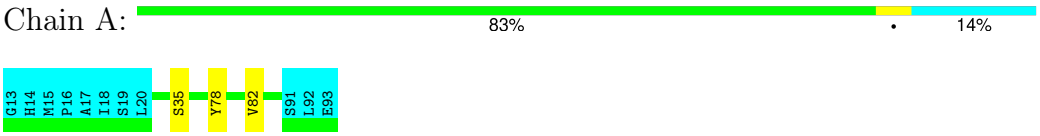
4 Residue-property plots

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: DNA (cytosine-5)-methyltransferase 1

Chain A:



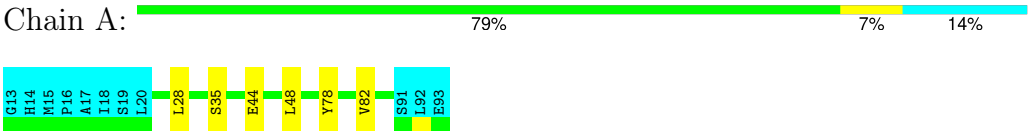
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

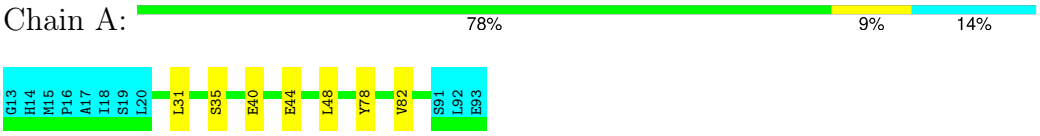
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

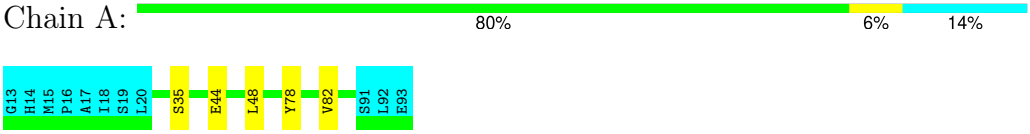
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

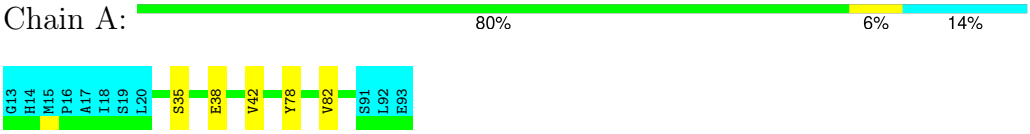
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

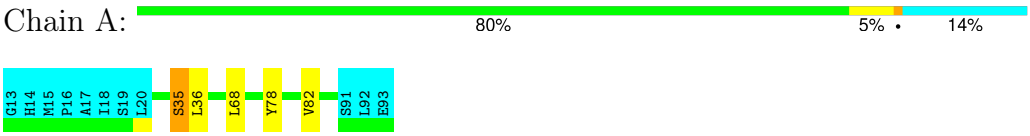
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

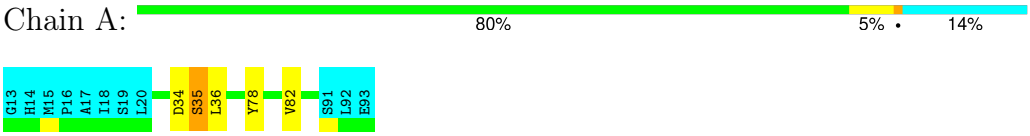
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

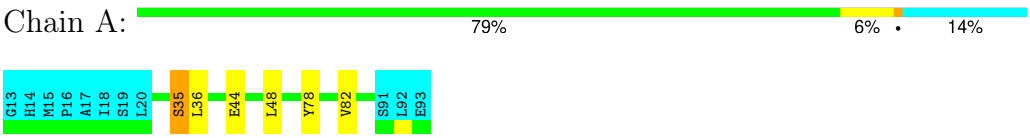
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

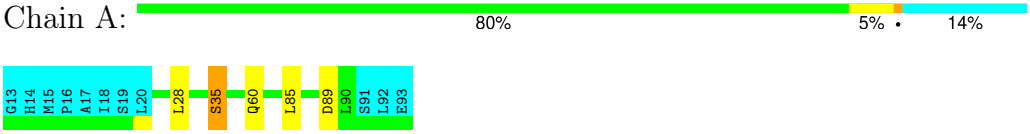
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

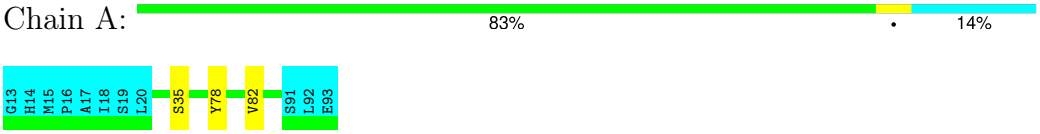
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

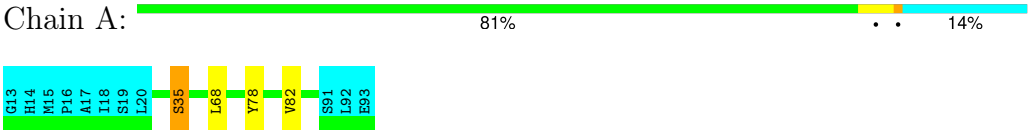
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

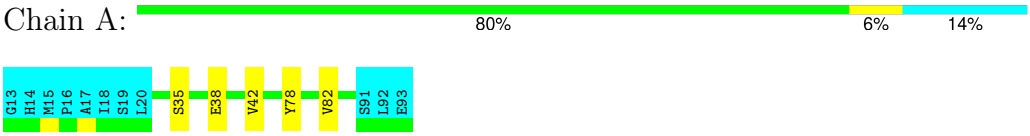
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

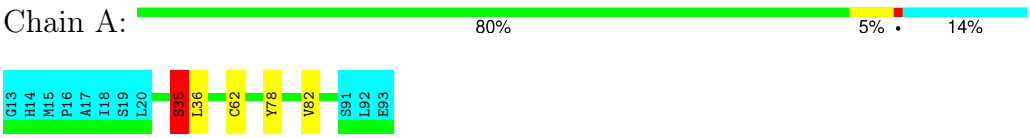
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

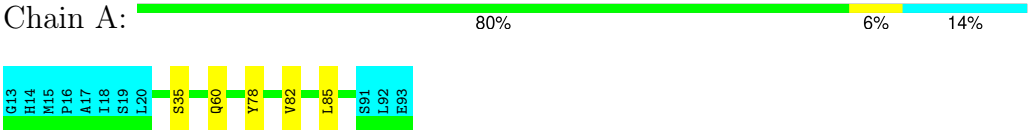
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

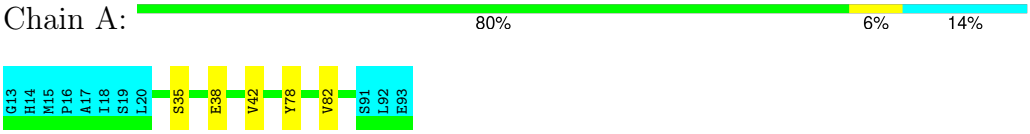
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

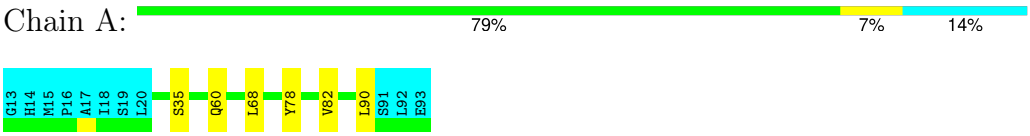
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

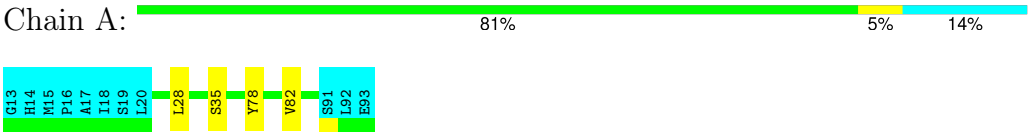
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

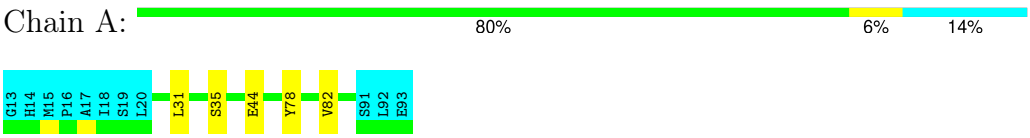
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

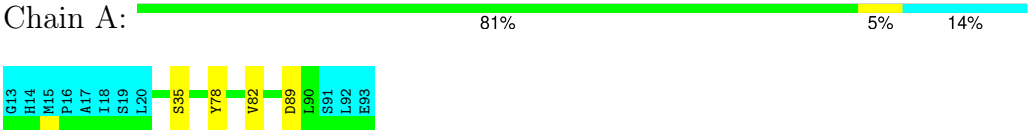
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

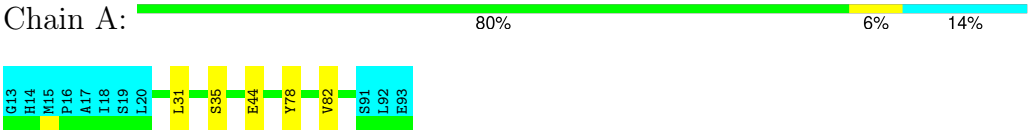
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

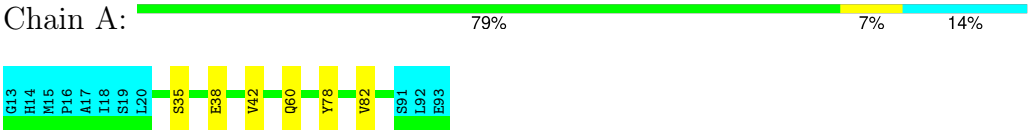
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

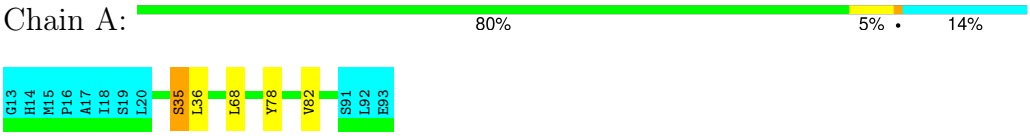
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

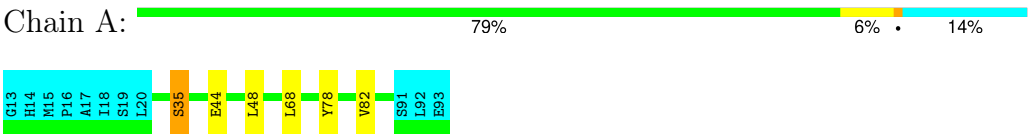
Chain A:



4.2.22 Score per residue for model 22 (medoid)

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

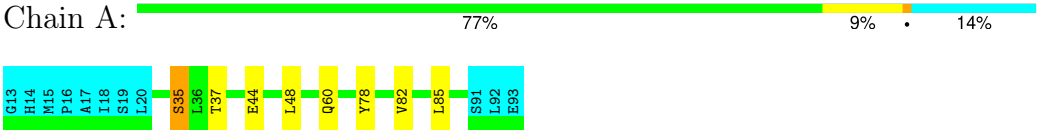
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

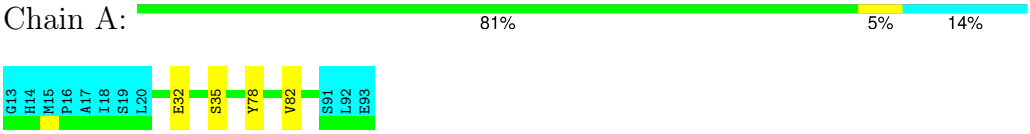
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

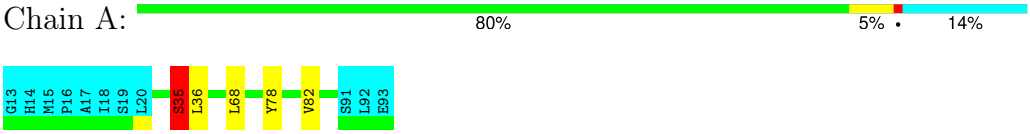
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

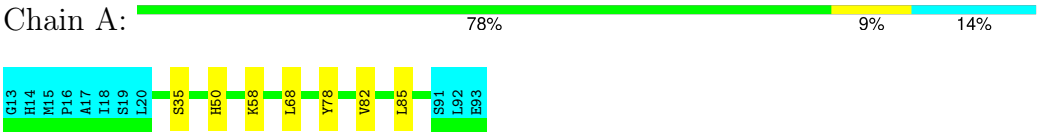
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

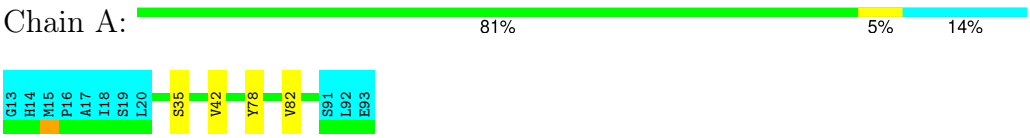
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

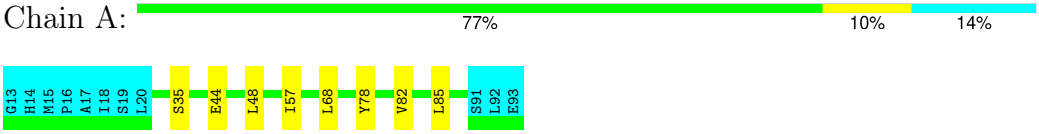
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

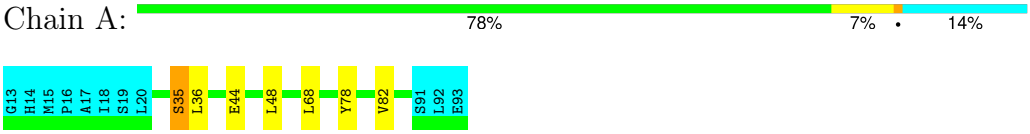
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

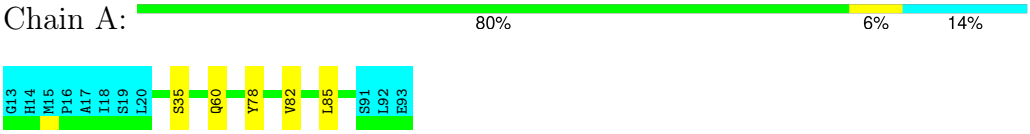
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
TALOS+	geometry optimization	
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1220
Number of shifts mapped to atoms	1030
Number of unparsed shifts	0
Number of shifts with mapping errors	190
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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	583	608	608	2±1
All	All	17490	18240	18240	71

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:TYR:O	1:A:82:VAL:HG23	0.59	1.97	26	29
1:A:68:LEU:HD11	1:A:78:TYR:CD2	0.55	2.37	22	3
1:A:31:LEU:HD13	1:A:44:GLU:OE1	0.52	2.04	2	2
1:A:60:GLN:OE1	1:A:85:LEU:HD11	0.51	2.07	30	4
1:A:68:LEU:HD11	1:A:78:TYR:CG	0.51	2.41	28	5
1:A:36:LEU:HD12	1:A:36:LEU:N	0.49	2.23	6	1
1:A:57:ILE:HG23	1:A:85:LEU:HD21	0.48	1.85	28	1
1:A:38:GLU:O	1:A:42:VAL:HG23	0.47	2.09	20	4
1:A:68:LEU:HD11	1:A:78:TYR:CD1	0.46	2.44	26	1
1:A:44:GLU:O	1:A:48:LEU:HD13	0.46	2.11	1	8
1:A:42:VAL:CG1	1:A:82:VAL:HG11	0.46	2.40	27	1
1:A:28:LEU:N	1:A:28:LEU:HD12	0.45	2.26	8	2
1:A:35:SER:C	1:A:36:LEU:HD12	0.43	2.34	12	5
1:A:31:LEU:HD13	1:A:44:GLU:OE2	0.42	2.15	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:HIS:CE1	1:A:58:LYS:HZ1	0.40	2.34	26	1
1:A:28:LEU:HD12	1:A:28:LEU:N	0.40	2.31	1	1
1:A:36:LEU:N	1:A:36:LEU:HD12	0.40	2.31	21	1
1:A:34:ASP:O	1:A:35:SER:C	0.40	2.60	6	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	70/81 (86%)	68±1 (98±1%)	1±1 (1±1%)	1±0 (1±1%)	15	64
All	All	2100/2430 (86%)	2051 (98%)	25 (1%)	24 (1%)	15	64

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	35	SER	24

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	68/77 (88%)	67±1 (99±1%)	1±1 (1±1%)	69	95
All	All	2040/2310 (88%)	2018 (99%)	22 (1%)	69	95

All 8 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	35	SER	13

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Mol	Chain	Res	Type	Models (Total)
1	A	89	ASP	2
1	A	60	GLN	2
1	A	40	GLU	1
1	A	62	CYS	1
1	A	37	THR	1
1	A	32	GLU	1
1	A	85	LEU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_ output*

7.1.1 Bookkeeping

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

Total number of shifts	1220
Number of shifts mapped to atoms	1030
Number of unparsed shifts	0
Number of shifts with mapping errors	190
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 4 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	VAL	HG12	0.883	.	1
1	A	120	VAL	HG13	0.883	.	1
1	A	120	VAL	HG22	0.883	.	1
1	A	120	VAL	HG23	0.883	.	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 190 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	ASN	H	8.407	.	1
1	A	94	ASN	HB2	2.768	.	1
1	A	94	ASN	HB3	2.768	.	1
1	A	94	ASN	HD22	6.891	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	ASN	C	175.823	.	1
1	A	94	ASN	CA	53.482	.	1
1	A	94	ASN	CB	38.908	.	1
1	A	94	ASN	N	119.353	.	1
1	A	94	ASN	ND2	112.633	.	1
1	A	95	GLY	H	8.379	.	1
1	A	95	GLY	C	174.195	.	1
1	A	95	GLY	CA	45.666	.	1
1	A	95	GLY	N	109.043	.	1
1	A	96	ALA	H	8.084	.	1
1	A	96	ALA	CA	52.73	.	1
1	A	96	ALA	CB	19.142	.	1
1	A	96	ALA	N	123.157	.	1
1	A	97	HIS	H	8.146	.	1
1	A	97	HIS	CA	56.309	.	1
1	A	97	HIS	CB	30.651	.	1
1	A	97	HIS	N	117.761	.	1
1	A	98	ALA	H	8.025	.	1
1	A	98	ALA	C	177.325	.	1
1	A	98	ALA	CA	52.509	.	1
1	A	98	ALA	CB	19.306	.	1
1	A	98	ALA	N	124.282	.	1
1	A	99	TYR	H	8.087	.	1
1	A	99	TYR	HA	4.498	.	1
1	A	99	TYR	HB2	3.008	.	2
1	A	99	TYR	HB3	2.938	.	2
1	A	99	TYR	HD1	7.059	.	1
1	A	99	TYR	HD2	7.059	.	1
1	A	99	TYR	HE1	6.783	.	1
1	A	99	TYR	HE2	6.783	.	1
1	A	99	TYR	C	175.437	.	1
1	A	99	TYR	CA	57.809	.	1
1	A	99	TYR	CB	38.632	.	1
1	A	99	TYR	CD1	133.044	.	1
1	A	99	TYR	CD2	133.044	.	1
1	A	99	TYR	CE1	118.016	.	1
1	A	99	TYR	CE2	118.016	.	1
1	A	99	TYR	N	119.03	.	1
1	A	100	ASN	H	8.255	.	1
1	A	100	ASN	C	174.91	.	1
1	A	100	ASN	CA	53.161	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	ASN	CB	38.769	.	1
1	A	100	ASN	N	120.445	.	1
1	A	101	ARG	H	8.182	.	1
1	A	101	ARG	C	176.358	.	1
1	A	101	ARG	CA	56.666	.	1
1	A	101	ARG	CB	30.803	.	1
1	A	101	ARG	N	121.353	.	1
1	A	102	GLU	H	8.153	.	1
1	A	102	GLU	C	174.762	.	1
1	A	102	GLU	CA	56.192	.	1
1	A	102	GLU	N	121.132	.	1
1	A	103	VAL	H	8.159	.	1
1	A	103	VAL	C	176.099	.	1
1	A	103	VAL	CA	62.608	.	1
1	A	103	VAL	CB	32.624	.	1
1	A	103	VAL	N	121.282	.	1
1	A	104	ASN	H	8.48	.	1
1	A	104	ASN	C	175.686	.	1
1	A	104	ASN	CA	53.674	.	1
1	A	104	ASN	CB	38.817	.	1
1	A	104	ASN	N	121.506	.	1
1	A	105	GLY	H	8.329	.	1
1	A	105	GLY	C	173.899	.	1
1	A	105	GLY	CA	45.588	.	1
1	A	105	GLY	N	108.918	.	1
1	A	106	ARG	H	8.071	.	1
1	A	106	ARG	C	176.077	.	1
1	A	106	ARG	CA	56.016	.	1
1	A	106	ARG	CB	30.794	.	1
1	A	106	ARG	N	120.236	.	1
1	A	107	LEU	H	8.28	.	1
1	A	107	LEU	C	177.449	.	1
1	A	107	LEU	CA	55.284	.	1
1	A	107	LEU	CB	42.232	.	1
1	A	107	LEU	N	123.163	.	1
1	A	108	GLU	H	8.466	.	1
1	A	108	GLU	C	176.269	.	1
1	A	108	GLU	CA	56.7	.	1
1	A	108	GLU	CB	30.222	.	1
1	A	108	GLU	N	121.794	.	1
1	A	109	ASN	H	8.23	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	ASN	C	177.012	.	1
1	A	109	ASN	CA	54.468	.	1
1	A	109	ASN	CB	41.369	.	1
1	A	109	ASN	N	121.131	.	1
1	A	110	GLY	H	8.369	.	1
1	A	110	GLY	C	174.215	.	1
1	A	110	GLY	CA	45.716	.	1
1	A	110	GLY	N	109.351	.	1
1	A	111	ASN	H	8.307	.	1
1	A	111	ASN	C	175.607	.	1
1	A	111	ASN	CA	53.647	.	1
1	A	111	ASN	CB	38.728	.	1
1	A	111	ASN	N	118.592	.	1
1	A	112	GLN	H	8.371	.	1
1	A	112	GLN	C	175.997	.	1
1	A	112	GLN	CA	56.236	.	1
1	A	112	GLN	CB	29.181	.	1
1	A	112	GLN	N	120.552	.	1
1	A	113	ALA	H	8.281	.	1
1	A	113	ALA	C	177.869	.	1
1	A	113	ALA	CA	52.771	.	1
1	A	113	ALA	CB	19.119	.	1
1	A	113	ALA	N	124.576	.	1
1	A	114	ARG	H	8.161	.	1
1	A	114	ARG	CA	56.337	.	1
1	A	114	ARG	CB	30.69	.	1
1	A	114	ARG	N	119.817	.	1
1	A	115	SER	H	8.292	.	1
1	A	115	SER	CA	58.76	.	1
1	A	115	SER	CB	63.578	.	1
1	A	115	SER	N	116.816	.	1
1	A	116	GLU	H	8.452	.	1
1	A	116	GLU	CA	56.884	.	1
1	A	116	GLU	CB	30.228	.	1
1	A	116	GLU	N	122.907	.	1
1	A	117	ALA	H	8.191	.	1
1	A	117	ALA	N	124.414	.	1
1	A	118	ARG	C	176.275	.	1
1	A	118	ARG	CB	30.716	.	1
1	A	119	ARG	H	8.362	.	1
1	A	119	ARG	C	176.753	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	119	ARG	CA	56.762	.	1
1	A	119	ARG	CB	30.297	.	1
1	A	119	ARG	N	121.442	.	1
1	A	120	VAL	H	8.122	.	1
1	A	120	VAL	HA	4.033	.	1
1	A	120	VAL	HB	2.021	.	1
1	A	120	VAL	HG11	0.883	.	1
1	A	120	VAL	HG12	0.883	.	1
1	A	120	VAL	HG13	0.883	.	1
1	A	120	VAL	HG21	0.883	.	1
1	A	120	VAL	HG22	0.883	.	1
1	A	120	VAL	HG23	0.883	.	1
1	A	120	VAL	C	176.652	.	1
1	A	120	VAL	CA	62.58	.	1
1	A	120	VAL	CB	32.752	.	1
1	A	120	VAL	N	120.691	.	1
1	A	121	GLY	H	8.498	.	1
1	A	121	GLY	HA2	4.072	.	1
1	A	121	GLY	HA3	3.934	.	1
1	A	121	GLY	C	174.154	.	1
1	A	121	GLY	CA	45.243	.	1
1	A	121	GLY	N	112.464	.	1
1	A	122	MET	H	8.146	.	1
1	A	122	MET	C	176.153	.	1
1	A	122	MET	CA	55.495	.	1
1	A	122	MET	CB	33.108	.	1
1	A	122	MET	N	119.787	.	1
1	A	123	ALA	H	8.366	.	1
1	A	123	ALA	C	177.402	.	1
1	A	123	ALA	CA	52.654	.	1
1	A	123	ALA	CB	19.235	.	1
1	A	123	ALA	N	125.011	.	1
1	A	124	ASP	H	8.254	.	1
1	A	124	ASP	C	176.27	.	1
1	A	124	ASP	CA	54.136	.	1
1	A	124	ASP	CB	41.329	.	1
1	A	124	ASP	N	119.648	.	1
1	A	125	ALA	H	8.253	.	1
1	A	125	ALA	C	177.647	.	1
1	A	125	ALA	CA	52.915	.	1
1	A	125	ALA	CB	19.154	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	ALA	N	124.412	.	1
1	A	126	ASN	H	8.381	.	1
1	A	126	ASN	C	174.9	.	1
1	A	126	ASN	N	116.719	.	1
1	A	127	SER	H	8.005	.	1
1	A	127	SER	N	117.024	.	1
1	A	131	PRO	C	176.773	.	1
1	A	132	LEU	H	8.378	.	1
1	A	132	LEU	C	177.436	.	1
1	A	132	LEU	CA	55.203	.	1
1	A	132	LEU	CB	42.386	.	1
1	A	132	LEU	N	122.535	.	1
1	A	133	SER	H	8.247	.	1
1	A	133	SER	C	173.339	.	1
1	A	133	SER	CA	58.219	.	1
1	A	133	SER	CB	63.946	.	1
1	A	133	SER	N	117.093	.	1
1	A	134	LYS	H	7.957	.	1
1	A	134	LYS	C	181.206	.	1
1	A	134	LYS	CA	57.871	.	1
1	A	134	LYS	CB	33.679	.	1
1	A	134	LYS	N	128.09	.	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	111	-0.48 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	106	0.03 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	101	-0.37 ± 0.12	None needed (< 0.5 ppm)
^{15}N	111	0.47 ± 0.30	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 90%, i.e. 926 atoms were assigned a chemical shift out of a possible 1030. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	341/349 (98%)	139/140 (99%)	134/140 (96%)	68/69 (99%)
Sidechain	568/655 (87%)	385/417 (92%)	178/208 (86%)	5/30 (17%)
Aromatic	17/26 (65%)	9/13 (69%)	8/12 (67%)	0/1 (0%)
Overall	926/1030 (90%)	533/570 (94%)	320/360 (89%)	73/100 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1024 atoms were assigned a chemical shift out of a possible 1169. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	376/403 (93%)	153/162 (94%)	148/162 (91%)	75/79 (95%)
Sidechain	631/733 (86%)	429/470 (91%)	197/233 (85%)	5/30 (17%)
Aromatic	17/33 (52%)	9/17 (53%)	8/14 (57%)	0/2 (0%)
Overall	1024/1169 (88%)	591/649 (91%)	353/409 (86%)	80/111 (72%)

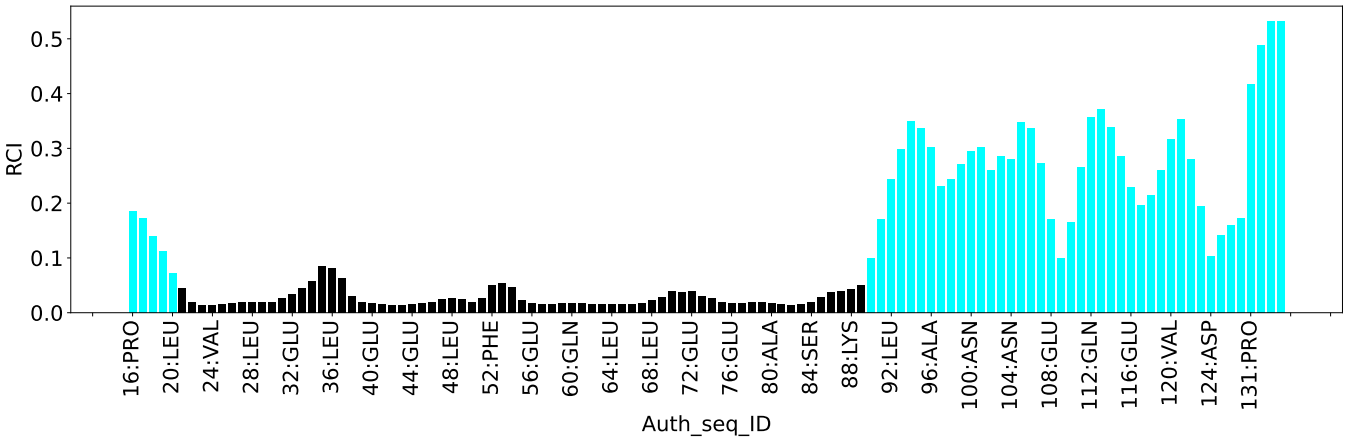
7.1.4 Statistically unusual chemical shifts (i)

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	937
Intra-residue (|i-j|=0)	243
Sequential (|i-j|=1)	288
Medium range (|i-j|>1 and |i-j|<5)	306
Long range (|i-j|≥5)	100
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	132
Number of unmapped restraints	0
Number of restraints per residue	13.2
Number of long range restraints per residue[1]	1.2

[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)	19.9	0.2
0.2-0.5 (Medium)	16.0	0.49
>0.5 (Large)	3.9	1.31

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)	2.2	4.61
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

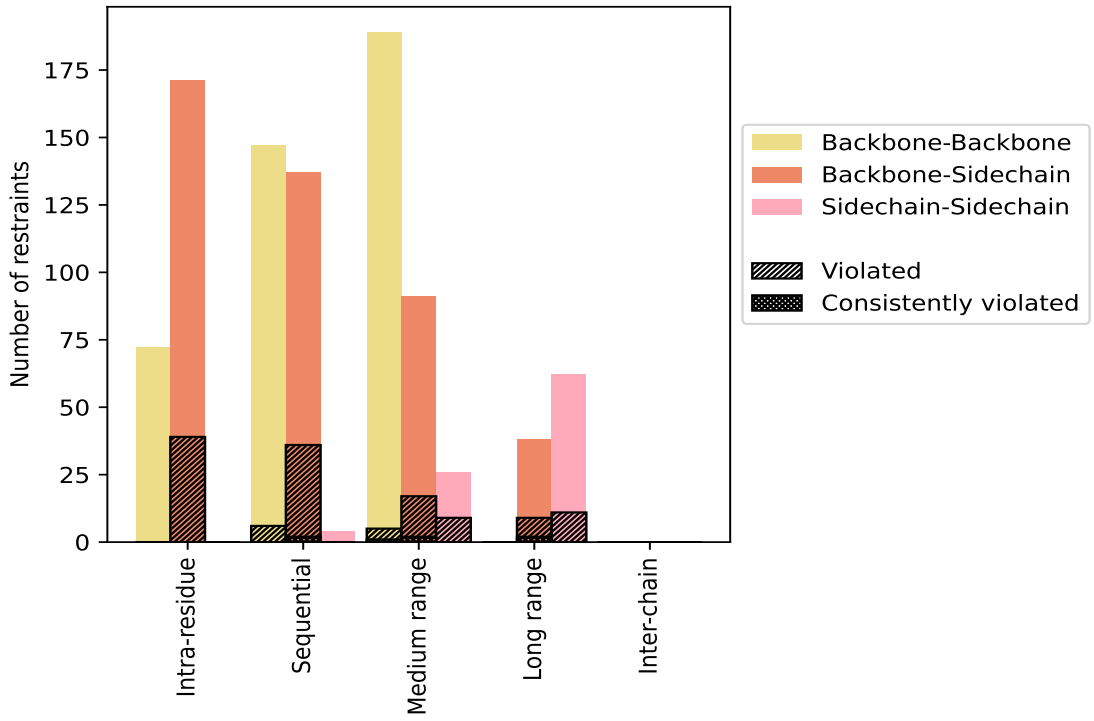
9.1 Summary of distance violations (i)

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)	243	25.9	39	16.0	4.2	0	0.0	0.0
Backbone-Backbone	72	7.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	171	18.2	39	22.8	4.2	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	288	30.7	42	14.6	4.5	2	0.7	0.2
Backbone-Backbone	147	15.7	6	4.1	0.6	0	0.0	0.0
Backbone-Sidechain	137	14.6	36	26.3	3.8	2	1.5	0.2
Sidechain-Sidechain	4	0.4	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	306	32.7	31	10.1	3.3	3	1.0	0.3
Backbone-Backbone	189	20.2	5	2.6	0.5	1	0.5	0.1
Backbone-Sidechain	91	9.7	17	18.7	1.8	2	2.2	0.2
Sidechain-Sidechain	26	2.8	9	34.6	1.0	0	0.0	0.0
Long range (|i-j|≥5)	100	10.7	20	20.0	2.1	2	2.0	0.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	38	4.1	9	23.7	1.0	2	5.3	0.2
Sidechain-Sidechain	62	6.6	11	17.7	1.2	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	937	100.0	132	14.1	14.1	7	0.7	0.7
Backbone-Backbone	408	43.5	11	2.7	1.2	1	0.2	0.1
Backbone-Sidechain	437	46.6	101	23.1	10.8	6	1.4	0.6
Sidechain-Sidechain	92	9.8	20	21.7	2.1	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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	13	13	7	8	0	41	0.28	1.15	0.22	0.18
2	7	17	8	9	0	41	0.28	0.91	0.2	0.21
3	7	12	10	7	0	36	0.26	1.14	0.22	0.2
4	11	17	13	9	0	50	0.24	0.81	0.15	0.2
5	13	18	6	6	0	43	0.25	0.96	0.2	0.16
6	6	16	8	5	0	35	0.24	0.9	0.17	0.15
7	8	16	11	9	0	44	0.27	1.16	0.25	0.16
8	8	19	7	9	0	43	0.26	1.2	0.2	0.21
9	14	12	6	9	0	41	0.31	1.12	0.24	0.23
10	6	14	7	6	0	33	0.29	1.21	0.25	0.22

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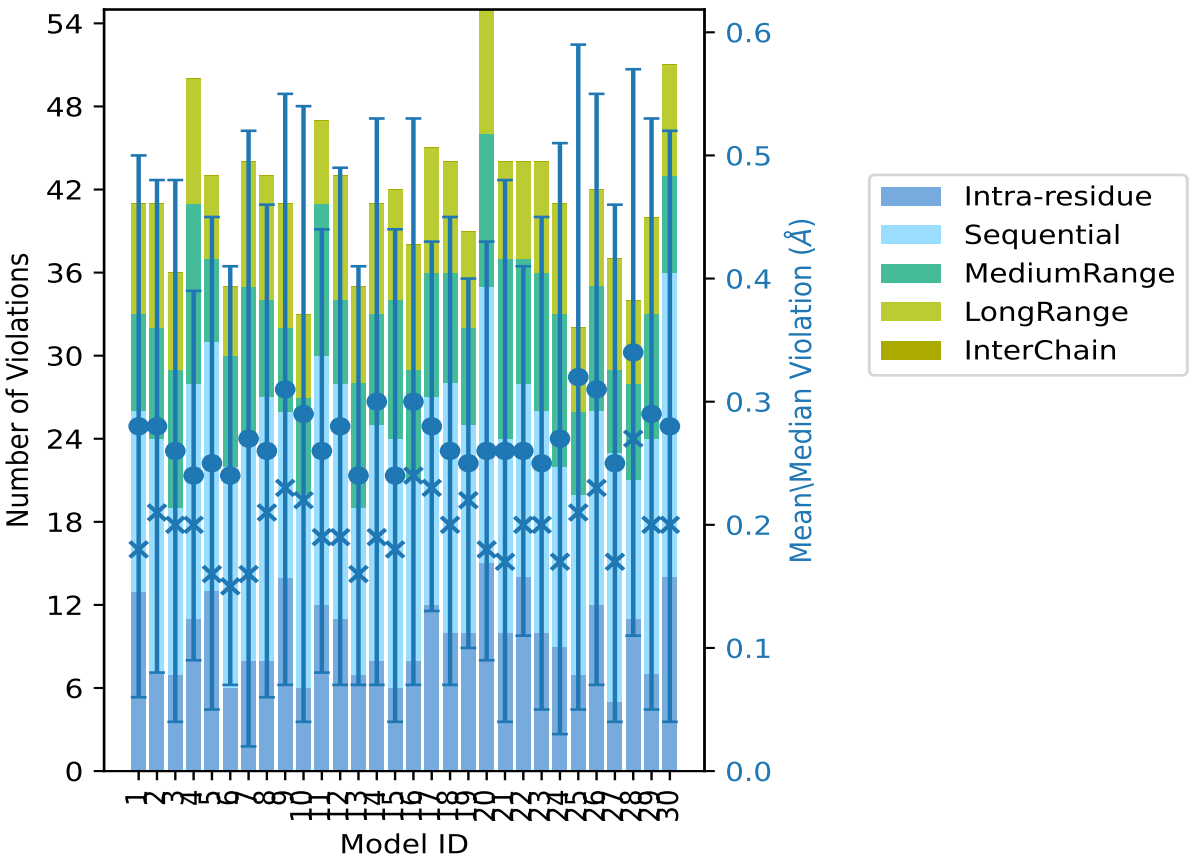
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	12	18	11	6	0	47	0.26	1.0	0.18	0.19
12	11	17	6	9	0	43	0.28	1.11	0.21	0.19
13	7	12	9	7	0	35	0.24	0.88	0.17	0.16
14	8	17	8	8	0	41	0.3	1.2	0.23	0.19
15	6	18	10	8	0	42	0.24	0.98	0.2	0.18
16	8	13	8	9	0	38	0.3	1.1	0.23	0.24
17	12	15	9	9	0	45	0.28	0.72	0.15	0.23
18	10	18	8	8	0	44	0.26	1.05	0.19	0.2
19	10	15	7	7	0	39	0.25	0.89	0.15	0.22
20	15	20	11	9	0	55	0.26	0.89	0.17	0.18
21	10	14	13	7	0	44	0.26	1.29	0.22	0.17
22	14	14	9	7	0	44	0.26	0.82	0.15	0.2
23	10	16	10	8	0	44	0.25	1.16	0.2	0.2
24	9	13	11	8	0	41	0.27	1.03	0.24	0.17
25	7	13	6	6	0	32	0.32	1.19	0.27	0.21
26	12	14	9	7	0	42	0.31	1.31	0.24	0.23
27	5	18	6	8	0	37	0.25	1.11	0.21	0.17
28	11	10	7	6	0	34	0.34	0.96	0.23	0.27
29	7	17	9	7	0	40	0.29	1.18	0.24	0.2
30	14	22	7	8	0	51	0.28	1.28	0.24	0.2

[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

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, 805(IR:204, SQ:246, MR:275, LR:80, 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]	%
7	5	7	4	0	23	1	3.3
3	3	5	4	0	15	2	6.7
3	6	5	0	0	14	3	10.0
1	3	2	1	0	7	4	13.3
4	2	0	0	0	6	5	16.7
3	0	0	0	0	3	6	20.0

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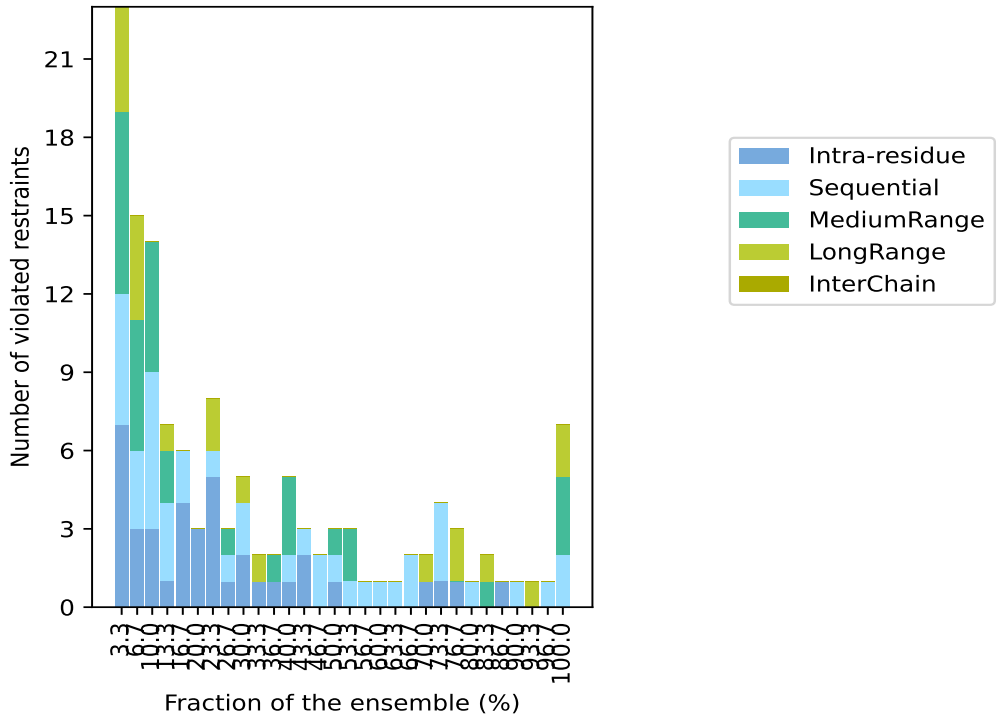
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
5	1	0	2	0	8	7	23.3
1	1	1	0	0	3	8	26.7
2	2	0	1	0	5	9	30.0
1	0	0	1	0	2	10	33.3
1	0	1	0	0	2	11	36.7
1	1	3	0	0	5	12	40.0
2	1	0	0	0	3	13	43.3
0	2	0	0	0	2	14	46.7
1	1	1	0	0	3	15	50.0
0	1	2	0	0	3	16	53.3
0	1	0	0	0	1	17	56.7
0	1	0	0	0	1	18	60.0
0	1	0	0	0	1	19	63.3
0	2	0	0	0	2	20	66.7
1	0	0	1	0	2	21	70.0
1	3	0	0	0	4	22	73.3
1	0	0	2	0	3	23	76.7
0	1	0	0	0	1	24	80.0
0	0	1	1	0	2	25	83.3
1	0	0	0	0	1	26	86.7
0	1	0	0	0	1	27	90.0
0	0	0	1	0	1	28	93.3
0	1	0	0	0	1	29	96.7
0	2	3	2	0	7	30	100.0

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

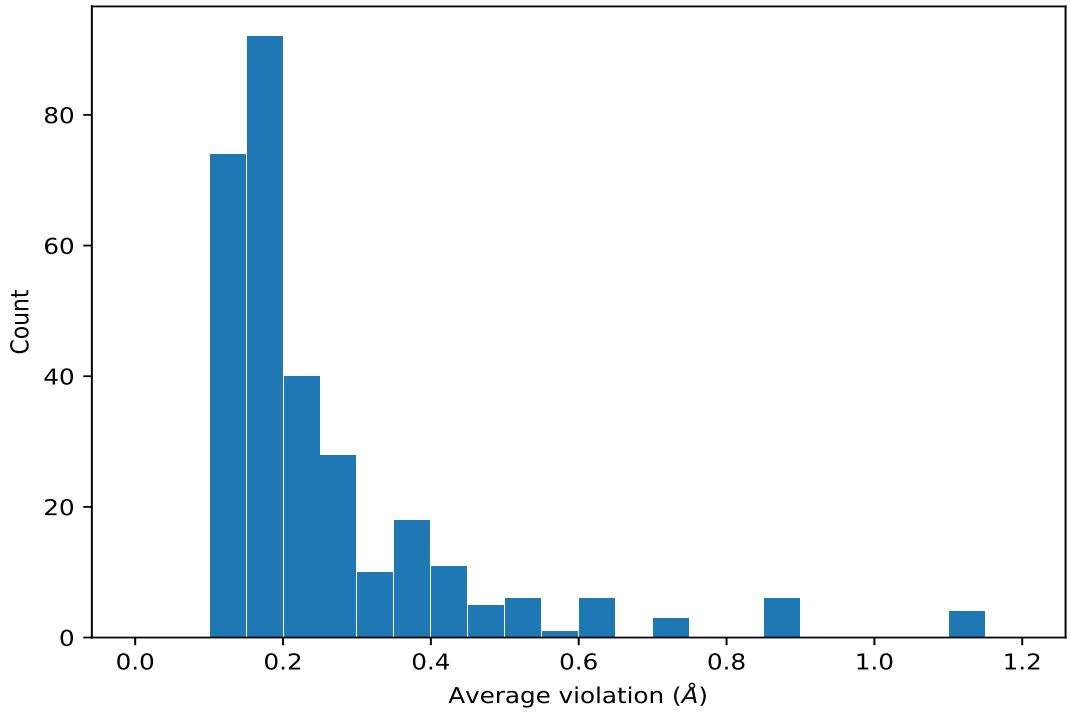
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	30	0.86	0.1	0.87
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	30	0.86	0.1	0.87
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	30	0.86	0.1	0.87
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	30	0.86	0.1	0.87
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	30	0.86	0.1	0.87
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	30	0.86	0.1	0.87
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	30	0.63	0.09	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	30	0.63	0.09	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	30	0.63	0.09	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	30	0.63	0.09	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	30	0.63	0.09	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	30	0.63	0.09	0.66
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	30	0.28	0.03	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	30	0.28	0.03	0.28
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	30	0.27	0.03	0.28
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	30	0.25	0.03	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	30	0.25	0.03	0.24
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	30	0.25	0.03	0.24
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	30	0.25	0.04	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	30	0.25	0.04	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	30	0.25	0.04	0.25
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	30	0.16	0.03	0.15
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	29	0.36	0.05	0.37
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	28	0.19	0.06	0.18
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	28	0.19	0.06	0.18
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	28	0.19	0.06	0.18
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	28	0.19	0.06	0.18
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	27	0.15	0.03	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	27	0.15	0.03	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	27	0.15	0.03	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	27	0.15	0.03	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	27	0.15	0.03	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	27	0.15	0.03	0.14
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	26	0.16	0.02	0.16
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	25	0.71	0.27	0.83
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	25	0.71	0.27	0.83
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	25	0.71	0.27	0.83
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	25	0.29	0.11	0.34
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	25	0.29	0.11	0.34
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	24	0.18	0.04	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	24	0.18	0.04	0.17
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	23	0.51	0.22	0.57
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	23	0.51	0.22	0.57
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	23	0.51	0.22	0.57
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	23	0.51	0.22	0.57
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	23	0.51	0.22	0.57
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	23	0.51	0.22	0.57
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	23	0.37	0.04	0.38
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	23	0.13	0.02	0.13
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	23	0.13	0.02	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	23	0.13	0.02	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	23	0.13	0.02	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	23	0.13	0.02	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	23	0.13	0.02	0.13
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	22	0.18	0.12	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	22	0.16	0.06	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	22	0.16	0.06	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	22	0.16	0.06	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	22	0.16	0.03	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	22	0.16	0.03	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	22	0.15	0.02	0.15
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	22	0.15	0.02	0.15
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	21	1.14	0.1	1.15
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	21	1.14	0.1	1.15
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	21	1.14	0.1	1.15
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	21	1.14	0.1	1.15
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	21	0.25	0.02	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	21	0.25	0.02	0.25
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	20	0.18	0.04	0.2
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	20	0.18	0.04	0.2
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	20	0.14	0.02	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	20	0.14	0.02	0.15
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	19	0.14	0.02	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	19	0.14	0.02	0.13
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	18	0.14	0.04	0.13
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	18	0.14	0.04	0.13
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	17	0.15	0.02	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	17	0.15	0.02	0.15
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	16	0.18	0.06	0.16
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	16	0.15	0.03	0.14
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	16	0.15	0.03	0.14
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	16	0.15	0.03	0.14
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	16	0.14	0.04	0.12
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	16	0.14	0.04	0.12
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	16	0.14	0.04	0.12
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	16	0.14	0.04	0.12
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	16	0.14	0.04	0.12
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	16	0.14	0.04	0.12
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	15	0.41	0.04	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	15	0.41	0.04	0.39
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	15	0.16	0.03	0.17
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	15	0.16	0.03	0.17
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	15	0.12	0.02	0.12
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	14	0.2	0.05	0.19
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	14	0.11	0.01	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	14	0.11	0.01	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	14	0.11	0.01	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	14	0.11	0.01	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	14	0.11	0.01	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	14	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	13	0.39	0.03	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	13	0.39	0.03	0.41
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	13	0.35	0.03	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	13	0.35	0.03	0.34
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	13	0.13	0.02	0.13
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	13	0.13	0.02	0.13
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	12	0.31	0.02	0.3
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	12	0.31	0.02	0.3
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	12	0.15	0.06	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	12	0.15	0.06	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	12	0.15	0.06	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	12	0.15	0.06	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	12	0.15	0.06	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	12	0.15	0.06	0.13
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	12	0.15	0.04	0.14
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	12	0.15	0.04	0.14
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	12	0.15	0.04	0.14
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	12	0.15	0.04	0.14
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	12	0.15	0.04	0.14
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	12	0.15	0.04	0.14
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	12	0.14	0.04	0.12
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	12	0.14	0.04	0.12
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	12	0.14	0.04	0.12
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	12	0.14	0.04	0.12
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	12	0.14	0.04	0.12
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	12	0.14	0.04	0.12
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	12	0.12	0.01	0.12
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	12	0.12	0.01	0.12
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	11	0.12	0.02	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	11	0.12	0.02	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	11	0.12	0.02	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	11	0.11	0.01	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	11	0.11	0.01	0.11
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	10	0.3	0.05	0.31
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	10	0.17	0.05	0.15
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	10	0.17	0.05	0.15
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	10	0.17	0.05	0.15
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	9	0.47	0.01	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	9	0.47	0.01	0.47
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	9	0.43	0.03	0.43
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	9	0.38	0.03	0.39
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	9	0.38	0.03	0.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	9	0.2	0.06	0.2
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	9	0.2	0.06	0.2
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	9	0.2	0.06	0.2
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	9	0.2	0.06	0.2
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	9	0.2	0.06	0.2
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	9	0.2	0.06	0.2
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	9	0.12	0.01	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	9	0.12	0.01	0.11
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	8	0.36	0.03	0.35
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	8	0.36	0.03	0.35
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	8	0.18	0.02	0.18
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	8	0.18	0.02	0.18
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	8	0.18	0.02	0.18
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	8	0.18	0.02	0.18
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	8	0.18	0.02	0.18
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	8	0.18	0.02	0.18
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	8	0.12	0.02	0.12
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	8	0.12	0.02	0.12
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG2	7	0.42	0.01	0.42
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG3	7	0.42	0.01	0.42
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB2	7	0.34	0.04	0.33
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB3	7	0.34	0.04	0.33
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE2	7	0.32	0.06	0.28
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE3	7	0.32	0.06	0.28
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD11	7	0.2	0.06	0.21
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD12	7	0.2	0.06	0.21
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD13	7	0.2	0.06	0.21
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB2	7	0.18	0.04	0.18
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB3	7	0.18	0.04	0.18
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB2	7	0.18	0.04	0.18
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB3	7	0.18	0.04	0.18
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB2	7	0.18	0.04	0.18
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB3	7	0.18	0.04	0.18
(1,18)	1:19:A:SER:H	1:18:A:ILE:HB	7	0.14	0.03	0.14
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD21	7	0.12	0.01	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD22	7	0.12	0.01	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD23	7	0.12	0.01	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG21	7	0.11	0.01	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG22	7	0.11	0.01	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG23	7	0.11	0.01	0.11
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG2	6	0.41	0.01	0.41
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG3	6	0.41	0.01	0.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG2	6	0.41	0.03	0.39
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG3	6	0.41	0.03	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG2	6	0.39	0.01	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG3	6	0.39	0.01	0.39
(1,24)	1:20:A:LEU:H	1:19:A:SER:HA	5	0.56	0.01	0.57
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG2	5	0.43	0.01	0.44
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG3	5	0.43	0.01	0.44
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD11	5	0.26	0.05	0.24
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD12	5	0.26	0.05	0.24
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD13	5	0.26	0.05	0.24
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG2	5	0.23	0.12	0.17
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG3	5	0.23	0.12	0.17
(1,12)	1:18:A:ILE:H	1:18:A:ILE:HB	5	0.2	0.08	0.24
(1,399)	1:50:A:HIS:H	1:50:A:HIS:HD2	5	0.19	0.05	0.19
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD2	4	0.28	0.06	0.26
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD3	4	0.28	0.06	0.26
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB2	4	0.26	0.02	0.26
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB3	4	0.26	0.02	0.26
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG12	4	0.22	0.11	0.18
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG13	4	0.22	0.11	0.18
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD11	4	0.15	0.03	0.15
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD12	4	0.15	0.03	0.15
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD13	4	0.15	0.03	0.15
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD11	4	0.15	0.03	0.15
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD12	4	0.15	0.03	0.15
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD13	4	0.15	0.03	0.15
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD21	4	0.14	0.01	0.14
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD22	4	0.14	0.01	0.14
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD23	4	0.14	0.01	0.14
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB2	4	0.12	0.01	0.12
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB3	4	0.12	0.01	0.12
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG2	4	0.11	0.01	0.11
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG3	4	0.11	0.01	0.11
(1,501)	1:60:A:GLN:H	1:60:A:GLN:HG2	3	0.35	0.17	0.47
(1,501)	1:60:A:GLN:H	1:60:A:GLN:HG3	3	0.35	0.17	0.47
(1,717)	1:76:A:GLU:H	1:75:A:GLU:HB2	3	0.25	0.02	0.23
(1,717)	1:76:A:GLU:H	1:75:A:GLU:HB3	3	0.25	0.02	0.23
(1,269)	1:40:A:GLU:H	1:40:A:GLU:HG2	3	0.23	0.14	0.14
(1,269)	1:40:A:GLU:H	1:40:A:GLU:HG3	3	0.23	0.14	0.14
(1,258)	1:39:A:LYS:H	1:38:A:GLU:HG2	3	0.2	0.13	0.11
(1,258)	1:39:A:LYS:H	1:38:A:GLU:HG3	3	0.2	0.13	0.11
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB1	3	0.19	0.04	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB2	3	0.19	0.04	0.21
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB3	3	0.19	0.04	0.21
(1,856)	1:86:A:LEU:HA	1:89:A:ASP:HB2	3	0.18	0.06	0.14
(1,856)	1:86:A:LEU:HA	1:89:A:ASP:HB3	3	0.18	0.06	0.14
(1,245)	1:37:A:THR:HG21	1:40:A:GLU:HG2	3	0.18	0.07	0.14
(1,245)	1:37:A:THR:HG21	1:40:A:GLU:HG3	3	0.18	0.07	0.14
(1,245)	1:37:A:THR:HG22	1:40:A:GLU:HG2	3	0.18	0.07	0.14
(1,245)	1:37:A:THR:HG22	1:40:A:GLU:HG3	3	0.18	0.07	0.14
(1,245)	1:37:A:THR:HG23	1:40:A:GLU:HG2	3	0.18	0.07	0.14
(1,245)	1:37:A:THR:HG23	1:40:A:GLU:HG3	3	0.18	0.07	0.14
(1,908)	1:92:A:LEU:H	1:91:A:SER:HB2	3	0.16	0.02	0.17
(1,908)	1:92:A:LEU:H	1:91:A:SER:HB3	3	0.16	0.02	0.17
(1,483)	1:59:A:ASN:H	1:58:A:LYS:HG2	3	0.11	0.0	0.11
(1,483)	1:59:A:ASN:H	1:58:A:LYS:HG3	3	0.11	0.0	0.11
(1,504)	1:60:A:GLN:HE21	1:57:A:ILE:HA	3	0.11	0.01	0.11
(1,504)	1:60:A:GLN:HE22	1:57:A:ILE:HA	3	0.11	0.01	0.11
(1,920)	1:93:A:GLU:H	1:93:A:GLU:HG2	3	0.11	0.01	0.11
(1,920)	1:93:A:GLU:H	1:93:A:GLU:HG3	3	0.11	0.01	0.11
(1,286)	1:42:A:VAL:H	1:39:A:LYS:HA	3	0.11	0.01	0.1
(1,764)	1:80:A:ALA:H	1:77:A:GLY:HA2	3	0.11	0.0	0.11
(1,764)	1:80:A:ALA:H	1:77:A:GLY:HA3	3	0.11	0.0	0.11
(1,906)	1:91:A:SER:H	1:92:A:LEU:H	3	0.1	0.0	0.1
(1,9)	1:18:A:ILE:H	1:17:A:ALA:HA	2	0.48	0.03	0.48
(1,473)	1:58:A:LYS:H	1:58:A:LYS:HD2	2	0.47	0.0	0.47
(1,473)	1:58:A:LYS:H	1:58:A:LYS:HD3	2	0.47	0.0	0.47
(1,257)	1:39:A:LYS:H	1:38:A:GLU:HB2	2	0.38	0.01	0.38
(1,257)	1:39:A:LYS:H	1:38:A:GLU:HB3	2	0.38	0.01	0.38
(1,261)	1:39:A:LYS:H	1:39:A:LYS:HG2	2	0.36	0.04	0.36
(1,261)	1:39:A:LYS:H	1:39:A:LYS:HG3	2	0.36	0.04	0.36
(1,239)	1:37:A:THR:H	1:37:A:THR:HG21	2	0.3	0.18	0.3
(1,239)	1:37:A:THR:H	1:37:A:THR:HG22	2	0.3	0.18	0.3
(1,239)	1:37:A:THR:H	1:37:A:THR:HG23	2	0.3	0.18	0.3
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD11	2	0.28	0.02	0.28
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD12	2	0.28	0.02	0.28
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD13	2	0.28	0.02	0.28
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD21	2	0.28	0.02	0.28
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD22	2	0.28	0.02	0.28
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD23	2	0.28	0.02	0.28
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG21	2	0.24	0.03	0.24
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG22	2	0.24	0.03	0.24
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG23	2	0.24	0.03	0.24
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG21	2	0.24	0.03	0.24

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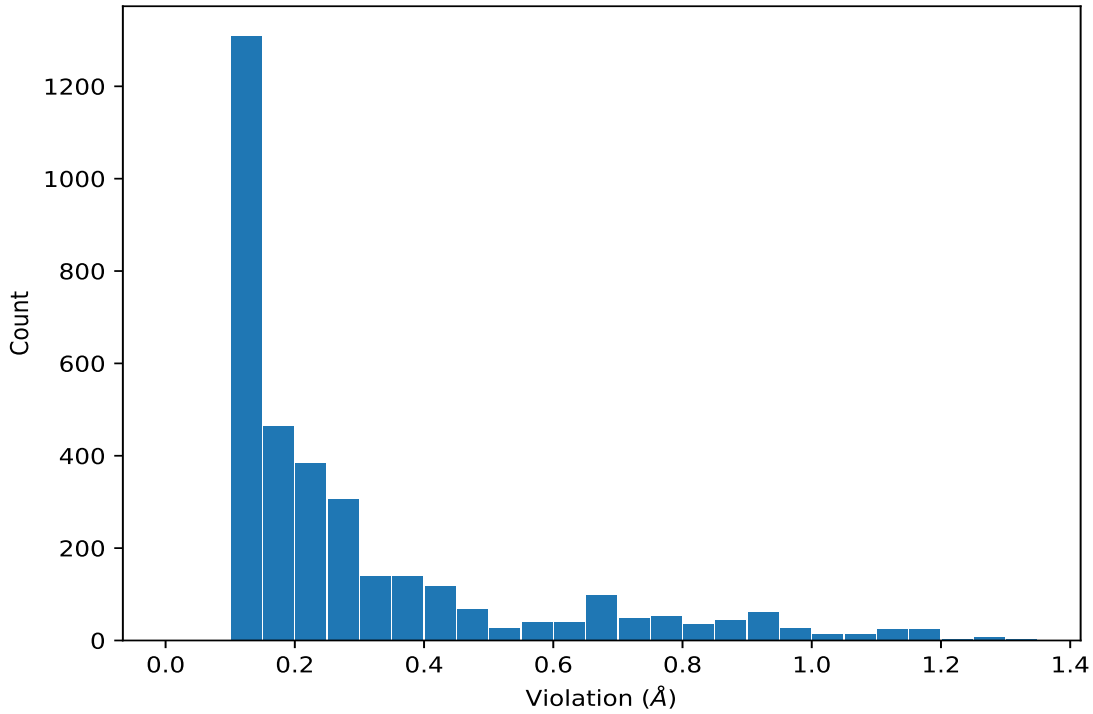
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG22	2	0.24	0.03	0.24
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG23	2	0.24	0.03	0.24
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD11	2	0.24	0.03	0.24
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD12	2	0.24	0.03	0.24
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD13	2	0.24	0.03	0.24
(1,81)	1:24:A:VAL:HG11	1:52:A:PHE:HD1	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG11	1:52:A:PHE:HD2	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG12	1:52:A:PHE:HD1	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG12	1:52:A:PHE:HD2	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG13	1:52:A:PHE:HD1	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG13	1:52:A:PHE:HD2	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG21	1:52:A:PHE:HD1	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG21	1:52:A:PHE:HD2	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG22	1:52:A:PHE:HD1	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG22	1:52:A:PHE:HD2	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG23	1:52:A:PHE:HD1	2	0.21	0.01	0.21
(1,81)	1:24:A:VAL:HG23	1:52:A:PHE:HD2	2	0.21	0.01	0.21
(1,297)	1:42:A:VAL:HA	1:45:A:LYS:HD2	2	0.18	0.02	0.18
(1,297)	1:42:A:VAL:HA	1:45:A:LYS:HD3	2	0.18	0.02	0.18
(1,48)	1:20:A:LEU:HB2	1:25:A:ARG:HD2	2	0.18	0.03	0.18
(1,48)	1:20:A:LEU:HB2	1:25:A:ARG:HD3	2	0.18	0.03	0.18
(1,48)	1:20:A:LEU:HB3	1:25:A:ARG:HD2	2	0.18	0.03	0.18
(1,48)	1:20:A:LEU:HB3	1:25:A:ARG:HD3	2	0.18	0.03	0.18
(1,727)	1:77:A:GLY:H	1:76:A:GLU:HB2	2	0.17	0.04	0.17
(1,727)	1:77:A:GLY:H	1:76:A:GLU:HB3	2	0.17	0.04	0.17
(1,870)	1:87:A:ASN:HD21	1:84:A:SER:HA	2	0.16	0.02	0.16
(1,870)	1:87:A:ASN:HD22	1:84:A:SER:HA	2	0.16	0.02	0.16
(1,926)	1:42:A:VAL:HG21	1:83:A:LYS:HA	2	0.15	0.03	0.15
(1,926)	1:42:A:VAL:HG22	1:83:A:LYS:HA	2	0.15	0.03	0.15
(1,926)	1:42:A:VAL:HG23	1:83:A:LYS:HA	2	0.15	0.03	0.15
(1,606)	1:66:A:THR:HG21	1:70:A:LYS:HE2	2	0.12	0.0	0.12
(1,606)	1:66:A:THR:HG21	1:70:A:LYS:HE3	2	0.12	0.0	0.12
(1,606)	1:66:A:THR:HG22	1:70:A:LYS:HE2	2	0.12	0.0	0.12
(1,606)	1:66:A:THR:HG22	1:70:A:LYS:HE3	2	0.12	0.0	0.12
(1,606)	1:66:A:THR:HG23	1:70:A:LYS:HE2	2	0.12	0.0	0.12
(1,606)	1:66:A:THR:HG23	1:70:A:LYS:HE3	2	0.12	0.0	0.12

[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)
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	26	1.31
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	26	1.31
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	26	1.31
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	26	1.31
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	21	1.29
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	21	1.29
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	21	1.29
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	21	1.29
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	30	1.28
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	30	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	30	1.28
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	30	1.28
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	10	1.21
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	10	1.21
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	10	1.21
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	10	1.21
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	8	1.2
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	8	1.2
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	8	1.2
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	8	1.2
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	14	1.2
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	14	1.2
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	14	1.2
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	14	1.2
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	25	1.19
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	25	1.19
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	25	1.19
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	25	1.19
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	29	1.18
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	29	1.18
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	29	1.18
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	29	1.18
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	7	1.16
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	7	1.16
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	7	1.16
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	7	1.16
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	23	1.16
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	23	1.16
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	23	1.16
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	23	1.16
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	1	1.15
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	1	1.15
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	1	1.15
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	1	1.15
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	3	1.14
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	3	1.14
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	3	1.14
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	3	1.14
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	9	1.12
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	9	1.12
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	9	1.12
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	9	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	12	1.11
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	12	1.11
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	12	1.11
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	12	1.11
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	27	1.11
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	27	1.11
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	27	1.11
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	27	1.11
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	16	1.1
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	16	1.1
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	16	1.1
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	16	1.1
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	7	1.09
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	7	1.09
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	7	1.09
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	10	1.06
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	10	1.06
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	10	1.06
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	10	1.06
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	10	1.06
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	10	1.06
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	18	1.05
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	18	1.05
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	18	1.05
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	18	1.05
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	24	1.03
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	24	1.03
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	24	1.03
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	24	1.03
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	16	1.01
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	16	1.01
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	16	1.01
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	16	1.01
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	16	1.01
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	16	1.01
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	11	1.0
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	11	1.0
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	11	1.0
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	26	0.98
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	26	0.98
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	26	0.98
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	26	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	26	0.98
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	26	0.98
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	15	0.98
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	15	0.98
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	15	0.98
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	15	0.98
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	9	0.97
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	9	0.97
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	9	0.97
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	9	0.97
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	9	0.97
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	9	0.97
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	24	0.97
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	24	0.97
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	24	0.97
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	5	0.96
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	5	0.96
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	5	0.96
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	28	0.96
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	28	0.96
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	28	0.96
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	28	0.96
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	3	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	3	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	3	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	3	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	3	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	3	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	15	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	15	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	15	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	15	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	15	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	15	0.95
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	1	0.94
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	1	0.94
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	1	0.94
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	1	0.94
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	1	0.94
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	1	0.94
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	25	0.94
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	25	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	25	0.94
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	30	0.94
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	30	0.94
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	30	0.94
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	8	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	8	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	8	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	8	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	8	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	8	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	25	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	25	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	25	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	25	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	25	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	25	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	27	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	27	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	27	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	27	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	27	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	27	0.91
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	28	0.91
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	28	0.91
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	28	0.91
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	29	0.91
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	29	0.91
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	29	0.91
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB2	2	0.91
(1,49)	1:20:A:LEU:HB2	1:25:A:ARG:HB3	2	0.91
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB2	2	0.91
(1,49)	1:20:A:LEU:HB3	1:25:A:ARG:HB3	2	0.91
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	6	0.9
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	6	0.9
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	6	0.9
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	6	0.9
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	6	0.9
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	6	0.9
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	9	0.9
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	9	0.9
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	9	0.9
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	19	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	19	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	19	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	19	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	19	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	19	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	28	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	28	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	28	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	28	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	28	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	28	0.89
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	20	0.89
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	20	0.89
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	20	0.89
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	7	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	7	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	7	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	7	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	7	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	7	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	13	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	13	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	13	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	13	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	13	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	13	0.88
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	12	0.88
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	12	0.88
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	12	0.88
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	24	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	24	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	24	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	24	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	24	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	24	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	30	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	30	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	30	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	30	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	30	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	30	0.86
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	26	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	26	0.86
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	26	0.86
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	23	0.85
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	23	0.85
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	23	0.85
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	23	0.85
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	23	0.85
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	23	0.85
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	11	0.83
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	11	0.83
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	11	0.83
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	11	0.83
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	11	0.83
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	11	0.83
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	14	0.83
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	14	0.83
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	14	0.83
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	22	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	22	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	22	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	22	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	22	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	22	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	29	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	29	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	29	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	29	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	29	0.82
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	29	0.82
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	4	0.81
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	4	0.81
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	4	0.81
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	21	0.8
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	21	0.8
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	21	0.8
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	21	0.8
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	21	0.8
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	21	0.8
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	12	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	12	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	12	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	12	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	12	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	12	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	14	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	14	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	14	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	14	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	14	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	14	0.78
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	2	0.78
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	2	0.78
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	2	0.78
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	2	0.78
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	2	0.78
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	2	0.78
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	30	0.78
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	30	0.78
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	30	0.78
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	30	0.78
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	30	0.78
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	30	0.78
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	5	0.76
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	5	0.76
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	5	0.76
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	5	0.76
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	5	0.76
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	5	0.76
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	7	0.76
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	7	0.76
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	7	0.76
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	7	0.76
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	7	0.76
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	7	0.76
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	2	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	2	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	2	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	2	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	2	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	2	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	20	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	20	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	20	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	20	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	20	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	20	0.75
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	15	0.75
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	15	0.75
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	15	0.75
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	15	0.75
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	15	0.75
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	15	0.75
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	18	0.74
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	18	0.74
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	18	0.74
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	18	0.74
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	18	0.74
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	18	0.74
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	29	0.74
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	29	0.74
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	29	0.74
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	29	0.74
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	29	0.74
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	29	0.74
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	14	0.73
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	2	0.73
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	2	0.73
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	2	0.73
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	25	0.72
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	25	0.72
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	25	0.72
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	25	0.72
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	25	0.72
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	25	0.72
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	16	0.72
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	16	0.72
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	16	0.72
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	17	0.72
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	17	0.72
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	17	0.72
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	17	0.72
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	17	0.72
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	17	0.72
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	21	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	21	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	21	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	21	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	21	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	21	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	24	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	24	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	24	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	24	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	24	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	24	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	30	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	30	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	30	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	30	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	30	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	30	0.71
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	2	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	2	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	2	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	2	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	2	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	2	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	5	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	5	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	5	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	5	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	5	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	5	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	6	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	6	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	6	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	6	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	6	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	6	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	10	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	10	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	10	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	10	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	10	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	10	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	23	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	23	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	23	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	23	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	23	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	23	0.7
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	24	0.7
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	24	0.7
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	24	0.7
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	24	0.7
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	24	0.7
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	24	0.7
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	9	0.69
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	9	0.69
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	9	0.69
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	9	0.69
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	9	0.69
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	9	0.69
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	4	0.68
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	4	0.68
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	4	0.68
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	4	0.68
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	4	0.68
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	4	0.68
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	16	0.68
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	16	0.68
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	16	0.68
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	16	0.68
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	16	0.68
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	16	0.68
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	20	0.67
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	20	0.67
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	20	0.67
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	20	0.67
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	20	0.67
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	20	0.67
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	28	0.67
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	28	0.67
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	28	0.67
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	28	0.67
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	28	0.67
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	28	0.67
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	7	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	7	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	7	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	7	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	7	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	7	0.66
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	13	0.66
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	13	0.66
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	13	0.66
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	5	0.66
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	5	0.66
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	5	0.66
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	5	0.66
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	5	0.66
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	5	0.66
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	27	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	27	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	27	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	27	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	27	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	27	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	28	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	28	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	28	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	28	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	28	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	28	0.65
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	25	0.65
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	25	0.65
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	25	0.65
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	25	0.65
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	25	0.65
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	25	0.65
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	1	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	1	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	1	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	1	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	1	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	1	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	3	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	3	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	3	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	3	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	3	0.64
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	19	0.63
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	19	0.63
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	19	0.63
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	19	0.63
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	19	0.63
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	19	0.63
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD11	17	0.62
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD12	17	0.62
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD13	17	0.62
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD21	17	0.62
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD22	17	0.62
(1,921)	1:38:A:GLU:HA	1:79:A:LEU:HD23	17	0.62
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	26	0.61
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	26	0.61
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	26	0.61
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	26	0.61
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	26	0.61
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	26	0.61
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	17	0.61
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	17	0.61
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	17	0.61
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	26	0.61
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	26	0.61
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	26	0.61
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	26	0.61
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	26	0.61
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	26	0.61
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	29	0.6
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	29	0.6
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	29	0.6
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	29	0.6
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	29	0.6
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	29	0.6
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	22	0.58
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	22	0.58
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	22	0.58
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	22	0.58
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	22	0.58
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	22	0.58
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	9	0.58
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	9	0.58
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	9	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	9	0.58
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	9	0.58
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	9	0.58
(1,24)	1:20:A:LEU:H	1:19:A:SER:HA	22	0.58
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	14	0.57
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	14	0.57
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	14	0.57
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	14	0.57
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	14	0.57
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	14	0.57
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	14	0.57
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	14	0.57
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	14	0.57
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	14	0.57
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	14	0.57
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	14	0.57
(1,24)	1:20:A:LEU:H	1:19:A:SER:HA	18	0.57
(1,24)	1:20:A:LEU:H	1:19:A:SER:HA	20	0.57
(1,24)	1:20:A:LEU:H	1:19:A:SER:HA	17	0.56
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	12	0.55
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	12	0.55
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	12	0.55
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	12	0.55
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	12	0.55
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	12	0.55
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	13	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	13	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	13	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	13	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	13	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	13	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	18	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	18	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	18	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	18	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	18	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	18	0.54
(1,24)	1:20:A:LEU:H	1:19:A:SER:HA	9	0.54
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	4	0.53
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	4	0.53
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	4	0.53
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	4	0.53
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	4	0.53
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	11	0.53
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	11	0.53
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	11	0.53
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	11	0.53
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	11	0.53
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	11	0.53
(1,9)	1:18:A:ILE:H	1:17:A:ALA:HA	11	0.51
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	11	0.49
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	11	0.49
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	11	0.48
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	11	0.48
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	11	0.48
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	11	0.48
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	11	0.48
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	11	0.48
(1,239)	1:37:A:THR:H	1:37:A:THR:HG21	1	0.48
(1,239)	1:37:A:THR:H	1:37:A:THR:HG22	1	0.48
(1,239)	1:37:A:THR:H	1:37:A:THR:HG23	1	0.48
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	22	0.48
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	22	0.48
(1,501)	1:60:A:GLN:H	1:60:A:GLN:HG2	21	0.47
(1,501)	1:60:A:GLN:H	1:60:A:GLN:HG3	21	0.47
(1,501)	1:60:A:GLN:H	1:60:A:GLN:HG2	28	0.47
(1,501)	1:60:A:GLN:H	1:60:A:GLN:HG3	28	0.47
(1,473)	1:58:A:LYS:H	1:58:A:LYS:HD2	1	0.47
(1,473)	1:58:A:LYS:H	1:58:A:LYS:HD3	1	0.47
(1,473)	1:58:A:LYS:H	1:58:A:LYS:HD2	5	0.47
(1,473)	1:58:A:LYS:H	1:58:A:LYS:HD3	5	0.47
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	17	0.47
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	17	0.47
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	5	0.47
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	5	0.47
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	19	0.47
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	19	0.47
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	2	0.47
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	14	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	1	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	1	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	20	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	20	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	23	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	23	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	29	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	29	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	30	0.47
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	30	0.47
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	6	0.46
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	21	0.46
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	21	0.46
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	30	0.46
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	30	0.46
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	17	0.46
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	3	0.46
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	3	0.46
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG2	28	0.46
(1,1)	1:16:A:PRO:HA	1:16:A:PRO:HG3	28	0.46
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG2	21	0.45
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG3	21	0.45
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	17	0.45
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	17	0.45
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	17	0.45
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	17	0.45
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	17	0.45
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	17	0.45
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	16	0.45
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	16	0.45
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	16	0.45
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	16	0.45
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	16	0.45
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	16	0.45
(1,187)	1:31:A:LEU:HA	1:34:A:ASP:HB2	6	0.45
(1,187)	1:31:A:LEU:HA	1:34:A:ASP:HB3	6	0.45
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE2	20	0.45
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE3	20	0.45
(1,9)	1:18:A:ILE:H	1:17:A:ALA:HA	29	0.45
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG2	22	0.44
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG3	22	0.44
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	12	0.44
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	12	0.44
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	12	0.44
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	12	0.44
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	12	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	12	0.44
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	19	0.44
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	19	0.44
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	4	0.44
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	4	0.44
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	4	0.44
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	4	0.44
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	4	0.44
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	4	0.44
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG2	16	0.44
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG3	16	0.44
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG2	24	0.44
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG3	24	0.44
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG2	28	0.44
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG3	28	0.44
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	18	0.44
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	18	0.43
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	18	0.43
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	18	0.43
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	20	0.43
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	20	0.43
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	20	0.43
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	20	0.43
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	20	0.43
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	20	0.43
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	23	0.43
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG2	12	0.43
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG3	12	0.43
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG2	30	0.43
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG3	30	0.43
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG2	9	0.43
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG3	9	0.43
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG2	26	0.43
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG3	26	0.43
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	8	0.43
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	28	0.43
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	7	0.42
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	7	0.42
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	13	0.42
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	13	0.42
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	13	0.42
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	13	0.42
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	13	0.42
(1,269)	1:40:A:GLU:H	1:40:A:GLU:HG2	17	0.42
(1,269)	1:40:A:GLU:H	1:40:A:GLU:HG3	17	0.42
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG2	9	0.42
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG3	9	0.42
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG2	11	0.42
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG3	11	0.42
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG2	12	0.42
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG3	12	0.42
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG2	17	0.42
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG3	17	0.42
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	4	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	4	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	12	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	12	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	16	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	16	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	21	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	21	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	25	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	25	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	26	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	26	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	28	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	28	0.41
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	14	0.41
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	14	0.41
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	14	0.41
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	24	0.41
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG2	1	0.41
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG3	1	0.41
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	8	0.41
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	8	0.41
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	1	0.41
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	1	0.41
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	17	0.41
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	17	0.41
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	21	0.41
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	21	0.41
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG2	1	0.41
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG3	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG2	16	0.41
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG3	16	0.41
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG2	20	0.41
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG3	20	0.41
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	12	0.41
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	12	0.41
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG2	2	0.41
(1,126)	1:27:A:ARG:H	1:27:A:ARG:HG3	2	0.41
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	4	0.41
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	4	0.41
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	6	0.41
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	6	0.41
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB2	8	0.41
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB3	8	0.41
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	22	0.4
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	22	0.4
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	6	0.4
(1,261)	1:39:A:LYS:H	1:39:A:LYS:HG2	9	0.4
(1,261)	1:39:A:LYS:H	1:39:A:LYS:HG3	9	0.4
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG2	22	0.4
(1,207)	1:33:A:ARG:H	1:33:A:ARG:HG3	22	0.4
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	20	0.4
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	20	0.4
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG2	24	0.4
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG3	24	0.4
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG2	28	0.4
(1,113)	1:26:A:ARG:H	1:26:A:ARG:HG3	28	0.4
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	3	0.4
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	9	0.39
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	10	0.39
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	23	0.39
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	30	0.39
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG2	4	0.39
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG3	4	0.39
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG2	12	0.39
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG3	12	0.39
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG2	26	0.39
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG3	26	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG2	10	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG3	10	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG2	12	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG3	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG2	22	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG3	22	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG2	28	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG3	28	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG2	30	0.39
(1,651)	1:69:A:ARG:H	1:69:A:ARG:HG3	30	0.39
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD11	8	0.39
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD12	8	0.39
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD13	8	0.39
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD21	8	0.39
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD22	8	0.39
(1,375)	1:48:A:LEU:H	1:28:A:LEU:HD23	8	0.39
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	4	0.39
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	4	0.39
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	16	0.39
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	16	0.39
(1,258)	1:39:A:LYS:H	1:38:A:GLU:HG2	20	0.39
(1,258)	1:39:A:LYS:H	1:38:A:GLU:HG3	20	0.39
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	8	0.39
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	20	0.39
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	21	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	1	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	1	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	2	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	2	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	4	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	4	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	17	0.39
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	17	0.39
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	18	0.39
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	18	0.39
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	5	0.39
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	5	0.39
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	20	0.39
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	20	0.39
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	22	0.39
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	22	0.39
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG12	26	0.39
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG13	26	0.39
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	20	0.39
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	1	0.38
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	15	0.38
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	18	0.38
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	20	0.38
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	25	0.38
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	16	0.38
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	16	0.38
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG2	16	0.38
(1,720)	1:76:A:GLU:H	1:76:A:GLU:HG3	16	0.38
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG2	15	0.38
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG3	15	0.38
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG2	20	0.38
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG3	20	0.38
(1,257)	1:39:A:LYS:H	1:38:A:GLU:HB2	8	0.38
(1,257)	1:39:A:LYS:H	1:38:A:GLU:HB3	8	0.38
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	12	0.38
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	18	0.38
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	26	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	7	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	7	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	8	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	8	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	9	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	9	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	10	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	10	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	26	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	26	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	27	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	27	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG2	28	0.38
(1,196)	1:32:A:GLU:H	1:32:A:GLU:HG3	28	0.38
(1,171)	1:30:A:ASP:HA	1:33:A:ARG:HB2	10	0.38
(1,171)	1:30:A:ASP:HA	1:33:A:ARG:HB3	10	0.38
(1,2)	1:17:A:ALA:H	1:16:A:PRO:HA	30	0.38
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	4	0.37
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	13	0.37
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	19	0.37
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	22	0.37
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	29	0.37
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD2	23	0.37
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD3	23	0.37
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	9	0.37
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	18	0.37
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	18	0.37
(1,257)	1:39:A:LYS:H	1:38:A:GLU:HB2	19	0.37
(1,257)	1:39:A:LYS:H	1:38:A:GLU:HB3	19	0.37
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	10	0.37
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	13	0.37
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	15	0.37
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	16	0.37
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	25	0.37
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	28	0.37
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	29	0.37
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB2	30	0.37
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB3	30	0.37
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	3	0.36
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	3	0.36
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	14	0.36
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	14	0.36
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	17	0.36
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	17	0.36
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	7	0.36
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	11	0.36
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	14	0.36
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	16	0.36
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	28	0.36
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	17	0.36
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	17	0.36
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	15	0.36
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	15	0.36
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	21	0.36
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	21	0.36
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	14	0.36
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	14	0.36
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	23	0.36
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	23	0.36
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	23	0.36
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	3	0.36
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	4	0.36
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	11	0.36
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	22	0.36
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	13	0.36
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	29	0.35
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	1	0.35
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	1	0.35
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	14	0.35
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	14	0.35
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	20	0.35
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	20	0.35
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	27	0.35
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	27	0.35
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	5	0.35
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	7	0.35
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE2	12	0.35
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE3	12	0.35
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	14	0.35
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	14	0.35
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	19	0.35
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	19	0.35
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	17	0.35
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	17	0.35
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	19	0.35
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	19	0.35
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB2	26	0.35
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB3	26	0.35
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	5	0.34
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	11	0.34
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	18	0.34
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG2	11	0.34
(1,879)	1:88:A:LYS:H	1:88:A:LYS:HG3	11	0.34
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	26	0.34
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	26	0.34
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	26	0.34
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	10	0.34
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	10	0.34
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	26	0.34
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	26	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	9	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	9	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	13	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	13	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	16	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	16	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	18	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	25	0.34
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	25	0.34
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	22	0.34
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	22	0.34
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	22	0.34
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	1	0.34
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	14	0.34
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	24	0.34
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	27	0.34
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	3	0.34
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	3	0.34
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	17	0.34
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	17	0.34
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG2	11	0.34
(1,99)	1:25:A:ARG:H	1:25:A:ARG:HG3	11	0.34
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	9	0.33
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	21	0.33
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	21	0.33
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	21	0.33
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	6	0.33
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	4	0.33
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	4	0.33
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	6	0.33
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	6	0.33
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	22	0.33
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	22	0.33
(1,261)	1:39:A:LYS:H	1:39:A:LYS:HG2	30	0.33
(1,261)	1:39:A:LYS:H	1:39:A:LYS:HG3	30	0.33
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	30	0.33
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD11	27	0.33
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD12	27	0.33
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD13	27	0.33
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE2	18	0.33
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE3	18	0.33
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG2	9	0.33
(1,156)	1:29:A:LYS:H	1:29:A:LYS:HG3	9	0.33
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB2	21	0.33
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB3	21	0.33
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	5	0.32
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	5	0.32
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:79:A:LEU:H	1:79:A:LEU:HG	19	0.32
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	18	0.32
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	18	0.32
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	11	0.32
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	12	0.32
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	12	0.32
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	13	0.32
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	13	0.32
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG2	26	0.32
(1,333)	1:45:A:LYS:H	1:45:A:LYS:HG3	26	0.32
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	19	0.32
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	10	0.31
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	10	0.31
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	10	0.31
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	10	0.31
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	18	0.31
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	18	0.31
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	18	0.31
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	18	0.31
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	18	0.31
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	18	0.31
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	5	0.31
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	5	0.31
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	12	0.31
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	12	0.31
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	26	0.31
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	26	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	4	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	4	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	9	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	9	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	15	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	15	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	20	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	20	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	24	0.31
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	24	0.31
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	1	0.31
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	1	0.31
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	1	0.31
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	1	0.31
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD11	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD12	3	0.31
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD13	3	0.31
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	17	0.31
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	17	0.31
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	17	0.31
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	17	0.31
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	17	0.31
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	17	0.31
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB2	23	0.31
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB3	23	0.31
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB2	25	0.31
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB3	25	0.31
(1,12)	1:18:A:ILE:H	1:18:A:ILE:HB	22	0.31
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	1	0.3
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	1	0.3
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	8	0.3
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	8	0.3
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	15	0.3
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	15	0.3
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	25	0.3
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	25	0.3
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	12	0.3
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	12	0.3
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	12	0.3
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	20	0.3
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	20	0.3
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	20	0.3
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	14	0.3
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	14	0.3
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	21	0.3
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	21	0.3
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	15	0.3
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	5	0.3
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	5	0.3
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	5	0.3
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD11	9	0.3
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD12	9	0.3
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD13	9	0.3
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD21	9	0.3
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD22	9	0.3
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD23	9	0.3
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	30	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	2	0.29
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	2	0.29
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	10	0.29
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	10	0.29
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	11	0.29
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	11	0.29
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG2	29	0.29
(1,813)	1:83:A:LYS:H	1:83:A:LYS:HG3	29	0.29
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	2	0.29
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	2	0.29
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	13	0.29
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	20	0.29
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	21	0.29
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	24	0.29
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	16	0.29
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	16	0.29
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	16	0.29
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	19	0.29
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	19	0.29
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	19	0.29
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	11	0.28
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	11	0.28
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	11	0.28
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	11	0.28
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB2	4	0.28
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB3	4	0.28
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	4	0.28
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	2	0.28
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	21	0.28
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	8	0.28
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	8	0.28
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	8	0.28
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	29	0.28
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	29	0.28
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	29	0.28
(1,717)	1:76:A:GLU:H	1:75:A:GLU:HB2	17	0.28
(1,717)	1:76:A:GLU:H	1:75:A:GLU:HB3	17	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	6	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	6	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	11	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	11	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	12	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	16	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	16	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	28	0.28
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	28	0.28
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	4	0.28
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	5	0.28
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	8	0.28
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	17	0.28
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	23	0.28
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	28	0.28
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	29	0.28
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	21	0.28
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	21	0.28
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	21	0.28
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE2	14	0.28
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE3	14	0.28
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE2	19	0.28
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE3	19	0.28
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD11	8	0.28
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD12	8	0.28
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD13	8	0.28
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD11	23	0.28
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD12	23	0.28
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD13	23	0.28
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	16	0.27
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	16	0.27
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	16	0.27
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	16	0.27
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	22	0.27
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	22	0.27
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	22	0.27
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	22	0.27
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	30	0.27
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	4	0.27
(1,856)	1:86:A:LEU:HA	1:89:A:ASP:HB2	22	0.27
(1,856)	1:86:A:LEU:HA	1:89:A:ASP:HB3	22	0.27
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	2	0.27
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	2	0.27
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	2	0.27
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	4	0.27
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	4	0.27
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	7	0.27
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	7	0.27
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	7	0.27
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	9	0.27
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	9	0.27
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	9	0.27
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	13	0.27
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	13	0.27
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	13	0.27
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	19	0.27
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	6	0.27
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	6	0.27
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	7	0.27
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	7	0.27
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	13	0.27
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	13	0.27
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	23	0.27
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	23	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	4	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	4	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	12	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	12	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	18	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	18	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	20	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	20	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	26	0.27
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	26	0.27
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	6	0.27
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	6	0.27
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	14	0.27
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	19	0.27
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	22	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	10	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	10	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	10	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	20	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	20	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	20	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	27	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	27	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	27	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	30	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	30	0.27
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	30	0.27
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD2	3	0.27
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD3	3	0.27
(1,245)	1:37:A:THR:HG21	1:40:A:GLU:HG2	17	0.27
(1,245)	1:37:A:THR:HG21	1:40:A:GLU:HG3	17	0.27
(1,245)	1:37:A:THR:HG22	1:40:A:GLU:HG2	17	0.27
(1,245)	1:37:A:THR:HG22	1:40:A:GLU:HG3	17	0.27
(1,245)	1:37:A:THR:HG23	1:40:A:GLU:HG2	17	0.27
(1,245)	1:37:A:THR:HG23	1:40:A:GLU:HG3	17	0.27
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	4	0.27
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE2	17	0.27
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE3	17	0.27
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB2	5	0.27
(1,27)	1:20:A:LEU:H	1:20:A:LEU:HB3	5	0.27
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB2	2	0.26
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB3	2	0.26
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB2	21	0.26
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB3	21	0.26
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	21	0.26
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD11	2	0.26
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD12	2	0.26
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD13	2	0.26
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	15	0.26
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	15	0.26
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	15	0.26
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	22	0.26
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	22	0.26
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	22	0.26
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	27	0.26
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	27	0.26
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	27	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	3	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	3	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	10	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	10	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	22	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	22	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	25	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	25	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	26	0.26
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	26	0.26
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	7	0.26
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	7	0.26
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	24	0.26
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	24	0.26
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	28	0.26
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	28	0.26
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	10	0.26
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	25	0.26
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	26	0.26
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	27	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	6	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	6	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	6	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	8	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	8	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	8	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	22	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	22	0.26
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	22	0.26
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG21	23	0.26
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG22	23	0.26
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG23	23	0.26
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG21	23	0.26
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG22	23	0.26
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG23	23	0.26
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD2	7	0.26
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD3	7	0.26
(1,399)	1:50:A:HIS:H	1:50:A:HIS:HD2	23	0.26
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD11	20	0.26
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD12	20	0.26
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD13	20	0.26
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD21	20	0.26
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD22	20	0.26
(1,311)	1:44:A:GLU:H	1:36:A:LEU:HD23	20	0.26
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	8	0.26
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	8	0.26
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	8	0.26
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	26	0.26
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	26	0.26
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	26	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	19	0.26
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	19	0.26
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	19	0.26
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	19	0.26
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	19	0.26
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	19	0.26
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE2	9	0.26
(1,157)	1:29:A:LYS:H	1:29:A:LYS:HE3	9	0.26
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	2	0.25
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	2	0.25
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	2	0.25
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	2	0.25
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	15	0.25
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	15	0.25
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	15	0.25
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	15	0.25
(1,817)	1:83:A:LYS:HA	1:86:A:LEU:HD11	14	0.25
(1,817)	1:83:A:LYS:HA	1:86:A:LEU:HD12	14	0.25
(1,817)	1:83:A:LYS:HA	1:86:A:LEU:HD13	14	0.25
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	18	0.25
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	18	0.25
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	18	0.25
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	5	0.25
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	5	0.25
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	8	0.25
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	8	0.25
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	27	0.25
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	27	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	3	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	3	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	10	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	10	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	11	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	11	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	30	0.25
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	30	0.25
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	4	0.25
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	4	0.25
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	11	0.25
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	11	0.25
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	3	0.25
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	16	0.25
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	30	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	11	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	11	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	11	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	12	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	12	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	12	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	25	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	25	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	25	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	28	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	28	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	28	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	29	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	29	0.25
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	29	0.25
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB2	11	0.25
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB3	11	0.25
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB2	11	0.25
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB3	11	0.25
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB2	11	0.25
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB3	11	0.25
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	15	0.25
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	15	0.25
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	15	0.25
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	17	0.24
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	17	0.24
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	17	0.24
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	17	0.24
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	3	0.24
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	3	0.24
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	3	0.24
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	11	0.24
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	11	0.24
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	11	0.24
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	14	0.24
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	14	0.24
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	14	0.24
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	16	0.24
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	16	0.24
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	19	0.24
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	19	0.24
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	29	0.24
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	29	0.24
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB2	30	0.24
(1,673)	1:72:A:GLU:H	1:71:A:GLU:HB3	30	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	5	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	5	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	8	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	8	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	19	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	19	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	22	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	22	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	27	0.24
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	27	0.24
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	4	0.24
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	4	0.24
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	4	0.24
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	15	0.24
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	15	0.24
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	15	0.24
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	17	0.24
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	17	0.24
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	17	0.24
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	15	0.24
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	24	0.24
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD11	2	0.24
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD12	2	0.24
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD13	2	0.24
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	21	0.24
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	21	0.24
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	21	0.24
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	9	0.24
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	9	0.24
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	9	0.24
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	9	0.24
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	9	0.24
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	9	0.24
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	10	0.24
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	10	0.24
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	16	0.24
(1,12)	1:18:A:ILE:H	1:18:A:ILE:HB	24	0.24
(1,12)	1:18:A:ILE:H	1:18:A:ILE:HB	27	0.24
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	18	0.23
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	18	0.23
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	18	0.23
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	18	0.23
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	19	0.23
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	19	0.23
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	19	0.23
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	19	0.23
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB2	30	0.23
(1,915)	1:93:A:GLU:H	1:92:A:LEU:HB3	30	0.23
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	12	0.23
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	26	0.23
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	1	0.23
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	1	0.23
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	1	0.23
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	6	0.23
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	6	0.23
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	6	0.23
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	17	0.23
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	17	0.23
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	17	0.23
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	26	0.23
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	26	0.23
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	26	0.23
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	30	0.23
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	30	0.23
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	30	0.23
(1,717)	1:76:A:GLU:H	1:75:A:GLU:HB2	29	0.23
(1,717)	1:76:A:GLU:H	1:75:A:GLU:HB3	29	0.23
(1,717)	1:76:A:GLU:H	1:75:A:GLU:HB2	30	0.23
(1,717)	1:76:A:GLU:H	1:75:A:GLU:HB3	30	0.23
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	2	0.23
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	2	0.23
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	23	0.23
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	23	0.23
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	29	0.23
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	29	0.23
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	23	0.23
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	23	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	2	0.23
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	9	0.23
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	12	0.23
(1,647)	1:69:A:ARG:H	1:68:A:LEU:HG	18	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	13	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	13	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	13	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	17	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	17	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	17	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	23	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	23	0.23
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	23	0.23
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	6	0.23
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	6	0.23
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	6	0.23
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	6	0.23
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	6	0.23
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	6	0.23
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	19	0.23
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	19	0.23
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	19	0.23
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	19	0.23
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	19	0.23
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	19	0.23
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	11	0.23
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	20	0.23
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	4	0.23
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	4	0.23
(1,39)	1:20:A:LEU:HD21	1:19:A:SER:HA	17	0.23
(1,39)	1:20:A:LEU:HD22	1:19:A:SER:HA	17	0.23
(1,39)	1:20:A:LEU:HD23	1:19:A:SER:HA	17	0.23
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD11	30	0.23
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD12	30	0.23
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD13	30	0.23
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	2	0.22
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	24	0.22
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	24	0.22
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	24	0.22
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	25	0.22
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	25	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	3	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	3	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	3	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	3	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	3	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	26	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	26	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	26	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	26	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	26	0.22
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	26	0.22
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	2	0.22
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	2	0.22
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	2	0.22
(1,399)	1:50:A:HIS:H	1:50:A:HIS:HD2	28	0.22
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD11	10	0.22
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD12	10	0.22
(1,284)	1:41:A:CYS:HA	1:36:A:LEU:HD13	10	0.22
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	13	0.22
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	13	0.22
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	13	0.22
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	13	0.22
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	13	0.22
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	13	0.22
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	23	0.22
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	23	0.22
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	23	0.22
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	23	0.22
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	23	0.22
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	23	0.22
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	18	0.22
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	23	0.22
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	17	0.22
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	8	0.22
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	8	0.22
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	27	0.22
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	27	0.22
(1,81)	1:24:A:VAL:HG11	1:52:A:PHE:HD1	19	0.22
(1,81)	1:24:A:VAL:HG11	1:52:A:PHE:HD2	19	0.22
(1,81)	1:24:A:VAL:HG12	1:52:A:PHE:HD1	19	0.22
(1,81)	1:24:A:VAL:HG12	1:52:A:PHE:HD2	19	0.22
(1,81)	1:24:A:VAL:HG13	1:52:A:PHE:HD1	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:24:A:VAL:HG13	1:52:A:PHE:HD2	19	0.22
(1,81)	1:24:A:VAL:HG21	1:52:A:PHE:HD1	19	0.22
(1,81)	1:24:A:VAL:HG21	1:52:A:PHE:HD2	19	0.22
(1,81)	1:24:A:VAL:HG22	1:52:A:PHE:HD1	19	0.22
(1,81)	1:24:A:VAL:HG22	1:52:A:PHE:HD2	19	0.22
(1,81)	1:24:A:VAL:HG23	1:52:A:PHE:HD1	19	0.22
(1,81)	1:24:A:VAL:HG23	1:52:A:PHE:HD2	19	0.22
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB1	8	0.22
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB2	8	0.22
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB3	8	0.22
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	24	0.21
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	24	0.21
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	24	0.21
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	24	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	8	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	8	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	8	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	8	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	8	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	8	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	22	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	22	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	22	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	22	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	22	0.21
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	22	0.21
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	2	0.21
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	2	0.21
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD11	21	0.21
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD12	21	0.21
(1,886)	1:89:A:ASP:H	1:85:A:LEU:HD13	21	0.21
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	10	0.21
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	10	0.21
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	10	0.21
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	19	0.21
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	19	0.21
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	19	0.21
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	23	0.21
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	23	0.21
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	23	0.21
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	25	0.21
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	25	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	25	0.21
(1,801)	1:82:A:VAL:HG11	1:79:A:LEU:HA	28	0.21
(1,801)	1:82:A:VAL:HG12	1:79:A:LEU:HA	28	0.21
(1,801)	1:82:A:VAL:HG13	1:79:A:LEU:HA	28	0.21
(1,727)	1:77:A:GLY:H	1:76:A:GLU:HB2	8	0.21
(1,727)	1:77:A:GLY:H	1:76:A:GLU:HB3	8	0.21
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	29	0.21
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	23	0.21
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	23	0.21
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	24	0.21
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	24	0.21
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	14	0.21
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	14	0.21
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	14	0.21
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	14	0.21
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	14	0.21
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	14	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	3	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	3	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	3	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	18	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	18	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	18	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	24	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	24	0.21
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	24	0.21
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG21	20	0.21
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG22	20	0.21
(1,489)	1:59:A:ASN:HD21	1:55:A:THR:HG23	20	0.21
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG21	20	0.21
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG22	20	0.21
(1,489)	1:59:A:ASN:HD22	1:55:A:THR:HG23	20	0.21
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB2	3	0.21
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB3	3	0.21
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB2	3	0.21
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB3	3	0.21
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB2	3	0.21
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB3	3	0.21
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD2	4	0.21
(1,435)	1:55:A:THR:HA	1:58:A:LYS:HD3	4	0.21
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD11	19	0.21
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD12	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD13	19	0.21
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	2	0.21
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	2	0.21
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	2	0.21
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	2	0.21
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	2	0.21
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	2	0.21
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	6	0.21
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	30	0.21
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	15	0.21
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	15	0.21
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	24	0.21
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	24	0.21
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	26	0.21
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	26	0.21
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	29	0.21
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	29	0.21
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD11	26	0.21
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD12	26	0.21
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD13	26	0.21
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB1	25	0.21
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB2	25	0.21
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB3	25	0.21
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	3	0.2
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	3	0.2
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	3	0.2
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	3	0.2
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	8	0.2
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	8	0.2
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	8	0.2
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	8	0.2
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	20	0.2
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	20	0.2
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	20	0.2
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	20	0.2
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	16	0.2
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	30	0.2
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB2	15	0.2
(1,669)	1:71:A:GLU:H	1:71:A:GLU:HB3	15	0.2
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	15	0.2
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	15	0.2
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	1	0.2
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	1	0.2
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	1	0.2
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	1	0.2
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	1	0.2
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	4	0.2
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	4	0.2
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	4	0.2
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	4	0.2
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	4	0.2
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	4	0.2
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	9	0.2
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	9	0.2
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	9	0.2
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	23	0.2
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	23	0.2
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	23	0.2
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	23	0.2
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	23	0.2
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	23	0.2
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	2	0.2
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	2	0.2
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	11	0.2
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	11	0.2
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	22	0.2
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	22	0.2
(1,297)	1:42:A:VAL:HA	1:45:A:LYS:HD2	15	0.2
(1,297)	1:42:A:VAL:HA	1:45:A:LYS:HD3	15	0.2
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	18	0.2
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	18	0.2
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	18	0.2
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	18	0.2
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	18	0.2
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	18	0.2
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	20	0.2
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	20	0.2
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	20	0.2
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	20	0.2
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	20	0.2
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	20	0.2
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	7	0.2
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	7	0.2
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	4	0.2
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	4	0.2
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	4	0.2
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	4	0.2
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	4	0.2
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	4	0.2
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	23	0.2
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	3	0.2
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	3	0.2
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	7	0.2
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	7	0.2
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	25	0.2
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	25	0.2
(1,81)	1:24:A:VAL:HG11	1:52:A:PHE:HD1	30	0.2
(1,81)	1:24:A:VAL:HG11	1:52:A:PHE:HD2	30	0.2
(1,81)	1:24:A:VAL:HG12	1:52:A:PHE:HD1	30	0.2
(1,81)	1:24:A:VAL:HG12	1:52:A:PHE:HD2	30	0.2
(1,81)	1:24:A:VAL:HG13	1:52:A:PHE:HD1	30	0.2
(1,81)	1:24:A:VAL:HG13	1:52:A:PHE:HD2	30	0.2
(1,81)	1:24:A:VAL:HG21	1:52:A:PHE:HD1	30	0.2
(1,81)	1:24:A:VAL:HG21	1:52:A:PHE:HD2	30	0.2
(1,81)	1:24:A:VAL:HG22	1:52:A:PHE:HD1	30	0.2
(1,81)	1:24:A:VAL:HG22	1:52:A:PHE:HD2	30	0.2
(1,81)	1:24:A:VAL:HG23	1:52:A:PHE:HD1	30	0.2
(1,81)	1:24:A:VAL:HG23	1:52:A:PHE:HD2	30	0.2
(1,48)	1:20:A:LEU:HB2	1:25:A:ARG:HD2	4	0.2
(1,48)	1:20:A:LEU:HB2	1:25:A:ARG:HD3	4	0.2
(1,48)	1:20:A:LEU:HB3	1:25:A:ARG:HD2	4	0.2
(1,48)	1:20:A:LEU:HB3	1:25:A:ARG:HD3	4	0.2
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG12	29	0.2
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG13	29	0.2
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	10	0.19
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	14	0.19
(1,911)	1:92:A:LEU:H	1:92:A:LEU:HG	1	0.19
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	1	0.19
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	1	0.19
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	20	0.19
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	20	0.19
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	23	0.19
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	23	0.19
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	18	0.19
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	18	0.19
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	13	0.19
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	17	0.19
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	27	0.19
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	9	0.19
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	9	0.19
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	6	0.19
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	6	0.19
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	6	0.19
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	6	0.19
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	6	0.19
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	6	0.19
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	27	0.19
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	27	0.19
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	27	0.19
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	27	0.19
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	27	0.19
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	27	0.19
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	7	0.19
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	7	0.19
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	7	0.19
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB2	7	0.19
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB3	7	0.19
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB2	7	0.19
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB3	7	0.19
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB2	7	0.19
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB3	7	0.19
(1,399)	1:50:A:HIS:H	1:50:A:HIS:HD2	5	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	2	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	2	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	2	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	7	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	7	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	7	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	13	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	13	0.19
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	13	0.19
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	11	0.19
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	11	0.19
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	11	0.19
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	11	0.19
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	11	0.19
(1,231)	1:36:A:LEU:H	1:37:A:THR:H	2	0.19
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD11	17	0.19
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD12	17	0.19
(1,230)	1:36:A:LEU:H	1:36:A:LEU:HD13	17	0.19
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	12	0.19
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	12	0.19
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	12	0.19
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	17	0.19
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	17	0.19
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	14	0.19
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	14	0.19
(1,20)	1:19:A:SER:H	1:18:A:ILE:HG21	29	0.19
(1,20)	1:19:A:SER:H	1:18:A:ILE:HG22	29	0.19
(1,20)	1:19:A:SER:H	1:18:A:ILE:HG23	29	0.19
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	14	0.18
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	14	0.18
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	14	0.18
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	14	0.18
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	21	0.18
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	21	0.18
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	21	0.18
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	21	0.18
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	29	0.18
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	29	0.18
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	29	0.18
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	29	0.18
(1,927)	1:42:A:VAL:HG21	1:83:A:LYS:HE2	8	0.18
(1,927)	1:42:A:VAL:HG21	1:83:A:LYS:HE3	8	0.18
(1,927)	1:42:A:VAL:HG22	1:83:A:LYS:HE2	8	0.18
(1,927)	1:42:A:VAL:HG22	1:83:A:LYS:HE3	8	0.18
(1,927)	1:42:A:VAL:HG23	1:83:A:LYS:HE2	8	0.18
(1,927)	1:42:A:VAL:HG23	1:83:A:LYS:HE3	8	0.18
(1,926)	1:42:A:VAL:HG21	1:83:A:LYS:HA	27	0.18
(1,926)	1:42:A:VAL:HG22	1:83:A:LYS:HA	27	0.18
(1,926)	1:42:A:VAL:HG23	1:83:A:LYS:HA	27	0.18
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	16	0.18
(1,908)	1:92:A:LEU:H	1:91:A:SER:HB2	5	0.18
(1,908)	1:92:A:LEU:H	1:91:A:SER:HB3	5	0.18
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	10	0.18
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:87:A:ASN:HD21	1:84:A:SER:HA	24	0.18
(1,870)	1:87:A:ASN:HD22	1:84:A:SER:HA	24	0.18
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	8	0.18
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	8	0.18
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	8	0.18
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	8	0.18
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	23	0.18
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	23	0.18
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	23	0.18
(1,837)	1:85:A:LEU:H	1:85:A:LEU:HG	26	0.18
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	10	0.18
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	10	0.18
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	19	0.18
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	19	0.18
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	27	0.18
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	27	0.18
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	15	0.18
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	11	0.18
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	11	0.18
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	29	0.18
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	29	0.18
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	29	0.18
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	29	0.18
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	29	0.18
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	29	0.18
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	22	0.18
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	22	0.18
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	22	0.18
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	22	0.18
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	22	0.18
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	22	0.18
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD11	28	0.18
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD12	28	0.18
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD13	28	0.18
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD11	28	0.18
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD12	28	0.18
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD13	28	0.18
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	16	0.18
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	16	0.18
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	16	0.18
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	16	0.18
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	16	0.18
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	14	0.18
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	14	0.18
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	14	0.18
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB2	17	0.18
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB3	17	0.18
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB2	17	0.18
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB3	17	0.18
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB2	17	0.18
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB3	17	0.18
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	1	0.18
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	1	0.18
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	1	0.18
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	1	0.18
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	1	0.18
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	1	0.18
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	2	0.18
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	2	0.18
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	19	0.18
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	19	0.18
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	30	0.18
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	30	0.18
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	25	0.18
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	25	0.18
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	25	0.18
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	25	0.18
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	25	0.18
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	25	0.18
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	1	0.18
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	1	0.18
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	1	0.18
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	1	0.18
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	1	0.18
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	1	0.18
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	4	0.18
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	15	0.18
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	25	0.18
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	20	0.18
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	20	0.18
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	1	0.18
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	1	0.18
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	4	0.18
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	1	0.18
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	1	0.18
(1,18)	1:19:A:SER:H	1:18:A:ILE:HB	29	0.18
(1,908)	1:92:A:LEU:H	1:91:A:SER:HB2	30	0.17
(1,908)	1:92:A:LEU:H	1:91:A:SER:HB3	30	0.17
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	15	0.17
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	15	0.17
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	18	0.17
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	18	0.17
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	27	0.17
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	27	0.17
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	5	0.17
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	18	0.17
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	21	0.17
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	23	0.17
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	30	0.17
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	1	0.17
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	1	0.17
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	1	0.17
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	24	0.17
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	24	0.17
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	24	0.17
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	15	0.17
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	15	0.17
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	7	0.17
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	8	0.17
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	14	0.17
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	25	0.17
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	15	0.17
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	15	0.17
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	27	0.17
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	27	0.17
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	14	0.17
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	14	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	7	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	7	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	14	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	14	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	18	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	18	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	20	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	26	0.17
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	26	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	8	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	8	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	8	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	8	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	8	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	8	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	16	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	16	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	16	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	16	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	16	0.17
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	16	0.17
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG2	17	0.17
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG3	17	0.17
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	7	0.17
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	7	0.17
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	7	0.17
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	7	0.17
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	7	0.17
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	7	0.17
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	29	0.17
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	29	0.17
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	29	0.17
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	29	0.17
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	29	0.17
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	29	0.17
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	4	0.17
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	4	0.17
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	4	0.17
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	4	0.17
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	4	0.17
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	4	0.17
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	28	0.17
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	28	0.17
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	28	0.17
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	28	0.17
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	28	0.17
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	28	0.17
(1,444)	1:57:A:ILE:H	1:56:A:GLU:HB2	26	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:57:A:ILE:H	1:56:A:GLU:HB3	26	0.17
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	17	0.17
(1,297)	1:42:A:VAL:HA	1:45:A:LYS:HD2	10	0.17
(1,297)	1:42:A:VAL:HA	1:45:A:LYS:HD3	10	0.17
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	22	0.17
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	22	0.17
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	22	0.17
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	22	0.17
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	22	0.17
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	22	0.17
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	26	0.17
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	26	0.17
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	26	0.17
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	26	0.17
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	26	0.17
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	26	0.17
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	14	0.17
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	5	0.17
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	5	0.17
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	5	0.17
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	12	0.17
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	9	0.17
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	9	0.17
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	14	0.17
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	14	0.17
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	25	0.17
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	25	0.17
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	18	0.17
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	18	0.17
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	9	0.17
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	9	0.17
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	21	0.17
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	21	0.17
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG12	14	0.17
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG13	14	0.17
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	9	0.16
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	9	0.16
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	9	0.16
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	9	0.16
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	25	0.16
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	25	0.16
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	25	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	25	0.16
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	26	0.16
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	26	0.16
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	26	0.16
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	26	0.16
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	30	0.16
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	30	0.16
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	30	0.16
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	30	0.16
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	7	0.16
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	13	0.16
(1,890)	1:89:A:ASP:H	1:88:A:LYS:HD2	5	0.16
(1,890)	1:89:A:ASP:H	1:88:A:LYS:HD3	5	0.16
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	19	0.16
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	19	0.16
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	30	0.16
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	30	0.16
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	19	0.16
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	20	0.16
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	22	0.16
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	24	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	4	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	4	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	4	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	5	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	5	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	5	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	16	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	16	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	16	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	19	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	19	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	19	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	20	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	20	0.16
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	20	0.16
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	22	0.16
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	22	0.16
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	22	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	1	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	1	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	7	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	18	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	18	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	24	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	24	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	25	0.16
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	25	0.16
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	24	0.16
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	24	0.16
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	24	0.16
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	6	0.16
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	6	0.16
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	6	0.16
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	6	0.16
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	6	0.16
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	6	0.16
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	8	0.16
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	8	0.16
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	8	0.16
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	8	0.16
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	8	0.16
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	8	0.16
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	2	0.16
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	2	0.16
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	3	0.16
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	3	0.16
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	7	0.16
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	7	0.16
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	15	0.16
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	15	0.16
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	3	0.16
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	3	0.16
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	29	0.16
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	29	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	10	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	10	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	10	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	10	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	10	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	10	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	13	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	13	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	13	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	13	0.16
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	13	0.16
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD11	15	0.16
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD12	15	0.16
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD13	15	0.16
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD11	15	0.16
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD12	15	0.16
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD13	15	0.16
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	14	0.16
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	14	0.16
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	14	0.16
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	14	0.16
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	14	0.16
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	14	0.16
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD11	21	0.16
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD12	21	0.16
(1,495)	1:60:A:GLN:H	1:57:A:ILE:HD13	21	0.16
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB2	16	0.16
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB3	16	0.16
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB2	16	0.16
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB3	16	0.16
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB2	16	0.16
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB3	16	0.16
(1,399)	1:50:A:HIS:H	1:50:A:HIS:HD2	1	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	3	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	3	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	7	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	7	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	11	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	11	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	12	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	12	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	28	0.16
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	28	0.16
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	12	0.16
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	12	0.16
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	12	0.16
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	28	0.16
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	13	0.16
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	13	0.16
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	23	0.16
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	23	0.16
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	23	0.16
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	23	0.16
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	23	0.16
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	23	0.16
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD21	9	0.16
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD22	9	0.16
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD23	9	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	3	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	7	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	11	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	14	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	18	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	20	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	21	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	28	0.16
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	29	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	7	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	7	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	18	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	18	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	21	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	21	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	23	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	23	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	26	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	26	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	27	0.16
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	27	0.16
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	2	0.16
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	2	0.16
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	18	0.16
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	18	0.16
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	13	0.15
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	13	0.15
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	13	0.15
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	13	0.15
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	27	0.15
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	27	0.15
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	27	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	27	0.15
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	20	0.15
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	25	0.15
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	5	0.15
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	5	0.15
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	9	0.15
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	9	0.15
(1,870)	1:87:A:ASN:HD21	1:84:A:SER:HA	6	0.15
(1,870)	1:87:A:ASN:HD22	1:84:A:SER:HA	6	0.15
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	1	0.15
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	6	0.15
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	9	0.15
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	12	0.15
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	13	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	7	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	7	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	7	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	9	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	9	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	9	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	12	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	12	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	12	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	13	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	13	0.15
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	13	0.15
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	20	0.15
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	20	0.15
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	20	0.15
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	3	0.15
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	3	0.15
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	9	0.15
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	9	0.15
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	17	0.15
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	17	0.15
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	10	0.15
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	11	0.15
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	12	0.15
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	22	0.15
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	7	0.15
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	7	0.15
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	7	0.15
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	7	0.15
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	7	0.15
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	12	0.15
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	12	0.15
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	12	0.15
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	12	0.15
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	12	0.15
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	12	0.15
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	14	0.15
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	14	0.15
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	14	0.15
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	14	0.15
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	14	0.15
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	14	0.15
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	19	0.15
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	19	0.15
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	19	0.15
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	19	0.15
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	19	0.15
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	19	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	4	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	4	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	8	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	8	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	11	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	11	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	12	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	12	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	20	0.15
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	20	0.15
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	2	0.15
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	2	0.15
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	5	0.15
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	5	0.15
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	17	0.15
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	17	0.15
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	21	0.15
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	21	0.15
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	26	0.15
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	26	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	1	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	1	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	1	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	1	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	1	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	15	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	15	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	15	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	15	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	15	0.15
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	15	0.15
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	2	0.15
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	3	0.15
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	3	0.15
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	24	0.15
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	24	0.15
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	29	0.15
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	29	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	5	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	5	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	8	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	8	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	10	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	10	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	29	0.15
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	29	0.15
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	11	0.15
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	11	0.15
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	11	0.15
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	27	0.15
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	27	0.15
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	27	0.15
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	3	0.15
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	3	0.15
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	3	0.15
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	3	0.15
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	3	0.15
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	3	0.15
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	16	0.15
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	16	0.15
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	16	0.15
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	16	0.15
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	16	0.15
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	22	0.15
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	6	0.15
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	6	0.15
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	27	0.15
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	27	0.15
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	2	0.15
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	17	0.15
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	19	0.15
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	22	0.15
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	24	0.15
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	26	0.15
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	6	0.15
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	6	0.15
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	11	0.15
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	11	0.15
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	12	0.15
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	12	0.15
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	15	0.15
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	15	0.15
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	20	0.15
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	20	0.15
(1,90)	1:25:A:ARG:H	1:20:A:LEU:HD11	23	0.15
(1,90)	1:25:A:ARG:H	1:20:A:LEU:HD12	23	0.15
(1,90)	1:25:A:ARG:H	1:20:A:LEU:HD13	23	0.15
(1,48)	1:20:A:LEU:HB2	1:25:A:ARG:HD2	24	0.15
(1,48)	1:20:A:LEU:HB2	1:25:A:ARG:HD3	24	0.15
(1,48)	1:20:A:LEU:HB3	1:25:A:ARG:HD2	24	0.15
(1,48)	1:20:A:LEU:HB3	1:25:A:ARG:HD3	24	0.15
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD11	5	0.15
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD12	5	0.15
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD13	5	0.15
(1,18)	1:19:A:SER:H	1:18:A:ILE:HB	1	0.15
(1,18)	1:19:A:SER:H	1:18:A:ILE:HB	30	0.15
(1,13)	1:18:A:ILE:H	1:18:A:ILE:HG13	11	0.15
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	6	0.14
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	6	0.14
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	6	0.14
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	6	0.14
(1,896)	1:90:A:LEU:H	1:89:A:ASP:HB2	22	0.14
(1,896)	1:90:A:LEU:H	1:89:A:ASP:HB3	22	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	11	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	11	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	11	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	11	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	11	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	11	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	17	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	17	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	17	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	17	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	17	0.14
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	17	0.14
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	4	0.14
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	7	0.14
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	11	0.14
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	15	0.14
(1,856)	1:86:A:LEU:HA	1:89:A:ASP:HB2	8	0.14
(1,856)	1:86:A:LEU:HA	1:89:A:ASP:HB3	8	0.14
(1,856)	1:86:A:LEU:HA	1:89:A:ASP:HB2	18	0.14
(1,856)	1:86:A:LEU:HA	1:89:A:ASP:HB3	18	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	6	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	6	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	6	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	11	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	11	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	11	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	15	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	15	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	15	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	22	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	22	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	22	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	30	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	30	0.14
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	30	0.14
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB2	1	0.14
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB3	1	0.14
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	2	0.14
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	2	0.14
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	5	0.14
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	5	0.14
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	14	0.14
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	2	0.14
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	5	0.14
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	6	0.14
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	26	0.14
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	10	0.14
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	10	0.14
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	3	0.14
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	3	0.14
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	3	0.14
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	3	0.14
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	3	0.14
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	3	0.14
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	22	0.14
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	22	0.14
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	22	0.14
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	22	0.14
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	22	0.14
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	22	0.14
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	24	0.14
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	24	0.14
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	24	0.14
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	24	0.14
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	24	0.14
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	24	0.14
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	17	0.14
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	17	0.14
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	30	0.14
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	30	0.14
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	13	0.14
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	13	0.14
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	16	0.14
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	16	0.14
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	27	0.14
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	27	0.14
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	7	0.14
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	7	0.14
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	14	0.14
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	14	0.14
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	21	0.14
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	21	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	12	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	12	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	12	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	12	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	12	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	17	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	17	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	17	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	17	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	17	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	17	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	18	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	18	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	18	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	18	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	18	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	18	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	19	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	19	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	19	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	19	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	19	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	19	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	30	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	30	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	30	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	30	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	30	0.14
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	30	0.14
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD11	11	0.14
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD12	11	0.14
(1,505)	1:60:A:GLN:HE21	1:57:A:ILE:HD13	11	0.14
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD11	11	0.14
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD12	11	0.14
(1,505)	1:60:A:GLN:HE22	1:57:A:ILE:HD13	11	0.14
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB2	20	0.14
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB3	20	0.14
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB2	20	0.14
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB3	20	0.14
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB2	20	0.14
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB3	20	0.14
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	2	0.14
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	2	0.14
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	2	0.14
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	2	0.14
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	2	0.14
(1,452)	1:57:A:ILE:HD11	1:53:A:LEU:HA	30	0.14
(1,452)	1:57:A:ILE:HD12	1:53:A:LEU:HA	30	0.14
(1,452)	1:57:A:ILE:HD13	1:53:A:LEU:HA	30	0.14
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	1	0.14
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	30	0.14
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	25	0.14
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	25	0.14
(1,269)	1:40:A:GLU:H	1:40:A:GLU:HG2	13	0.14
(1,269)	1:40:A:GLU:H	1:40:A:GLU:HG3	13	0.14
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	4	0.14
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	4	0.14
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	4	0.14
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	15	0.14
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	15	0.14
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	15	0.14
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	21	0.14
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	21	0.14
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	21	0.14
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	21	0.14
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	21	0.14
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	21	0.14
(1,245)	1:37:A:THR:HG21	1:40:A:GLU:HG2	7	0.14
(1,245)	1:37:A:THR:HG21	1:40:A:GLU:HG3	7	0.14
(1,245)	1:37:A:THR:HG22	1:40:A:GLU:HG2	7	0.14
(1,245)	1:37:A:THR:HG22	1:40:A:GLU:HG3	7	0.14
(1,245)	1:37:A:THR:HG23	1:40:A:GLU:HG2	7	0.14
(1,245)	1:37:A:THR:HG23	1:40:A:GLU:HG3	7	0.14
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	2	0.14
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	2	0.14
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	2	0.14
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD21	6	0.14
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD22	6	0.14
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD23	6	0.14
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	7	0.14
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	7	0.14
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	19	0.14
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	22	0.14
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	22	0.14
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	10	0.14
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	10	0.14
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	23	0.14
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	23	0.14
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	12	0.14
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	12	0.14
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	30	0.14
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	30	0.14
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	30	0.14
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	30	0.14
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD21	20	0.14
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD22	20	0.14
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD23	20	0.14
(1,18)	1:19:A:SER:H	1:18:A:ILE:HB	9	0.14
(1,14)	1:18:A:ILE:H	1:18:A:ILE:HG12	8	0.14
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG21	9	0.13
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG22	9	0.13
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG23	9	0.13
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	12	0.13
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	12	0.13
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	12	0.13
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	12	0.13
(1,913)	1:92:A:LEU:H	1:93:A:GLU:H	23	0.13
(1,908)	1:92:A:LEU:H	1:91:A:SER:HB2	20	0.13
(1,908)	1:92:A:LEU:H	1:91:A:SER:HB3	20	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	2	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	2	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	2	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	2	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	2	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	2	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	4	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	4	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	4	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	4	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	4	0.13
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	4	0.13
(1,885)	1:89:A:ASP:H	1:86:A:LEU:HA	21	0.13
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	16	0.13
(1,862)	1:87:A:ASN:H	1:86:A:LEU:HG	29	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	1	0.13
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	1	0.13
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	1	0.13
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	16	0.13
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	16	0.13
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	16	0.13
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	4	0.13
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	4	0.13
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	24	0.13
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	24	0.13
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	11	0.13
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	11	0.13
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	13	0.13
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	13	0.13
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	20	0.13
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	20	0.13
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	28	0.13
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	28	0.13
(1,727)	1:77:A:GLY:H	1:76:A:GLU:HB2	29	0.13
(1,727)	1:77:A:GLY:H	1:76:A:GLU:HB3	29	0.13
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	1	0.13
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	3	0.13
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	9	0.13
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	28	0.13
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	25	0.13
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	25	0.13
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	26	0.13
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	26	0.13
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	28	0.13
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	28	0.13
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	4	0.13
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	4	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	4	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	4	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	4	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	4	0.13
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	13	0.13
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	13	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	13	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	13	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	13	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	15	0.13
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	15	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	15	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	15	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	15	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	15	0.13
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	27	0.13
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	27	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	27	0.13
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	27	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	27	0.13
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	27	0.13
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	18	0.13
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	18	0.13
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	23	0.13
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	23	0.13
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	26	0.13
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	26	0.13
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	28	0.13
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	28	0.13
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	12	0.13
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	12	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	12	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	12	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	12	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	12	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	12	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	12	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	20	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	20	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	20	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	20	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	20	0.13
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	20	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	5	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	5	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	5	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	5	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	5	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	5	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	23	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	23	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	23	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	23	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	23	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	23	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	27	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	27	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	27	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	27	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	27	0.13
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	27	0.13
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD11	2	0.13
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD12	2	0.13
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD13	2	0.13
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD11	2	0.13
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD12	2	0.13
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD13	2	0.13
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	5	0.13
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	5	0.13
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	5	0.13
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	5	0.13
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	5	0.13
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	5	0.13
(1,399)	1:50:A:HIS:H	1:50:A:HIS:HD2	26	0.13
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	18	0.13
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	24	0.13
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	20	0.13
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	20	0.13
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	27	0.13
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	27	0.13
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	23	0.13
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	23	0.13
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	23	0.13
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	23	0.13
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	23	0.13
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	23	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	10	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	10	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	10	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	18	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	18	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	18	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	22	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	22	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	22	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	24	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	24	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	24	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	30	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	30	0.13
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	30	0.13
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	11	0.13
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	11	0.13
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	11	0.13
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	11	0.13
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	11	0.13
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	11	0.13
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	18	0.13
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	18	0.13
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	18	0.13
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	18	0.13
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	18	0.13
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	18	0.13
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	5	0.13
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	3	0.13
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	3	0.13
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	23	0.13
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	23	0.13
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	1	0.13
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	1	0.13
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	1	0.13
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	18	0.13
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	18	0.13
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	18	0.13
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	22	0.13
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	22	0.13
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	22	0.13
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	22	0.13
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	22	0.13
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	22	0.13
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD21	20	0.13
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD22	20	0.13
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD23	20	0.13
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	21	0.13
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	22	0.13
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	22	0.13
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	26	0.13
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	26	0.13
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	30	0.13
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	30	0.13
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	9	0.13
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	13	0.13
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	5	0.13
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	5	0.13
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	8	0.13
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	8	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	5	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	5	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	14	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	14	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	16	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	16	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	25	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	25	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	30	0.13
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	30	0.13
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	28	0.13
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	28	0.13
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	16	0.13
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	16	0.13
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	22	0.13
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	22	0.13
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD11	25	0.13
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD12	25	0.13
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD13	25	0.13
(1,18)	1:19:A:SER:H	1:18:A:ILE:HB	16	0.13
(1,12)	1:18:A:ILE:H	1:18:A:ILE:HB	20	0.13
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB1	1	0.13
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB2	1	0.13
(1,10)	1:18:A:ILE:H	1:17:A:ALA:HB3	1	0.13
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG21	12	0.12
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG22	12	0.12
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG23	12	0.12
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	1	0.12
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	1	0.12
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	1	0.12
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	4	0.12
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	4	0.12
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	4	0.12
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	4	0.12
(1,926)	1:42:A:VAL:HG21	1:83:A:LYS:HA	6	0.12
(1,926)	1:42:A:VAL:HG22	1:83:A:LYS:HA	6	0.12
(1,926)	1:42:A:VAL:HG23	1:83:A:LYS:HA	6	0.12
(1,920)	1:93:A:GLU:H	1:93:A:GLU:HG2	5	0.12
(1,920)	1:93:A:GLU:H	1:93:A:GLU:HG3	5	0.12
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	27	0.12
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	27	0.12
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	27	0.12
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	27	0.12
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	27	0.12
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	27	0.12
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	13	0.12
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	13	0.12
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	21	0.12
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	21	0.12
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	21	0.12
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	6	0.12
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	6	0.12
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	6	0.12
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	30	0.12
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	30	0.12
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB2	17	0.12
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB3	17	0.12
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB2	20	0.12
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB3	20	0.12
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	30	0.12
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	30	0.12
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	4	0.12
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	18	0.12
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	20	0.12
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	13	0.12
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	13	0.12
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	14	0.12
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	14	0.12
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	16	0.12
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	16	0.12
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	22	0.12
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	2	0.12
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	2	0.12
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	2	0.12
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	2	0.12
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	2	0.12
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	2	0.12
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	21	0.12
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	21	0.12
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	21	0.12
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	21	0.12
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	21	0.12
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	21	0.12
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	30	0.12
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	30	0.12
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	30	0.12
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	30	0.12
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	30	0.12
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	30	0.12
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	1	0.12
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	1	0.12
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	19	0.12
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	19	0.12
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	24	0.12
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	24	0.12
(1,606)	1:66:A:THR:HG21	1:70:A:LYS:HE2	17	0.12
(1,606)	1:66:A:THR:HG21	1:70:A:LYS:HE3	17	0.12
(1,606)	1:66:A:THR:HG22	1:70:A:LYS:HE2	17	0.12
(1,606)	1:66:A:THR:HG22	1:70:A:LYS:HE3	17	0.12
(1,606)	1:66:A:THR:HG23	1:70:A:LYS:HE2	17	0.12
(1,606)	1:66:A:THR:HG23	1:70:A:LYS:HE3	17	0.12
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	8	0.12
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	8	0.12
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	27	0.12
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	27	0.12
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG2	12	0.12
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG3	12	0.12
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG2	27	0.12
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG3	27	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	2	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	2	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	2	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	2	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	2	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	6	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	6	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	6	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	6	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	6	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	6	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	15	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	15	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	15	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	15	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	15	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	15	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	24	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	24	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	24	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	24	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	24	0.12
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	24	0.12
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	25	0.12
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	25	0.12
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	25	0.12
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	25	0.12
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	25	0.12
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	25	0.12
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG2	12	0.12
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG3	12	0.12
(1,504)	1:60:A:GLN:HE21	1:57:A:ILE:HA	3	0.12
(1,504)	1:60:A:GLN:HE22	1:57:A:ILE:HA	3	0.12
(1,483)	1:59:A:ASN:H	1:58:A:LYS:HG2	9	0.12
(1,483)	1:59:A:ASN:H	1:58:A:LYS:HG3	9	0.12
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	17	0.12
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	17	0.12
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	17	0.12
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	17	0.12
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	17	0.12
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	17	0.12
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	20	0.12
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	20	0.12
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	20	0.12
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	20	0.12
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	20	0.12
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	4	0.12
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	9	0.12
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	15	0.12
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	15	0.12
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	15	0.12
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	23	0.12
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	23	0.12
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG2	24	0.12
(1,342)	1:46:A:LEU:H	1:45:A:LYS:HG3	24	0.12
(1,286)	1:42:A:VAL:H	1:39:A:LYS:HA	26	0.12
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	8	0.12
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	8	0.12
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	8	0.12
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	8	0.12
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	8	0.12
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	8	0.12
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD11	15	0.12
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD12	15	0.12
(1,283)	1:41:A:CYS:HB2	1:36:A:LEU:HD13	15	0.12
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD11	15	0.12
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD12	15	0.12
(1,283)	1:41:A:CYS:HB3	1:36:A:LEU:HD13	15	0.12
(1,269)	1:40:A:GLU:H	1:40:A:GLU:HG2	7	0.12
(1,269)	1:40:A:GLU:H	1:40:A:GLU:HG3	7	0.12
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	5	0.12
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	5	0.12
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	5	0.12
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	17	0.12
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	17	0.12
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	17	0.12
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	17	0.12
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	17	0.12
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	17	0.12
(1,245)	1:37:A:THR:HG21	1:40:A:GLU:HG2	13	0.12
(1,245)	1:37:A:THR:HG21	1:40:A:GLU:HG3	13	0.12
(1,245)	1:37:A:THR:HG22	1:40:A:GLU:HG2	13	0.12
(1,245)	1:37:A:THR:HG22	1:40:A:GLU:HG3	13	0.12
(1,245)	1:37:A:THR:HG23	1:40:A:GLU:HG2	13	0.12
(1,245)	1:37:A:THR:HG23	1:40:A:GLU:HG3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	21	0.12
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	21	0.12
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	21	0.12
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	21	0.12
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	21	0.12
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	21	0.12
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	25	0.12
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	25	0.12
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	25	0.12
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	25	0.12
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	25	0.12
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	25	0.12
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	29	0.12
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	29	0.12
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	29	0.12
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	29	0.12
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	29	0.12
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	29	0.12
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	7	0.12
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	14	0.12
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	14	0.12
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	19	0.12
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	19	0.12
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	19	0.12
(1,186)	1:31:A:LEU:HD11	1:44:A:GLU:HA	27	0.12
(1,186)	1:31:A:LEU:HD12	1:44:A:GLU:HA	27	0.12
(1,186)	1:31:A:LEU:HD13	1:44:A:GLU:HA	27	0.12
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG2	20	0.12
(1,185)	1:31:A:LEU:HD11	1:44:A:GLU:HG3	20	0.12
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG2	20	0.12
(1,185)	1:31:A:LEU:HD12	1:44:A:GLU:HG3	20	0.12
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG2	20	0.12
(1,185)	1:31:A:LEU:HD13	1:44:A:GLU:HG3	20	0.12
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD21	22	0.12
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD22	22	0.12
(1,180)	1:31:A:LEU:H	1:31:A:LEU:HD23	22	0.12
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	6	0.12
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	6	0.12
(1,140)	1:28:A:LEU:H	1:28:A:LEU:HG	10	0.12
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	3	0.12
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	3	0.12
(1,127)	1:27:A:ARG:H	1:27:A:ARG:HD2	30	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:27:A:ARG:H	1:27:A:ARG:HD3	30	0.12
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	8	0.12
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	8	0.12
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	21	0.12
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	21	0.12
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	27	0.12
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	27	0.12
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	29	0.12
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	29	0.12
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	2	0.12
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	2	0.12
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD21	1	0.12
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD22	1	0.12
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD23	1	0.12
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD21	24	0.12
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD22	24	0.12
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD23	24	0.12
(1,934)	1:46:A:LEU:HG	1:86:A:LEU:HD11	14	0.11
(1,934)	1:46:A:LEU:HG	1:86:A:LEU:HD12	14	0.11
(1,934)	1:46:A:LEU:HG	1:86:A:LEU:HD13	14	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG21	3	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG22	3	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG23	3	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG21	8	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG22	8	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG23	8	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG21	16	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG22	16	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG23	16	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG21	27	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG22	27	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG23	27	0.11
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	23	0.11
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	23	0.11
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	23	0.11
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	23	0.11
(1,920)	1:93:A:GLU:H	1:93:A:GLU:HG2	7	0.11
(1,920)	1:93:A:GLU:H	1:93:A:GLU:HG3	7	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	12	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	12	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	12	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	12	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	12	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	20	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	20	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	20	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	20	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	20	0.11
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	20	0.11
(1,880)	1:88:A:LYS:H	1:88:A:LYS:HD2	14	0.11
(1,880)	1:88:A:LYS:H	1:88:A:LYS:HD3	14	0.11
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD21	27	0.11
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD22	27	0.11
(1,853)	1:86:A:LEU:H	1:86:A:LEU:HD23	27	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	4	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	4	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	4	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	7	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	7	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	7	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	11	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	11	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	11	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	24	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	24	0.11
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	24	0.11
(1,764)	1:80:A:ALA:H	1:77:A:GLY:HA2	4	0.11
(1,764)	1:80:A:ALA:H	1:77:A:GLY:HA3	4	0.11
(1,764)	1:80:A:ALA:H	1:77:A:GLY:HA2	12	0.11
(1,764)	1:80:A:ALA:H	1:77:A:GLY:HA3	12	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	9	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	9	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	11	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	11	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	13	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	13	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	17	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	17	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	18	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	18	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	23	0.11
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	23	0.11
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	6	0.11
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG2	23	0.11
(1,728)	1:77:A:GLY:H	1:76:A:GLU:HG3	23	0.11
(1,715)	1:76:A:GLU:H	1:74:A:SER:HB2	3	0.11
(1,715)	1:76:A:GLU:H	1:74:A:SER:HB3	3	0.11
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	21	0.11
(1,704)	1:74:A:SER:H	1:76:A:GLU:H	23	0.11
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	4	0.11
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	4	0.11
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	30	0.11
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	30	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	5	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	5	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	5	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	5	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	5	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	5	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	10	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	10	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	10	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	10	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	10	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	10	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	16	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	16	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	16	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	16	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	16	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	16	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	17	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	17	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	17	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	17	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	17	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	17	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	18	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	18	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	18	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	18	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	18	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	18	0.11
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE1	28	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:73:A:LEU:HD21	1:78:A:TYR:HE2	28	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE1	28	0.11
(1,690)	1:73:A:LEU:HD22	1:78:A:TYR:HE2	28	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE1	28	0.11
(1,690)	1:73:A:LEU:HD23	1:78:A:TYR:HE2	28	0.11
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG2	10	0.11
(1,682)	1:73:A:LEU:H	1:72:A:GLU:HG3	10	0.11
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	8	0.11
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	8	0.11
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG2	19	0.11
(1,660)	1:70:A:LYS:H	1:69:A:ARG:HG3	19	0.11
(1,606)	1:66:A:THR:HG21	1:70:A:LYS:HE2	24	0.11
(1,606)	1:66:A:THR:HG21	1:70:A:LYS:HE3	24	0.11
(1,606)	1:66:A:THR:HG22	1:70:A:LYS:HE2	24	0.11
(1,606)	1:66:A:THR:HG22	1:70:A:LYS:HE3	24	0.11
(1,606)	1:66:A:THR:HG23	1:70:A:LYS:HE2	24	0.11
(1,606)	1:66:A:THR:HG23	1:70:A:LYS:HE3	24	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	5	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	5	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	13	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	13	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	22	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	22	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	28	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	28	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD2	30	0.11
(1,603)	1:66:A:THR:HB	1:70:A:LYS:HD3	30	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	5	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	5	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	5	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	5	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	5	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	5	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	19	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	19	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	19	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	19	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	19	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	19	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	27	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	27	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	27	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	27	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	27	0.11
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	27	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	7	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	7	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	7	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	7	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	7	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	7	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	11	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	11	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	11	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	11	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	11	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	11	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	20	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	20	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	20	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	20	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	20	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	20	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	29	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	29	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	29	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	29	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	29	0.11
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	29	0.11
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD11	21	0.11
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD12	21	0.11
(1,507)	1:60:A:GLN:HG2	1:57:A:ILE:HD13	21	0.11
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD11	21	0.11
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD12	21	0.11
(1,507)	1:60:A:GLN:HG3	1:57:A:ILE:HD13	21	0.11
(1,504)	1:60:A:GLN:HE21	1:57:A:ILE:HA	21	0.11
(1,504)	1:60:A:GLN:HE22	1:57:A:ILE:HA	21	0.11
(1,501)	1:60:A:GLN:H	1:60:A:GLN:HG2	20	0.11
(1,501)	1:60:A:GLN:H	1:60:A:GLN:HG3	20	0.11
(1,483)	1:59:A:ASN:H	1:58:A:LYS:HG2	6	0.11
(1,483)	1:59:A:ASN:H	1:58:A:LYS:HG3	6	0.11
(1,483)	1:59:A:ASN:H	1:58:A:LYS:HG2	26	0.11
(1,483)	1:59:A:ASN:H	1:58:A:LYS:HG3	26	0.11
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:57:A:ILE:HD11	1:89:A:ASP:HB3	1	0.11
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB2	1	0.11
(1,457)	1:57:A:ILE:HD12	1:89:A:ASP:HB3	1	0.11
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB2	1	0.11
(1,457)	1:57:A:ILE:HD13	1:89:A:ASP:HB3	1	0.11
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	3	0.11
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	3	0.11
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	3	0.11
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	3	0.11
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	3	0.11
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	3	0.11
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	9	0.11
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	9	0.11
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	9	0.11
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	9	0.11
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	9	0.11
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	9	0.11
(1,417)	1:52:A:PHE:H	1:52:A:PHE:HE1	20	0.11
(1,417)	1:52:A:PHE:H	1:52:A:PHE:HE2	20	0.11
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	19	0.11
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	20	0.11
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	22	0.11
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	29	0.11
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	30	0.11
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	30	0.11
(1,258)	1:39:A:LYS:H	1:38:A:GLU:HG2	18	0.11
(1,258)	1:39:A:LYS:H	1:38:A:GLU:HG3	18	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	4	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	4	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	4	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	4	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	4	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	4	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	7	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	7	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	7	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	7	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	7	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	7	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	8	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	8	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	8	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	8	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	8	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	10	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	10	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	10	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	10	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	10	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	10	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	15	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	15	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	15	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	15	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	15	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	15	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	20	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	20	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	20	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	20	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	20	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	20	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	26	0.11
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	26	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	26	0.11
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	26	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	26	0.11
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	26	0.11
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	4	0.11
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	4	0.11
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	4	0.11
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	4	0.11
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	4	0.11
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	4	0.11
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	16	0.11
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	16	0.11
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	16	0.11
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	16	0.11
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	16	0.11
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	16	0.11
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	24	0.11
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	24	0.11
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	24	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	24	0.11
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	24	0.11
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	24	0.11
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	19	0.11
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	26	0.11
(1,239)	1:37:A:THR:H	1:37:A:THR:HG21	23	0.11
(1,239)	1:37:A:THR:H	1:37:A:THR:HG22	23	0.11
(1,239)	1:37:A:THR:H	1:37:A:THR:HG23	23	0.11
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	16	0.11
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	16	0.11
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	22	0.11
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	22	0.11
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	4	0.11
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	4	0.11
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	10	0.11
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	10	0.11
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	13	0.11
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	13	0.11
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	25	0.11
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	25	0.11
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG2	1	0.11
(1,137)	1:28:A:LEU:H	1:27:A:ARG:HG3	1	0.11
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	6	0.11
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	6	0.11
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG2	19	0.11
(1,123)	1:27:A:ARG:H	1:26:A:ARG:HG3	19	0.11
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG2	15	0.11
(1,109)	1:26:A:ARG:H	1:25:A:ARG:HG3	15	0.11
(1,72)	1:24:A:VAL:H	1:21:A:PRO:HG2	23	0.11
(1,72)	1:24:A:VAL:H	1:21:A:PRO:HG3	23	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	8	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	8	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	19	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	19	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	27	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	27	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	29	0.11
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	29	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD21	9	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD22	9	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD23	9	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD21	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD22	15	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD23	15	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD21	18	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD22	18	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD23	18	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD21	22	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD22	22	0.11
(1,30)	1:20:A:LEU:H	1:20:A:LEU:HD23	22	0.11
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD11	21	0.11
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD12	21	0.11
(1,29)	1:20:A:LEU:H	1:20:A:LEU:HD13	21	0.11
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG21	5	0.1
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG22	5	0.1
(1,932)	1:82:A:VAL:HB	1:42:A:VAL:HG23	5	0.1
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD2	7	0.1
(1,929)	1:47:A:ASN:HD21	1:58:A:LYS:HD3	7	0.1
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD2	7	0.1
(1,929)	1:47:A:ASN:HD22	1:58:A:LYS:HD3	7	0.1
(1,920)	1:93:A:GLU:H	1:93:A:GLU:HG2	17	0.1
(1,920)	1:93:A:GLU:H	1:93:A:GLU:HG3	17	0.1
(1,906)	1:91:A:SER:H	1:92:A:LEU:H	6	0.1
(1,906)	1:91:A:SER:H	1:92:A:LEU:H	14	0.1
(1,906)	1:91:A:SER:H	1:92:A:LEU:H	21	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	5	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	5	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	5	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	5	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	5	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	5	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD11	29	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD12	29	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD13	29	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD21	29	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD22	29	0.1
(1,894)	1:89:A:ASP:HA	1:90:A:LEU:HD23	29	0.1
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	6	0.1
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	6	0.1
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG2	8	0.1
(1,889)	1:89:A:ASP:H	1:88:A:LYS:HG3	8	0.1
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	13	0.1
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	13	0.1
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD21	23	0.1
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD22	23	0.1
(1,818)	1:83:A:LYS:HA	1:86:A:LEU:HD23	23	0.1
(1,794)	1:82:A:VAL:H	1:64:A:LEU:HD11	4	0.1
(1,794)	1:82:A:VAL:H	1:64:A:LEU:HD12	4	0.1
(1,794)	1:82:A:VAL:H	1:64:A:LEU:HD13	4	0.1
(1,794)	1:82:A:VAL:H	1:64:A:LEU:HD21	4	0.1
(1,794)	1:82:A:VAL:H	1:64:A:LEU:HD22	4	0.1
(1,794)	1:82:A:VAL:H	1:64:A:LEU:HD23	4	0.1
(1,764)	1:80:A:ALA:H	1:77:A:GLY:HA2	21	0.1
(1,764)	1:80:A:ALA:H	1:77:A:GLY:HA3	21	0.1
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	5	0.1
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	5	0.1
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD1	29	0.1
(1,743)	1:78:A:TYR:H	1:78:A:TYR:HD2	29	0.1
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB2	15	0.1
(1,736)	1:78:A:TYR:H	1:73:A:LEU:HB3	15	0.1
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	12	0.1
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	12	0.1
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB2	21	0.1
(1,697)	1:74:A:SER:H	1:73:A:LEU:HB3	21	0.1
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG2	4	0.1
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG3	4	0.1
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG2	7	0.1
(1,595)	1:66:A:THR:H	1:65:A:GLU:HG3	7	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	8	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	8	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	8	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	8	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	8	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	8	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	11	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	11	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	11	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	11	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	11	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	11	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	18	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	18	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	18	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	18	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	18	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	23	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	23	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	23	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	23	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	23	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	23	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD11	30	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD12	30	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD13	30	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD21	30	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD22	30	0.1
(1,573)	1:65:A:GLU:H	1:64:A:LEU:HD23	30	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	4	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	4	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	4	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	4	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	4	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	4	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	21	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	21	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	21	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	21	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	21	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	21	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD11	24	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD12	24	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD13	24	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD21	24	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD22	24	0.1
(1,531)	1:62:A:CYS:H	1:61:A:LEU:HD23	24	0.1
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG2	5	0.1
(1,515)	1:61:A:LEU:H	1:60:A:GLN:HG3	5	0.1
(1,504)	1:60:A:GLN:HE21	1:57:A:ILE:HA	11	0.1
(1,504)	1:60:A:GLN:HE22	1:57:A:ILE:HA	11	0.1
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG2	24	0.1
(1,453)	1:57:A:ILE:HD11	1:54:A:GLN:HG3	24	0.1
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG2	24	0.1
(1,453)	1:57:A:ILE:HD12	1:54:A:GLN:HG3	24	0.1
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG2	24	0.1
(1,453)	1:57:A:ILE:HD13	1:54:A:GLN:HG3	24	0.1
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:48:A:LEU:H	1:46:A:LEU:HA	11	0.1
(1,363)	1:47:A:ASN:HD21	1:44:A:GLU:HA	7	0.1
(1,363)	1:47:A:ASN:HD22	1:44:A:GLU:HA	7	0.1
(1,286)	1:42:A:VAL:H	1:39:A:LYS:HA	3	0.1
(1,286)	1:42:A:VAL:H	1:39:A:LYS:HA	13	0.1
(1,258)	1:39:A:LYS:H	1:38:A:GLU:HG2	11	0.1
(1,258)	1:39:A:LYS:H	1:38:A:GLU:HG3	11	0.1
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG21	28	0.1
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG22	28	0.1
(1,248)	1:38:A:GLU:H	1:37:A:THR:HG23	28	0.1
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE2	29	0.1
(1,246)	1:37:A:THR:HG21	1:39:A:LYS:HE3	29	0.1
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE2	29	0.1
(1,246)	1:37:A:THR:HG22	1:39:A:LYS:HE3	29	0.1
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE2	29	0.1
(1,246)	1:37:A:THR:HG23	1:39:A:LYS:HE3	29	0.1
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB2	15	0.1
(1,244)	1:37:A:THR:HG21	1:40:A:GLU:HB3	15	0.1
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB2	15	0.1
(1,244)	1:37:A:THR:HG22	1:40:A:GLU:HB3	15	0.1
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB2	15	0.1
(1,244)	1:37:A:THR:HG23	1:40:A:GLU:HB3	15	0.1
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	21	0.1
(1,240)	1:37:A:THR:H	1:41:A:CYS:HG	29	0.1
(1,208)	1:33:A:ARG:H	1:33:A:ARG:HD2	20	0.1
(1,208)	1:33:A:ARG:H	1:33:A:ARG:HD3	20	0.1
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	11	0.1
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	11	0.1
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG2	12	0.1
(1,204)	1:33:A:ARG:H	1:32:A:GLU:HG3	12	0.1
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG2	2	0.1
(1,166)	1:30:A:ASP:H	1:29:A:LYS:HG3	2	0.1
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	7	0.1
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	7	0.1
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG2	15	0.1
(1,57)	1:22:A:ASP:H	1:21:A:PRO:HG3	15	0.1
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG12	9	0.1
(1,19)	1:19:A:SER:H	1:18:A:ILE:HG13	9	0.1
(1,18)	1:19:A:SER:H	1:18:A:ILE:HB	4	0.1
(1,18)	1:19:A:SER:H	1:18:A:ILE:HB	11	0.1
(1,12)	1:18:A:ILE:H	1:18:A:ILE:HB	3	0.1

10 Dihedral-angle violation analysis

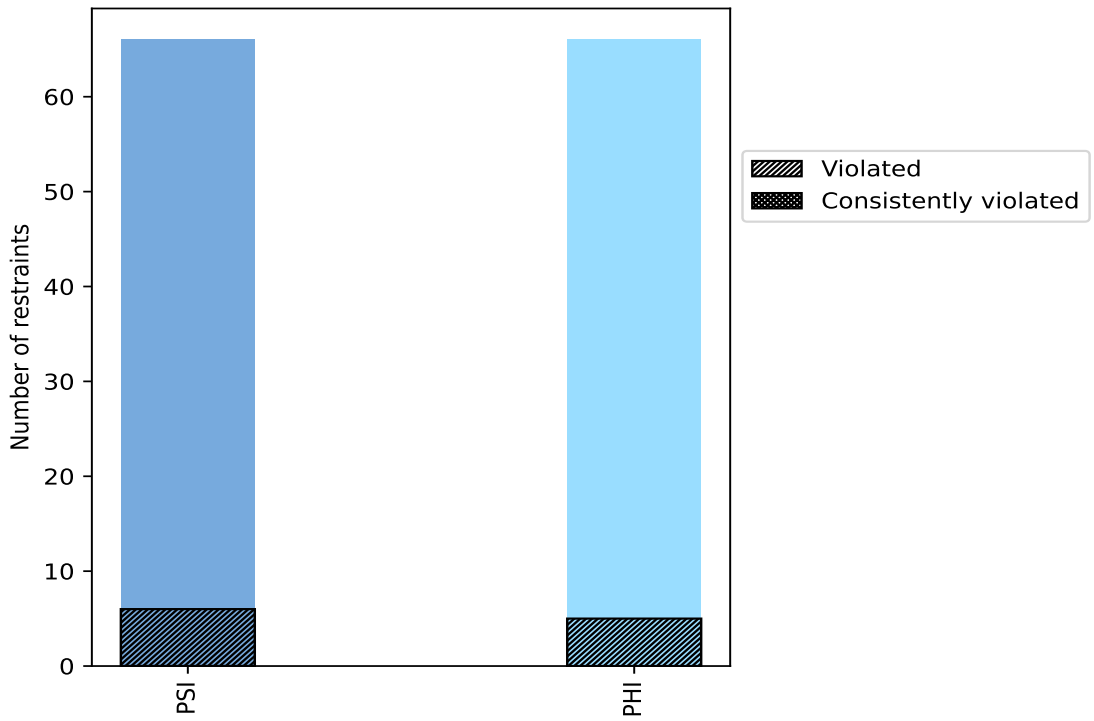
10.1 Summary of dihedral-angle violations

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	66	50.0	6	9.1	4.5	0	0.0	0.0
PHI	66	50.0	5	7.6	3.8	0	0.0	0.0
Total	132	100.0	11	8.3	8.3	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



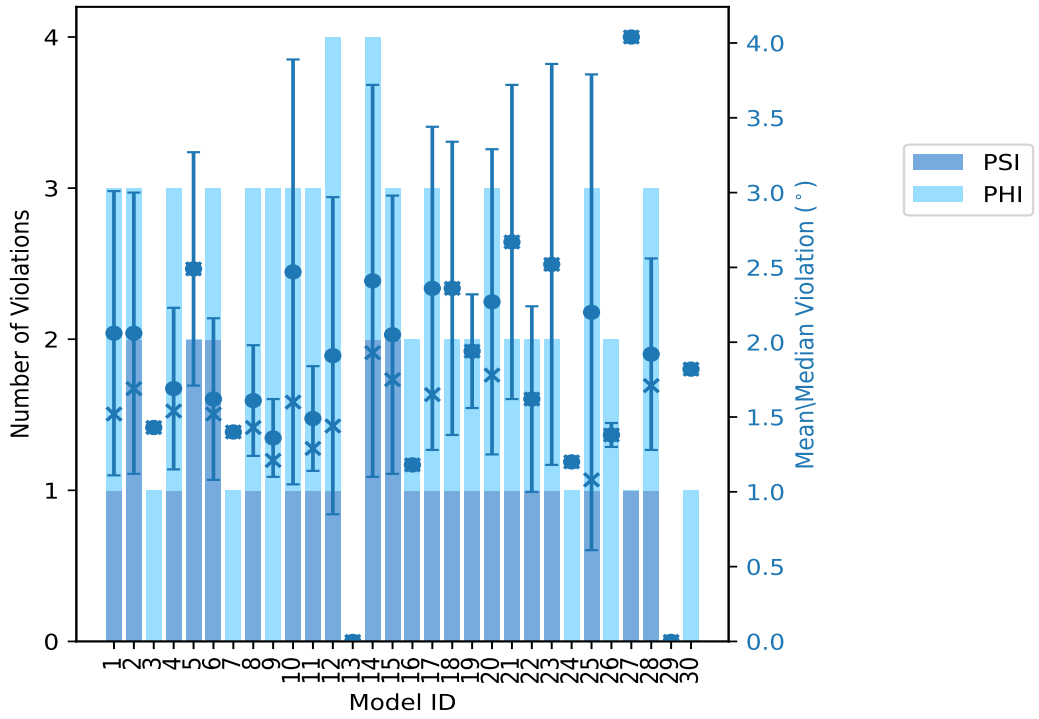
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	1	2	3	2.06	3.39	0.95	1.52
2	2	1	3	2.06	3.35	0.94	1.69
3	0	1	1	1.43	1.43	0.0	1.43
4	1	2	3	1.69	2.41	0.54	1.54
5	2	0	2	2.49	3.27	0.78	2.49
6	2	1	3	1.62	2.33	0.54	1.52
7	0	1	1	1.4	1.4	0.0	1.4
8	1	2	3	1.61	2.13	0.37	1.43
9	0	3	3	1.36	1.72	0.26	1.21
10	1	2	3	2.47	4.47	1.42	1.6
11	1	2	3	1.49	1.98	0.35	1.29
12	1	3	4	1.91	3.72	1.06	1.44
13	0	0	0	0.0	0.0	0.0	0.0
14	2	2	4	2.41	4.61	1.31	1.93
15	2	1	3	2.05	3.3	0.93	1.75
16	1	1	2	1.18	1.21	0.03	1.18
17	1	2	3	2.36	3.88	1.08	1.65
18	1	1	2	2.36	3.33	0.98	2.36
19	1	1	2	1.94	2.33	0.38	1.94
20	1	2	3	2.27	3.7	1.02	1.78
21	1	1	2	2.67	3.72	1.05	2.67
22	1	1	2	1.62	2.23	0.62	1.62
23	1	1	2	2.52	3.85	1.34	2.52
24	0	1	1	1.2	1.2	0.0	1.2
25	1	2	3	2.2	4.44	1.59	1.08
26	0	2	2	1.38	1.46	0.08	1.38
27	1	0	1	4.04	4.04	0.0	4.04
28	1	2	3	1.92	2.79	0.64	1.71
29	0	0	0	0.0	0.0	0.0	0.0
30	0	1	1	1.82	1.82	0.0	1.82

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]	%
3	2	5	1	3.3
0	0	0	2	6.7
2	0	2	3	10.0
0	1	1	4	13.3
0	0	0	5	16.7
0	0	0	6	20.0
0	0	0	7	23.3
0	0	0	8	26.7
0	0	0	9	30.0
0	0	0	10	33.3
0	1	1	11	36.7

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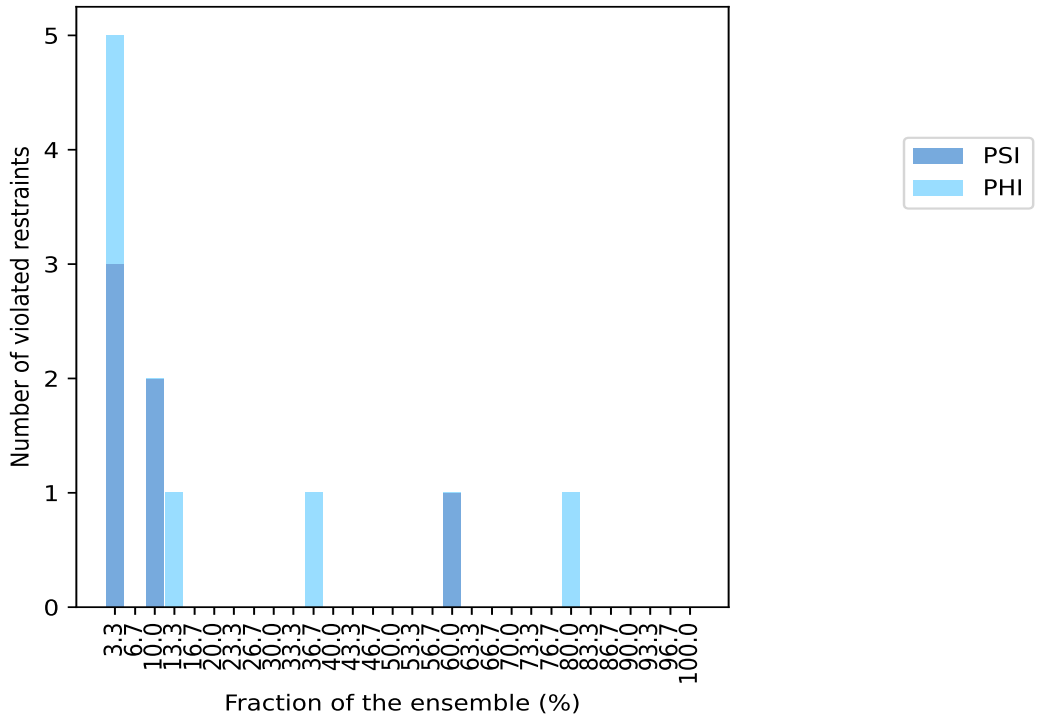
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	40.0
0	0	0	13	43.3
0	0	0	14	46.7
0	0	0	15	50.0
0	0	0	16	53.3
0	0	0	17	56.7
1	0	1	18	60.0
0	0	0	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
0	0	0	22	73.3
0	0	0	23	76.7
0	1	1	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
0	0	0	27	90.0
0	0	0	28	93.3
0	0	0	29	96.7
0	0	0	30	100.0

[1] Number of models with violations

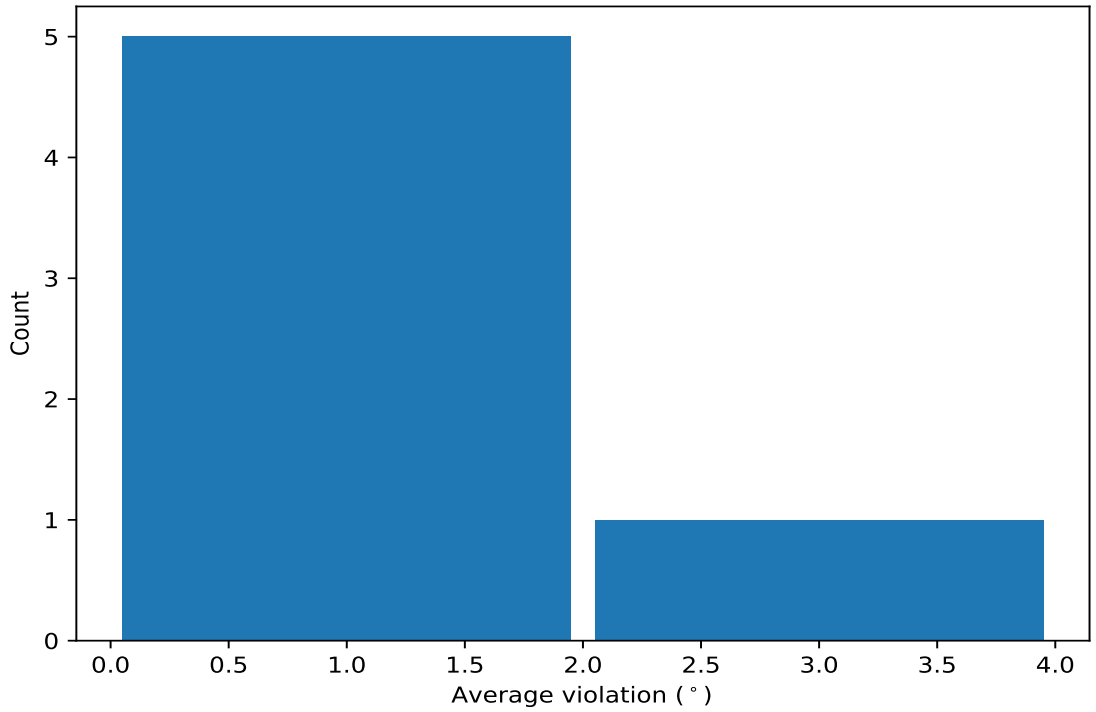
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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.

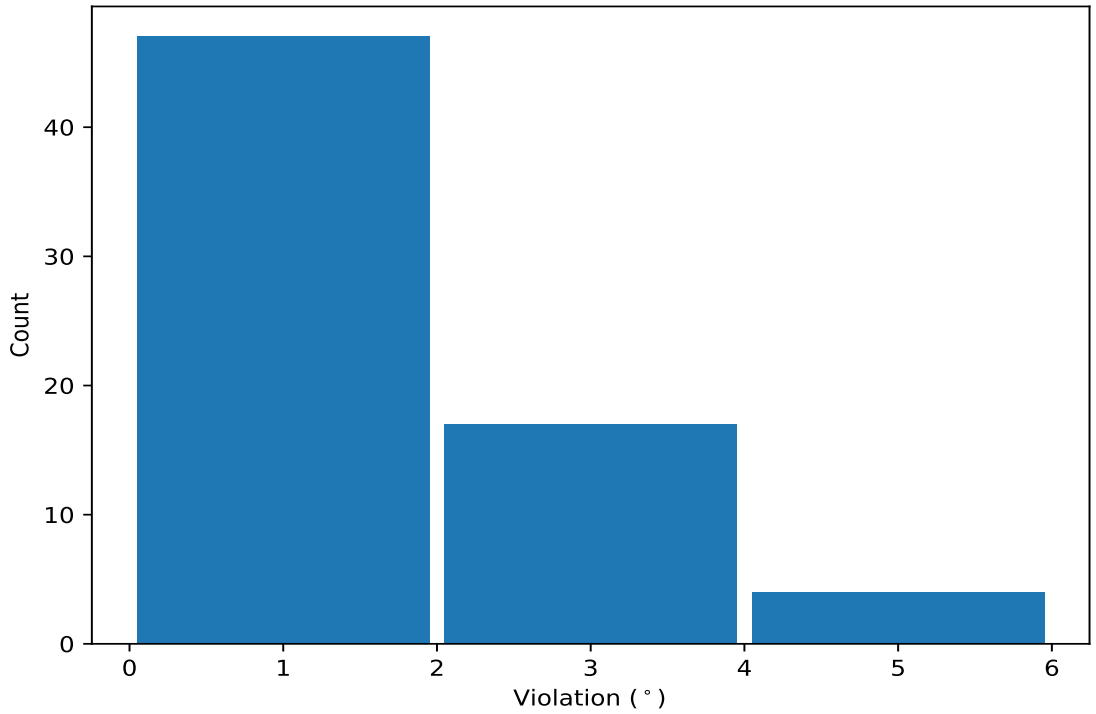
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	24	1.56	0.29	1.53
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	18	3.43	0.82	3.54
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	11	1.33	0.18	1.34
(1,55)	1:51:A:GLU:C	1:52:A:PHE:N	1:52:A:PHE:CA	1:52:A:PHE:C	4	1.13	0.11	1.12
(1,104)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	1:77:A:GLY:N	3	1.63	0.38	1.56
(1,130)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:LEU:N	3	1.31	0.28	1.13

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	14	4.61
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	10	4.47
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	25	4.44
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	27	4.04
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	17	3.88
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	23	3.85
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	12	3.72
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	21	3.72
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	20	3.7
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	1	3.39
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	2	3.35
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	18	3.33
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	15	3.3
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	5	3.27
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	28	2.79
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	4	2.41
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	19	2.33
(1,26)	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	1:35:A:SER:N	6	2.33
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	22	2.23
(1,104)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	1:77:A:GLY:N	8	2.13
(1,124)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:ASN:N	14	2.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	11	1.98
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	14	1.84
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	30	1.82
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	20	1.78
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	15	1.75
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	9	1.72
(1,130)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:LEU:N	5	1.71
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	28	1.71
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	2	1.69
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	17	1.65
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	21	1.62
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	10	1.6
(1,104)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	1:77:A:GLY:N	19	1.56
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	4	1.54
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	17	1.54
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	1	1.52
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	6	1.52
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	12	1.51
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	26	1.46
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	3	1.43
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	8	1.43
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	7	1.4
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	18	1.38
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	12	1.36
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	10	1.35
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	20	1.34
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	26	1.3
(1,132)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:SER:N	11	1.29
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	8	1.27
(1,59)	1:53:A:LEU:C	1:54:A:GLN:N	1:54:A:GLN:CA	1:54:A:GLN:C	28	1.27
(1,55)	1:51:A:GLU:C	1:52:A:PHE:N	1:52:A:PHE:CA	1:52:A:PHE:C	1	1.27
(1,104)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	1:77:A:GLY:N	16	1.21
(1,55)	1:51:A:GLU:C	1:52:A:PHE:N	1:52:A:PHE:CA	1:52:A:PHE:C	9	1.21
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	24	1.2
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	11	1.19
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	23	1.18
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	16	1.16
(1,131)	1:89:A:ASP:C	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	14	1.15
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	9	1.14
(1,130)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:LEU:N	2	1.13
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	4	1.12
(1,130)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:LEU:N	15	1.09
(1,97)	1:72:A:GLU:C	1:73:A:LEU:N	1:73:A:LEU:CA	1:73:A:LEU:C	25	1.08
(1,25)	1:33:A:ARG:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	25	1.07
(1,55)	1:51:A:GLU:C	1:52:A:PHE:N	1:52:A:PHE:CA	1:52:A:PHE:C	12	1.03
(1,90)	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	1:70:A:LYS:N	6	1.01
(1,55)	1:51:A:GLU:C	1:52:A:PHE:N	1:52:A:PHE:CA	1:52:A:PHE:C	22	1.0