



Full wwPDB NMR Structure Validation Report ⓘ

Feb 28, 2026 – 10:11 PM UTC

PDB ID : 2PNG / pdb_00002png
Title : Type I rat fatty acid synthase acyl carrier protein (ACP) domain
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Deposited on : 2007-04-24

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

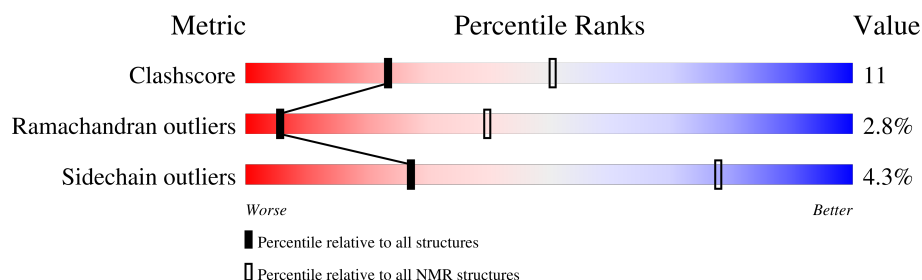
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	89	

2 Ensemble composition and analysis

This entry contains 30 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:74 (67)	0.91	1

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1386 atoms, of which 708 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fatty acid synthase (EC 2.3.1.85).

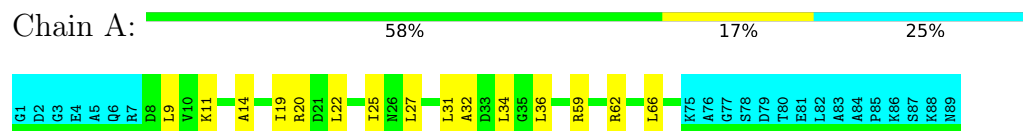
Mol	Chain	Residues	Atoms						Trace
1	A	89	Total	C	H	N	O	S	0
			1386	416	708	125	135	2	

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: Fatty acid synthase (EC 2.3.1.85)

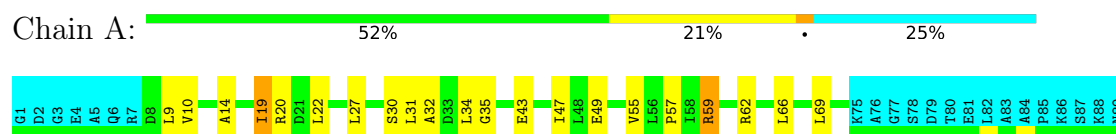


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

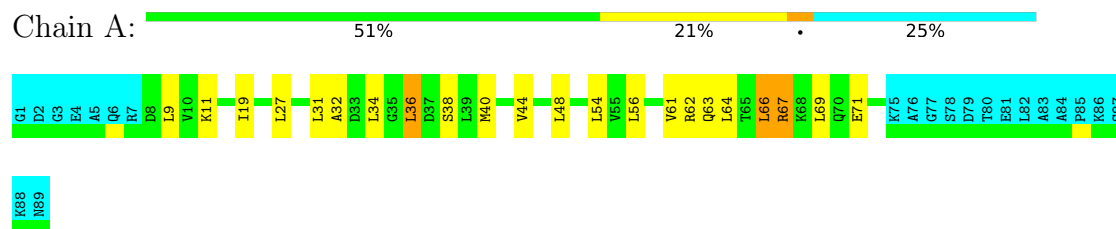
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



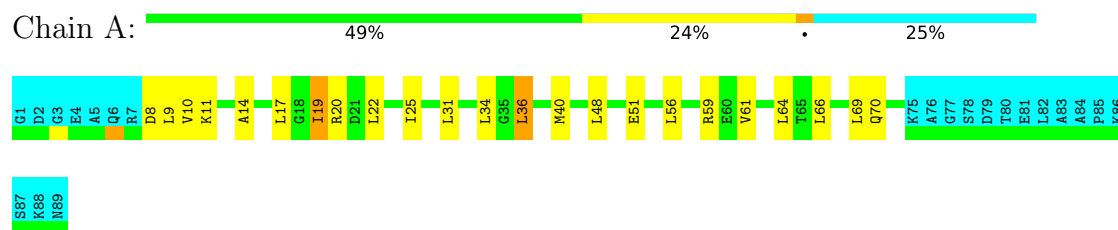
4.2.2 Score per residue for model 2

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



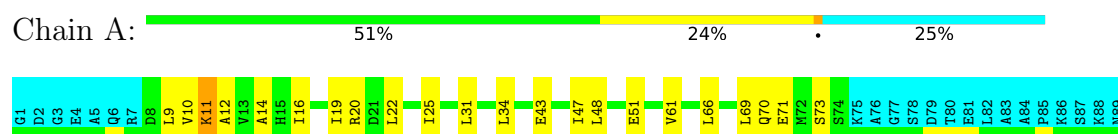
4.2.3 Score per residue for model 3

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



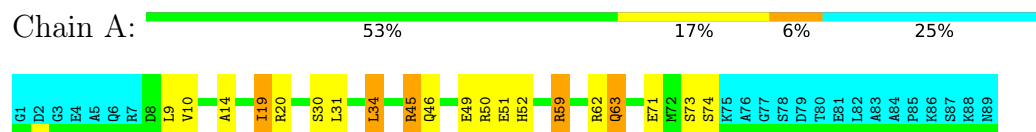
4.2.4 Score per residue for model 4

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



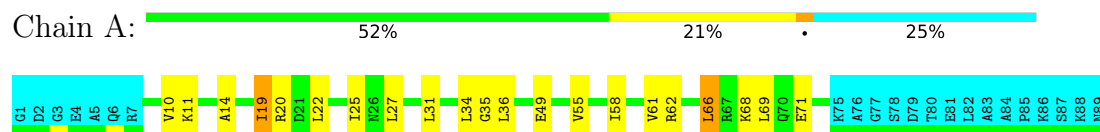
4.2.5 Score per residue for model 5

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



4.2.6 Score per residue for model 6

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



4.2.7 Score per residue for model 7

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)





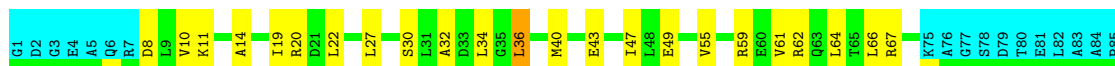
4.2.8 Score per residue for model 8

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



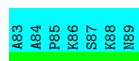
4.2.9 Score per residue for model 9

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



4.2.10 Score per residue for model 10

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



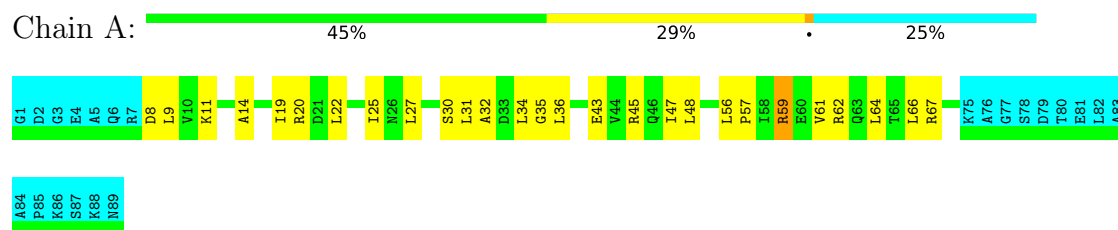
4.2.11 Score per residue for model 11

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



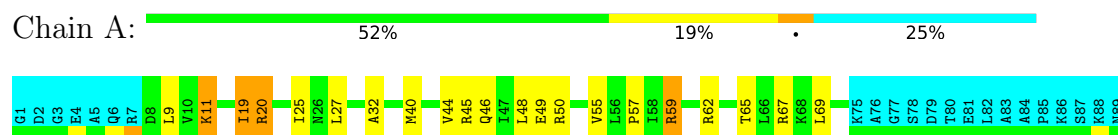
4.2.12 Score per residue for model 12

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



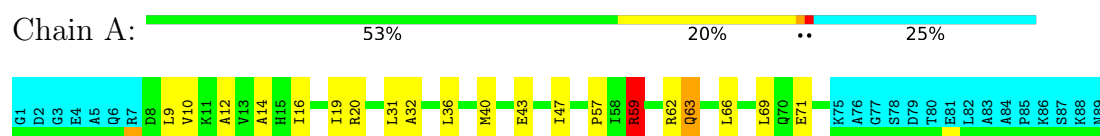
4.2.16 Score per residue for model 16

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



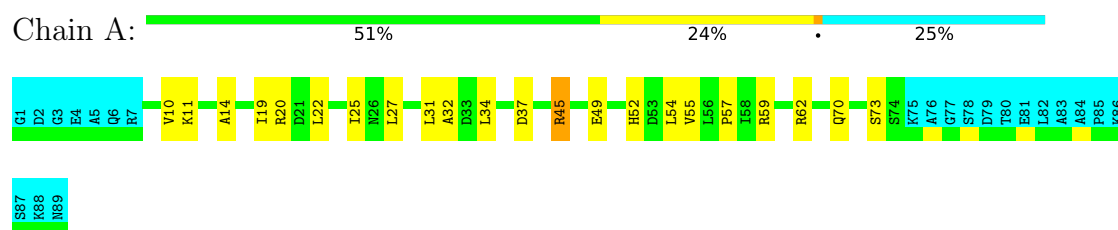
4.2.17 Score per residue for model 17

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



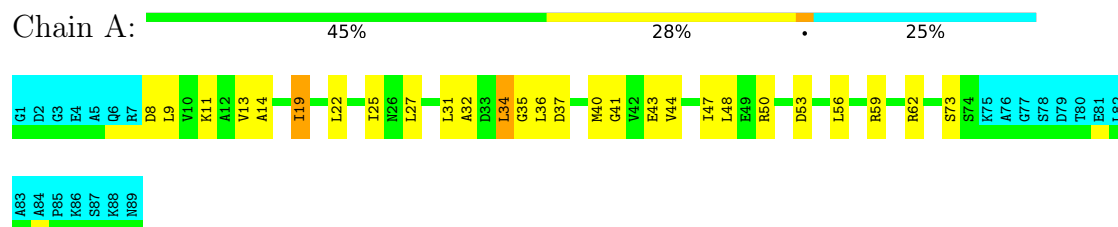
4.2.18 Score per residue for model 18

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



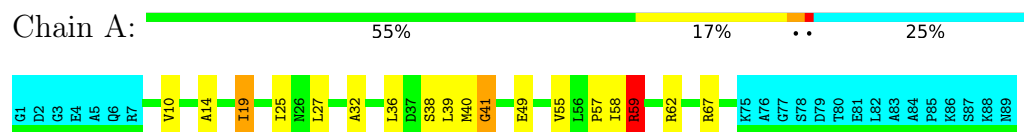
4.2.19 Score per residue for model 19

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



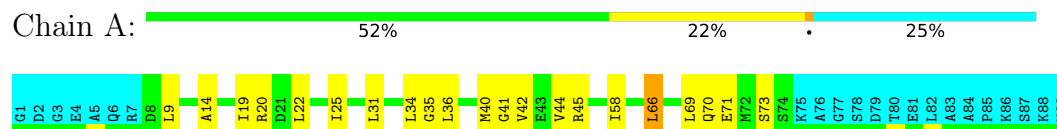
4.2.20 Score per residue for model 20

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



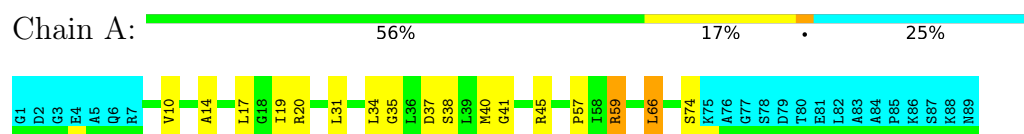
4.2.21 Score per residue for model 21

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



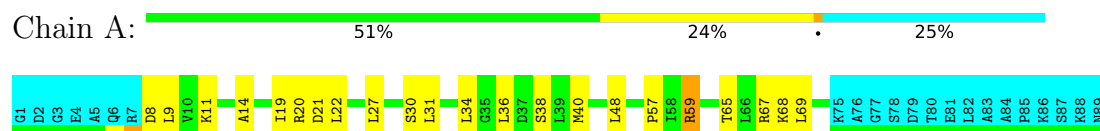
4.2.22 Score per residue for model 22

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



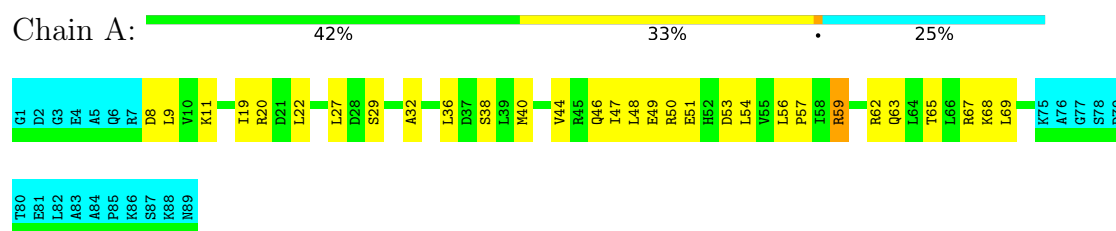
4.2.23 Score per residue for model 23

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



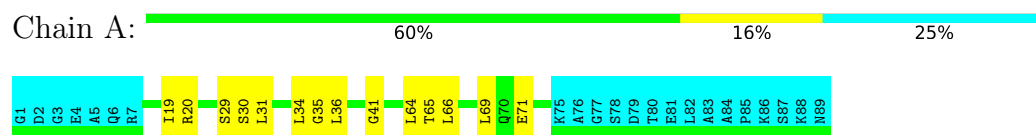
4.2.24 Score per residue for model 24

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



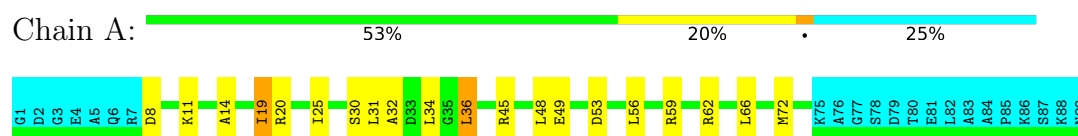
4.2.25 Score per residue for model 25

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



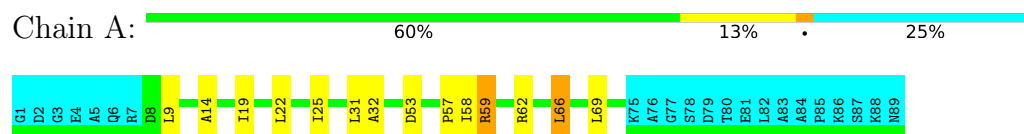
4.2.26 Score per residue for model 26

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



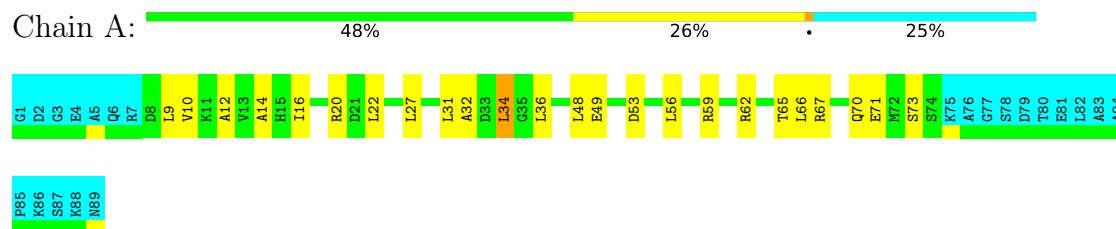
4.2.27 Score per residue for model 27

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



4.2.28 Score per residue for model 28

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



4.2.29 Score per residue for model 29

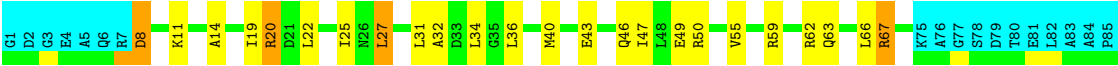
- Molecule 1: Fatty acid synthase (EC 2.3.1.85)





4.2.30 Score per residue for model 30

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



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
CNS	refinement	1.1
ARIA	structure solution	1.2

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	980
Number of shifts mapped to atoms	980
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.98±0.04	0±0/525 (0.0± 0.0%)	1.00±0.04	0±0/708 (0.1± 0.1%)
All	All	0.98	0/15750 (0.0%)	1.00	12/21240 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.6±0.7
All	All	0	19

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	71	GLU	N-CA-C	-6.01	106.10	113.50	10	8
1	A	37	ASP	N-CA-C	-5.35	108.52	114.62	19	2
1	A	74	SER	N-CA-C	-5.32	106.09	112.58	13	1
1	A	27	LEU	N-CA-C	-5.16	106.98	113.28	30	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	45	ARG	Sidechain	6
1	A	67	ARG	Sidechain	5
1	A	59	ARG	Sidechain	5
1	A	20	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	62	ARG	Sidechain	1

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	522	556	554	12±3
All	All	15660	16680	16620	356

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ASP:HB2	1:A:11:LYS:HG2	0.89	1.45	13	6
1:A:31:LEU:HD12	1:A:34:LEU:HD12	0.79	1.54	4	9
1:A:32:ALA:HB2	1:A:62:ARG:HG2	0.79	1.53	24	8
1:A:27:LEU:HD22	1:A:67:ARG:HG2	0.72	1.62	10	2
1:A:22:LEU:HG	1:A:27:LEU:HD21	0.72	1.62	14	6
1:A:48:LEU:HG	1:A:56:LEU:HD12	0.71	1.61	24	8
1:A:9:LEU:HB2	1:A:69:LEU:HB3	0.69	1.63	2	5
1:A:19:ILE:HG21	1:A:25:ILE:HG13	0.69	1.63	29	11
1:A:9:LEU:HG	1:A:47:ILE:HG21	0.69	1.64	13	1
1:A:22:LEU:HD12	1:A:27:LEU:HD21	0.68	1.63	23	1
1:A:49:GLU:HG2	1:A:55:VAL:HB	0.67	1.64	1	1
1:A:9:LEU:HG	1:A:73:SER:HA	0.66	1.65	5	4
1:A:48:LEU:HD22	1:A:54:LEU:HD23	0.65	1.67	2	1
1:A:32:ALA:HB2	1:A:62:ARG:HG3	0.65	1.67	9	3
1:A:45:ARG:HD3	1:A:57:PRO:HA	0.65	1.69	18	1
1:A:9:LEU:HD11	1:A:48:LEU:HD21	0.64	1.68	10	6
1:A:14:ALA:HB1	1:A:19:ILE:HG13	0.63	1.69	27	17
1:A:36:LEU:HA	1:A:40:MET:HE3	0.63	1.69	20	2
1:A:14:ALA:HB2	1:A:66:LEU:HD11	0.63	1.67	8	10
1:A:63:GLN:N	1:A:63:GLN:HE21	0.63	1.91	17	4
1:A:11:LYS:HA	1:A:11:LYS:HE2	0.62	1.70	8	1
1:A:49:GLU:HG2	1:A:55:VAL:HA	0.61	1.71	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:GLN:HA	1:A:73:SER:HB2	0.61	1.73	14	1
1:A:9:LEU:HB3	1:A:69:LEU:HB3	0.61	1.71	23	4
1:A:36:LEU:HB2	1:A:40:MET:HB2	0.61	1.72	17	5
1:A:57:PRO:HB2	1:A:59:ARG:HD2	0.59	1.72	17	7
1:A:61:VAL:HA	1:A:64:LEU:HG	0.59	1.73	2	5
1:A:22:LEU:HG	1:A:67:ARG:HE	0.59	1.54	23	2
1:A:31:LEU:HA	1:A:34:LEU:HD12	0.58	1.75	11	13
1:A:36:LEU:HA	1:A:40:MET:SD	0.58	2.39	24	2
1:A:22:LEU:HD11	1:A:66:LEU:HG	0.58	1.76	21	1
1:A:34:LEU:HD21	1:A:66:LEU:HD23	0.58	1.76	26	1
1:A:19:ILE:HD12	1:A:22:LEU:HD11	0.57	1.76	7	3
1:A:9:LEU:HD12	1:A:69:LEU:HD12	0.57	1.74	24	3
1:A:72:MET:HE2	1:A:72:MET:HA	0.57	1.75	26	2
1:A:22:LEU:HD13	1:A:25:ILE:HB	0.56	1.77	30	6
1:A:27:LEU:HD22	1:A:67:ARG:HG3	0.56	1.78	24	3
1:A:70:GLN:HA	1:A:73:SER:HB3	0.55	1.76	13	5
1:A:10:VAL:HG21	1:A:70:GLN:CG	0.55	2.31	3	1
1:A:9:LEU:HD22	1:A:69:LEU:HB3	0.54	1.78	3	1
1:A:32:ALA:HB2	1:A:62:ARG:CG	0.54	2.33	27	6
1:A:8:ASP:HB3	1:A:11:LYS:HG2	0.54	1.78	30	1
1:A:22:LEU:HD12	1:A:25:ILE:HB	0.54	1.79	18	3
1:A:49:GLU:HG3	1:A:55:VAL:HG22	0.54	1.79	9	7
1:A:57:PRO:HB2	1:A:59:ARG:CD	0.53	2.34	20	6
1:A:58:ILE:HA	1:A:61:VAL:HB	0.53	1.80	29	3
1:A:46:GLN:O	1:A:50:ARG:HG3	0.52	2.03	14	1
1:A:45:ARG:O	1:A:49:GLU:HB3	0.51	2.04	5	4
1:A:19:ILE:HG21	1:A:25:ILE:HG12	0.51	1.81	19	2
1:A:27:LEU:O	1:A:65:THR:HB	0.51	2.06	28	2
1:A:41:GLY:HA3	1:A:58:ILE:HG13	0.51	1.82	21	2
1:A:57:PRO:HB2	1:A:59:ARG:HD3	0.51	1.81	27	4
1:A:32:ALA:HB2	1:A:62:ARG:HB3	0.51	1.82	18	6
1:A:40:MET:O	1:A:44:VAL:HG23	0.51	2.06	24	4
1:A:31:LEU:HB2	1:A:64:LEU:O	0.51	2.06	8	2
1:A:68:LYS:HA	1:A:71:GLU:HB3	0.50	1.82	6	1
1:A:31:LEU:HD23	1:A:34:LEU:HD23	0.50	1.82	5	1
1:A:31:LEU:HD11	1:A:69:LEU:HD21	0.50	1.82	17	1
1:A:43:GLU:O	1:A:47:ILE:HG13	0.50	2.06	30	13
1:A:8:ASP:OD2	1:A:11:LYS:HG2	0.50	2.06	24	1
1:A:31:LEU:HD23	1:A:61:VAL:HG12	0.49	1.83	4	2
1:A:8:ASP:HB3	1:A:11:LYS:HE3	0.49	1.84	14	1
1:A:36:LEU:HA	1:A:40:MET:HB2	0.49	1.82	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HA	1:A:34:LEU:HD22	0.49	1.84	28	2
1:A:10:VAL:O	1:A:14:ALA:HB3	0.49	2.08	1	10
1:A:10:VAL:HG21	1:A:70:GLN:HG2	0.49	1.83	3	1
1:A:17:LEU:HD11	1:A:34:LEU:HD13	0.49	1.83	22	1
1:A:52:HIS:CD2	1:A:74:SER:HB2	0.48	2.43	5	1
1:A:12:ALA:O	1:A:16:ILE:HG12	0.48	2.09	13	5
1:A:42:VAL:HG22	1:A:45:ARG:HH21	0.48	1.69	21	1
1:A:66:LEU:HA	1:A:69:LEU:HD23	0.47	1.86	17	4
1:A:36:LEU:HD23	1:A:62:ARG:HA	0.47	1.84	12	2
1:A:14:ALA:HB2	1:A:66:LEU:HD21	0.47	1.86	11	2
1:A:36:LEU:HD13	1:A:41:GLY:N	0.47	2.24	25	3
1:A:29:SER:O	1:A:65:THR:HA	0.47	2.10	25	5
1:A:30:SER:HB3	1:A:62:ARG:O	0.47	2.10	5	2
1:A:34:LEU:HD13	1:A:66:LEU:HD23	0.47	1.87	10	1
1:A:46:GLN:O	1:A:50:ARG:HB3	0.46	2.11	30	3
1:A:30:SER:O	1:A:34:LEU:HG	0.46	2.10	23	6
1:A:9:LEU:CG	1:A:73:SER:HA	0.46	2.39	5	1
1:A:22:LEU:HB3	1:A:27:LEU:HD21	0.46	1.87	11	3
1:A:27:LEU:HD22	1:A:67:ARG:CG	0.46	2.40	29	2
1:A:31:LEU:HD23	1:A:36:LEU:HD22	0.46	1.86	26	1
1:A:8:ASP:OD2	1:A:11:LYS:HG3	0.45	2.12	3	1
1:A:48:LEU:HD13	1:A:56:LEU:HB2	0.45	1.88	2	1
1:A:49:GLU:O	1:A:53:ASP:HA	0.45	2.11	24	3
1:A:41:GLY:O	1:A:45:ARG:HG3	0.44	2.11	15	1
1:A:22:LEU:HG	1:A:67:ARG:HG2	0.44	1.88	28	1
1:A:11:LYS:HE2	1:A:20:ARG:HD3	0.44	1.88	16	1
1:A:8:ASP:HB2	1:A:11:LYS:CG	0.44	2.39	7	1
1:A:8:ASP:HB3	1:A:11:LYS:CG	0.44	2.42	30	1
1:A:65:THR:OG1	1:A:68:LYS:HB2	0.44	2.12	24	3
1:A:9:LEU:CB	1:A:69:LEU:HB3	0.44	2.43	17	1
1:A:58:ILE:O	1:A:62:ARG:HB2	0.44	2.12	27	1
1:A:36:LEU:HB2	1:A:40:MET:CB	0.44	2.43	30	1
1:A:48:LEU:HD12	1:A:54:LEU:HD23	0.43	1.90	24	1
1:A:30:SER:O	1:A:34:LEU:HD13	0.43	2.13	26	1
1:A:59:ARG:H	1:A:59:ARG:HD2	0.43	1.73	5	3
1:A:9:LEU:HD11	1:A:48:LEU:HD11	0.43	1.90	12	1
1:A:46:GLN:HA	1:A:50:ARG:HB2	0.43	1.90	16	1
1:A:68:LYS:O	1:A:72:MET:HG2	0.43	2.13	13	1
1:A:27:LEU:HD13	1:A:67:ARG:HG3	0.43	1.91	20	1
1:A:66:LEU:O	1:A:69:LEU:HB2	0.43	2.13	17	3
1:A:64:LEU:HB3	1:A:69:LEU:HD22	0.42	1.91	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LYS:HD2	1:A:11:LYS:N	0.42	2.29	6	1
1:A:19:ILE:HB	1:A:22:LEU:HD13	0.42	1.90	18	1
1:A:47:ILE:O	1:A:51:GLU:HB2	0.42	2.14	24	1
1:A:31:LEU:HD12	1:A:34:LEU:HD22	0.42	1.92	3	1
1:A:11:LYS:N	1:A:11:LYS:HE3	0.42	2.29	4	1
1:A:46:GLN:OE1	1:A:50:ARG:HD2	0.42	2.14	8	1
1:A:22:LEU:HG	1:A:27:LEU:CD2	0.42	2.41	14	2
1:A:44:VAL:O	1:A:48:LEU:HG	0.41	2.15	2	1
1:A:36:LEU:HG	1:A:62:ARG:HG3	0.41	1.92	12	1
1:A:42:VAL:HG13	1:A:45:ARG:NH2	0.41	2.30	15	1
1:A:49:GLU:HG2	1:A:55:VAL:HG22	0.41	1.92	15	1
1:A:8:ASP:CB	1:A:11:LYS:HD3	0.41	2.45	23	1
1:A:52:HIS:HB3	1:A:54:LEU:HD13	0.41	1.90	18	1
1:A:17:LEU:HD12	1:A:19:ILE:HD11	0.41	1.93	3	1
1:A:31:LEU:HG	1:A:64:LEU:O	0.41	2.16	15	2
1:A:59:ARG:HD2	1:A:59:ARG:H	0.41	1.76	15	2
1:A:31:LEU:HA	1:A:34:LEU:CD1	0.41	2.46	2	1
1:A:22:LEU:HB3	1:A:27:LEU:HD23	0.41	1.92	12	1
1:A:39:LEU:C	1:A:41:GLY:H	0.40	2.24	20	1
1:A:13:VAL:HG22	1:A:44:VAL:HG22	0.40	1.93	19	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	67/89 (75%)	56±2 (84±3%)	9±2 (13±3%)	2±1 (3±2%)	6	40
All	All	2010/2670 (75%)	1687 (84%)	266 (13%)	57 (3%)	6	40

All 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	20	ARG	22
1	A	35	GLY	10

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Mol	Chain	Res	Type	Models (Total)
1	A	38	SER	8
1	A	37	ASP	5
1	A	66	LEU	2
1	A	8	ASP	2
1	A	41	GLY	2
1	A	39	LEU	1
1	A	53	ASP	1
1	A	58	ILE	1
1	A	40	MET	1
1	A	74	SER	1
1	A	31	LEU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/74 (80%)	56±1 (96±2%)	3±1 (4±2%)	27	78
All	All	1770/2220 (80%)	1694 (96%)	76 (4%)	27	78

All 13 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	19	ILE	18
1	A	59	ARG	18
1	A	66	LEU	9
1	A	63	GLN	9
1	A	11	LYS	7
1	A	36	LEU	6
1	A	34	LEU	3
1	A	67	ARG	1
1	A	50	ARG	1
1	A	70	GLN	1
1	A	21	ASP	1
1	A	53	ASP	1
1	A	72	MET	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_bmr15449.str*

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	980
Number of shifts mapped to atoms	980
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	87	-0.35 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	80	-0.10 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	84	-0.19 ± 0.44	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 82%, i.e. 790 atoms were assigned a chemical shift out of a possible 962. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	268/337 (80%)	136/137 (99%)	67/134 (50%)	65/66 (98%)
Sidechain	522/609 (86%)	359/399 (90%)	160/186 (86%)	3/24 (12%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/16 (0%)	0/8 (0%)	0/4 (0%)	0/4 (0%)
Overall	790/962 (82%)	495/544 (91%)	227/324 (70%)	68/94 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 980 atoms were assigned a chemical shift out of a possible 1219. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	343/448 (77%)	172/183 (94%)	87/178 (49%)	84/87 (97%)
Sidechain	637/755 (84%)	437/491 (89%)	196/232 (84%)	4/32 (12%)
Aromatic	0/16 (0%)	0/8 (0%)	0/4 (0%)	0/4 (0%)
Overall	980/1219 (80%)	609/682 (89%)	283/414 (68%)	88/123 (72%)

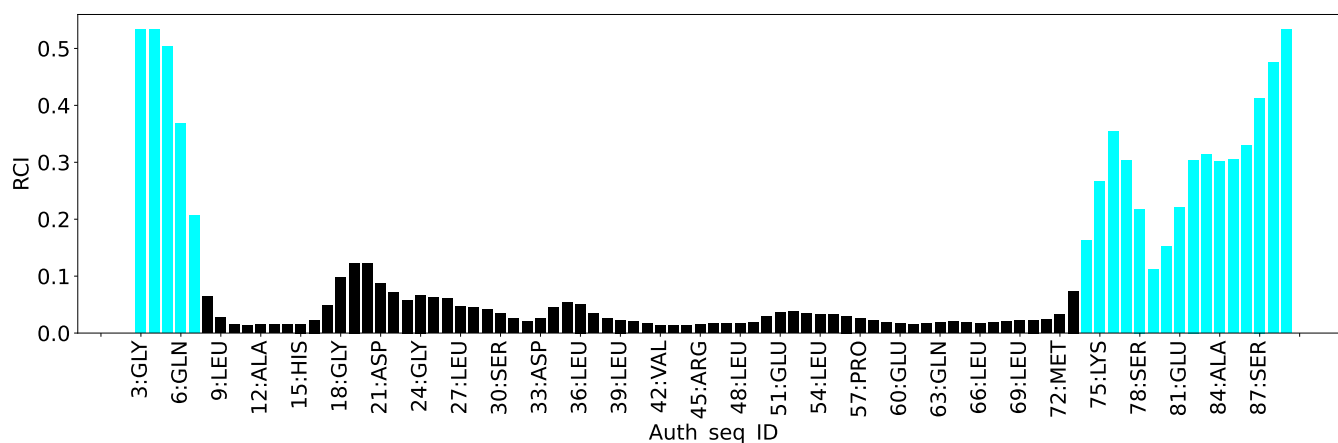
7.1.4 Statistically unusual chemical shifts [i](#)

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	1732
Intra-residue ($ i-j =0$)	697
Sequential ($ i-j =1$)	396
Medium range ($ i-j >1$ and $ i-j <5$)	425
Long range ($ i-j \geq 5$)	214
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	19.5
Number of long range restraints per residue ¹	2.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	10.4	0.2
0.2-0.5 (Medium)	12.1	0.5
>0.5 (Large)	23.6	3.2

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

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

9 Distance violation analysis ⓘ

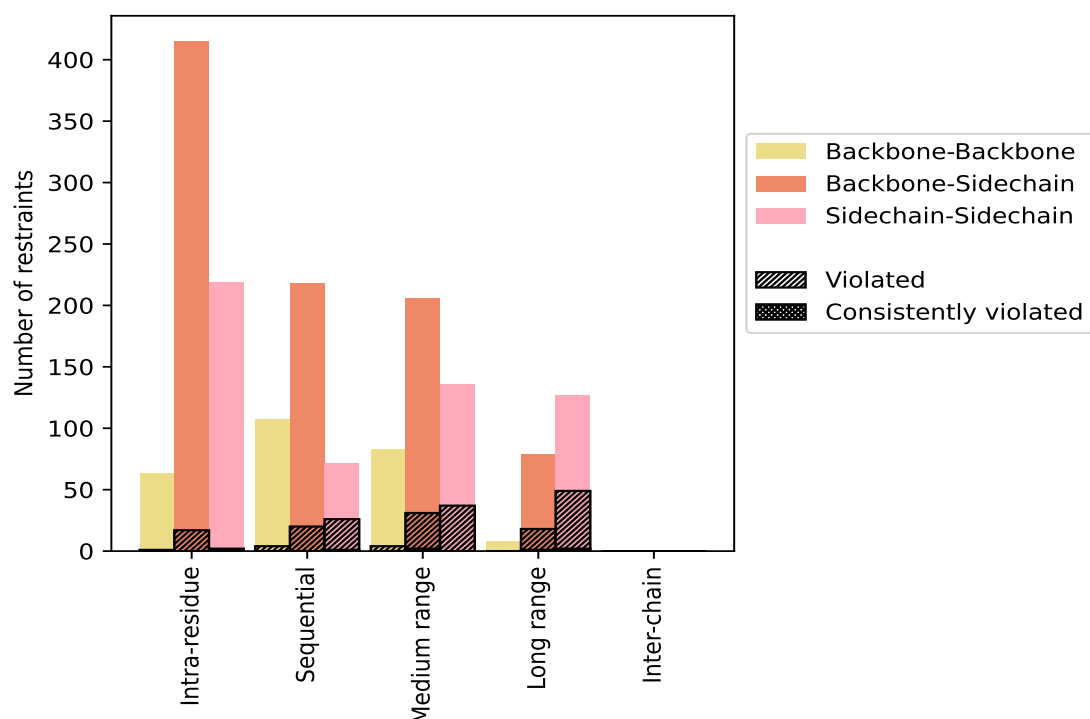
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	697	40.2	20	2.9	1.2	1	0.1	0.1
Backbone-Backbone	63	3.6	1	1.6	0.1	0	0.0	0.0
Backbone-Sidechain	415	24.0	17	4.1	1.0	0	0.0	0.0
Sidechain-Sidechain	219	12.6	2	0.9	0.1	1	0.5	0.1
Sequential (i-j =1)	396	22.9	50	12.6	2.9	1	0.3	0.1
Backbone-Backbone	107	6.2	4	3.7	0.2	0	0.0	0.0
Backbone-Sidechain	218	12.6	20	9.2	1.2	0	0.0	0.0
Sidechain-Sidechain	71	4.1	26	36.6	1.5	1	1.4	0.1
Medium range (i-j >1 & i-j <5)	425	24.5	72	16.9	4.2	2	0.5	0.1
Backbone-Backbone	83	4.8	4	4.8	0.2	0	0.0	0.0
Backbone-Sidechain	206	11.9	31	15.0	1.8	2	1.0	0.1
Sidechain-Sidechain	136	7.9	37	27.2	2.1	0	0.0	0.0
Long range (i-j ≥5)	214	12.4	67	31.3	3.9	3	1.4	0.2
Backbone-Backbone	8	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	79	4.6	18	22.8	1.0	1	1.3	0.1
Sidechain-Sidechain	127	7.3	49	38.6	2.8	2	1.6	0.1
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	1732	100.0	209	12.1	12.1	7	0.4	0.4
Backbone-Backbone	261	15.1	9	3.4	0.5	0	0.0	0.0
Backbone-Sidechain	918	53.0	86	9.4	5.0	3	0.3	0.2
Sidechain-Sidechain	553	31.9	114	20.6	6.6	4	0.7	0.2

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	2	10	17	19	0	48	0.67	1.58	0.44	0.51
2	2	8	22	19	0	51	0.75	3.01	0.55	0.72
3	3	8	17	20	0	48	0.59	1.56	0.42	0.48
4	1	5	10	15	0	31	0.6	1.72	0.47	0.5
5	4	6	16	25	0	51	0.59	1.62	0.41	0.52
6	3	4	15	20	0	42	0.58	1.95	0.5	0.38
7	3	7	16	21	0	47	0.45	1.39	0.35	0.34
8	4	10	14	16	0	44	0.58	1.69	0.44	0.53
9	2	6	9	18	0	35	0.62	1.64	0.5	0.48
10	2	4	17	15	0	38	0.61	1.51	0.43	0.52

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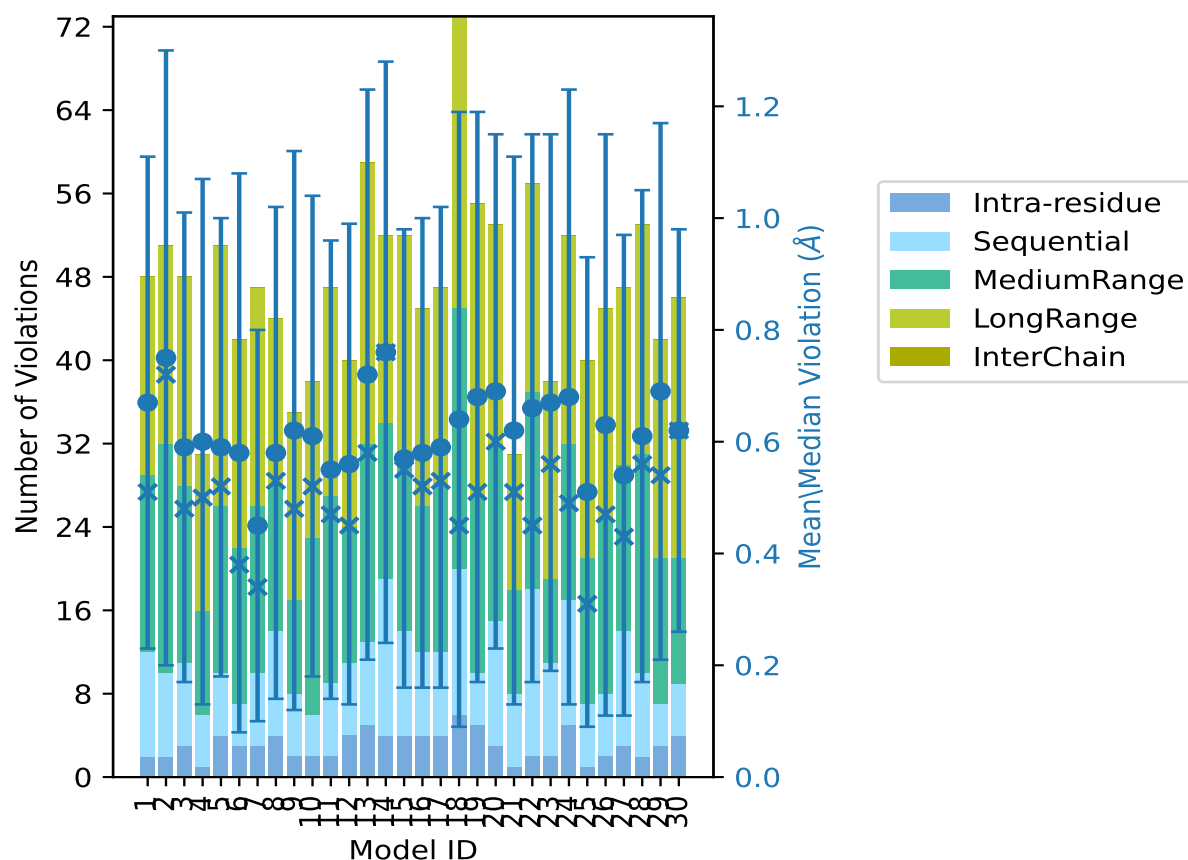
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	7	18	20	0	47	0.55	1.78	0.41	0.47
12	4	7	13	16	0	40	0.56	1.73	0.43	0.45
13	5	8	19	27	0	59	0.72	2.37	0.51	0.58
14	4	15	15	18	0	52	0.76	2.01	0.52	0.76
15	4	10	16	22	0	52	0.57	1.65	0.41	0.55
16	4	8	14	19	0	45	0.58	1.74	0.42	0.52
17	4	8	16	19	0	47	0.59	1.89	0.43	0.53
18	6	14	25	28	0	73	0.64	3.2	0.55	0.45
19	5	5	17	28	0	55	0.68	2.37	0.51	0.51
20	3	12	17	21	0	53	0.69	1.67	0.46	0.6
21	1	7	10	13	0	31	0.62	1.82	0.49	0.51
22	2	16	19	20	0	57	0.66	1.67	0.49	0.45
23	2	9	8	19	0	38	0.67	1.71	0.48	0.56
24	5	12	15	20	0	52	0.68	2.3	0.55	0.49
25	1	6	14	19	0	40	0.51	1.61	0.42	0.31
26	2	6	17	20	0	45	0.63	2.31	0.52	0.47
27	3	11	16	17	0	47	0.54	1.98	0.43	0.43
28	2	8	21	22	0	53	0.61	1.72	0.44	0.56
29	3	4	14	21	0	42	0.69	1.72	0.48	0.54
30	4	5	12	25	0	46	0.62	1.57	0.36	0.62

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1523(IR:677, SQ:346, MR:353, LR:147, 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	15	25	15	0	62	1	3.3
4	6	8	8	0	26	2	6.7
3	8	10	4	0	25	3	10.0
0	7	3	3	0	13	4	13.3
1	0	4	2	0	7	5	16.7
1	1	0	6	0	8	6	20.0

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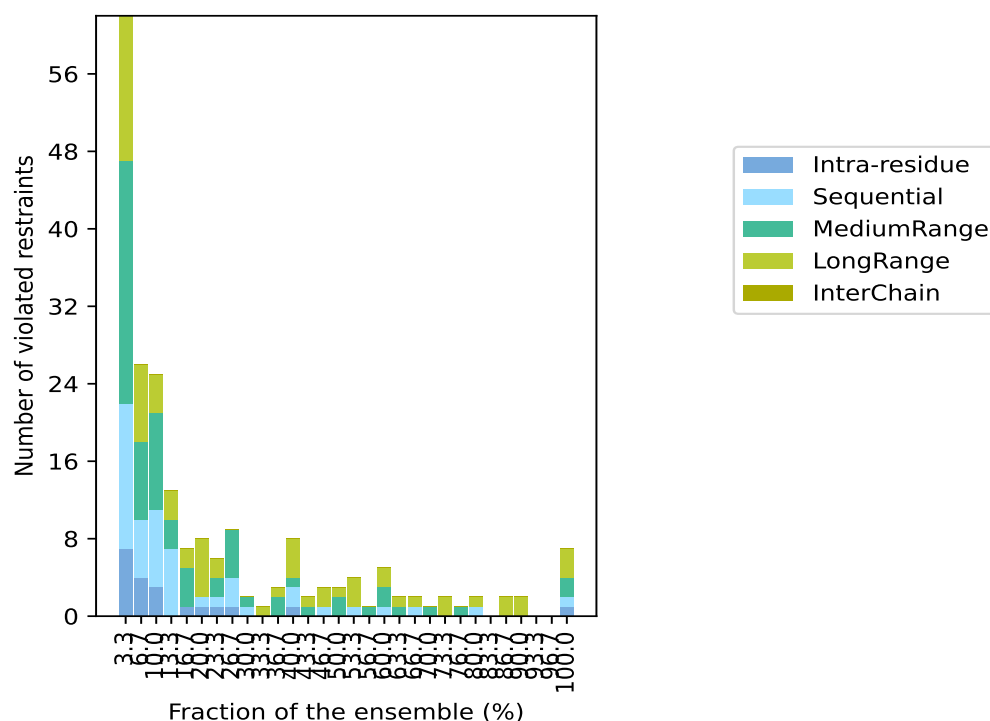
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	1	2	2	0	6	7	23.3
1	3	5	0	0	9	8	26.7
0	1	1	0	0	2	9	30.0
0	0	0	1	0	1	10	33.3
0	0	2	1	0	3	11	36.7
1	2	1	4	0	8	12	40.0
0	0	1	1	0	2	13	43.3
0	1	0	2	0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

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

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

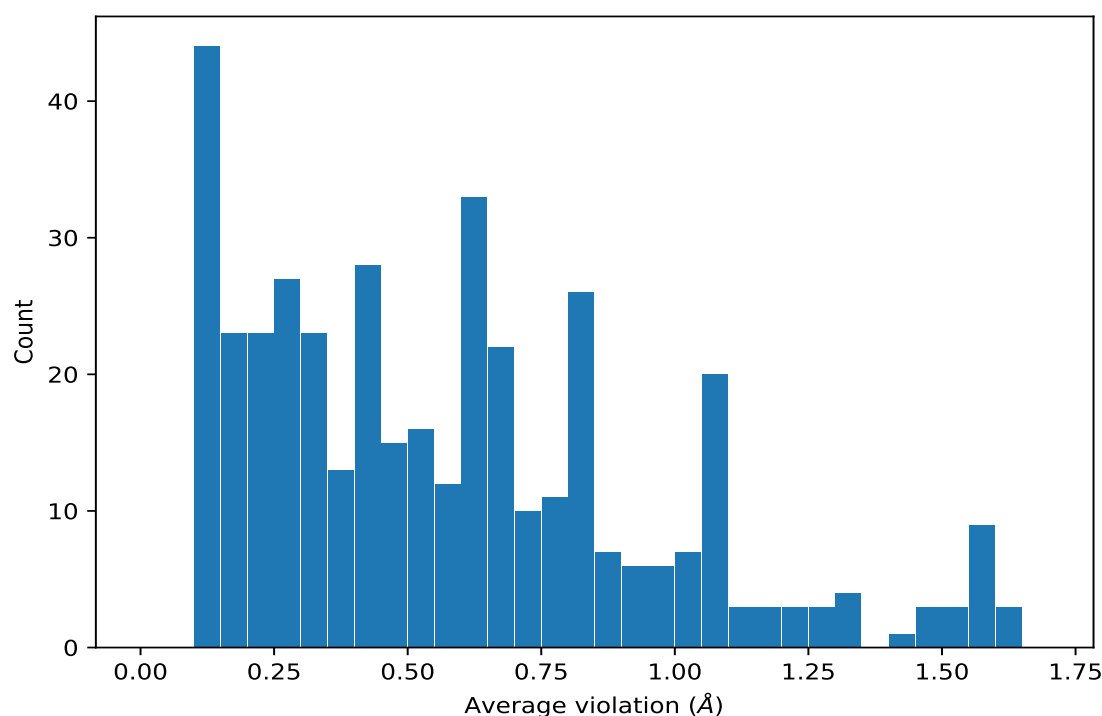
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	30	1.46	0.35	1.54
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	30	1.46	0.35	1.54
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	30	1.46	0.35	1.54
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	30	1.28	0.21	1.3
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	30	1.28	0.21	1.3
(1,43)	1:13:A:VAL:HG23	1:17:A:LEU:H	30	1.28	0.21	1.3
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE2	30	0.93	0.41	1.02
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE2	30	0.93	0.41	1.02
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE3	30	0.93	0.41	1.02
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE2	30	0.93	0.41	1.02
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE3	30	0.93	0.41	1.02
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE3	30	0.93	0.41	1.02
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	30	0.86	0.32	1.01
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	30	0.8	0.3	0.82
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	30	0.8	0.3	0.82
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	30	0.8	0.3	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	30	0.7	0.07	0.7
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HG2	30	0.7	0.07	0.7
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	30	0.2	0.01	0.2
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	27	1.23	0.43	1.35
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	27	1.23	0.43	1.35
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	27	1.23	0.43	1.35
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	27	1.01	0.25	1.02
(1,58)	1:66:A:LEU:HD22	1:10:A:VAL:HB	27	1.01	0.25	1.02
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	27	1.01	0.25	1.02
(1,58)	1:36:A:LEU:HD13	1:43:A:GLU:HB2	27	1.01	0.25	1.02
(1,64)	1:12:A:ALA:HB1	1:6:A:GLN:HG3	26	1.05	0.38	1.13
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG3	26	1.05	0.38	1.13
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	26	1.05	0.38	1.13
(1,64)	1:12:A:ALA:HB2	1:6:A:GLN:HG2	26	1.05	0.38	1.13
(1,64)	1:12:A:ALA:HB2	1:6:A:GLN:HG3	26	1.05	0.38	1.13
(1,64)	1:12:A:ALA:HB1	1:6:A:GLN:HG2	26	1.05	0.38	1.13
(1,32)	1:27:A:LEU:HD11	1:70:A:GLN:HE21	26	0.81	0.39	0.76
(1,32)	1:66:A:LEU:HD11	1:70:A:GLN:HE21	26	0.81	0.39	0.76
(1,32)	1:66:A:LEU:HD13	1:70:A:GLN:HE21	26	0.81	0.39	0.76
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	26	0.81	0.39	0.76
(1,32)	1:66:A:LEU:HD12	1:70:A:GLN:HE21	26	0.81	0.39	0.76
(1,32)	1:27:A:LEU:HD12	1:70:A:GLN:HE21	26	0.81	0.39	0.76
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	24	1.01	0.59	0.72
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	24	1.01	0.59	0.72
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	24	1.01	0.59	0.72
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	24	0.58	0.29	0.54
(1,59)	1:66:A:LEU:HD22	1:64:A:LEU:HB2	24	0.58	0.29	0.54
(1,59)	1:66:A:LEU:HD21	1:64:A:LEU:HB2	24	0.58	0.29	0.54
(1,59)	1:36:A:LEU:HD11	1:64:A:LEU:HB2	24	0.58	0.29	0.54
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	23	0.68	0.46	0.53
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	23	0.68	0.46	0.53
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD13	23	0.68	0.46	0.53
(1,9)	1:16:A:ILE:HG22	1:43:A:GLU:H	22	0.84	0.39	0.86
(1,9)	1:47:A:ILE:HG21	1:50:A:ARG:HE	22	0.84	0.39	0.86
(1,9)	1:16:A:ILE:HG23	1:43:A:GLU:H	22	0.84	0.39	0.86
(1,9)	1:16:A:ILE:HG21	1:43:A:GLU:H	22	0.84	0.39	0.86
(1,9)	1:47:A:ILE:HG23	1:50:A:ARG:HE	22	0.84	0.39	0.86
(1,9)	1:47:A:ILE:HG22	1:50:A:ARG:HE	22	0.84	0.39	0.86
(1,82)	1:73:A:SER:HB2	1:7:A:ARG:HG3	22	0.38	0.23	0.31
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	22	0.38	0.23	0.31
(1,82)	1:73:A:SER:HB2	1:7:A:ARG:HG2	22	0.38	0.23	0.31
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	21	0.29	0.12	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	20	0.58	0.28	0.55
(1,54)	1:7:A:ARG:HG3	1:10:A:VAL:HA	20	0.58	0.28	0.55
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	20	0.18	0.05	0.19
(1,50)	1:16:A:ILE:HG22	1:36:A:LEU:HA	19	0.65	0.36	0.59
(1,50)	1:16:A:ILE:HG21	1:39:A:LEU:HA	19	0.65	0.36	0.59
(1,50)	1:16:A:ILE:HG23	1:39:A:LEU:HA	19	0.65	0.36	0.59
(1,50)	1:16:A:ILE:HG21	1:36:A:LEU:HA	19	0.65	0.36	0.59
(1,50)	1:16:A:ILE:HG22	1:39:A:LEU:HA	19	0.65	0.36	0.59
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	19	0.42	0.17	0.48
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	19	0.42	0.17	0.48
(1,49)	1:47:A:ILE:HG23	1:43:A:GLU:HG3	18	1.08	0.29	1.14
(1,49)	1:47:A:ILE:HG21	1:43:A:GLU:HG3	18	1.08	0.29	1.14
(1,49)	1:47:A:ILE:HG22	1:43:A:GLU:HG3	18	1.08	0.29	1.14
(1,49)	1:16:A:ILE:HG21	1:43:A:GLU:HG3	18	1.08	0.29	1.14
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	18	1.05	0.42	1.06
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	18	0.84	0.41	0.97
(1,48)	1:44:A:VAL:HG13	1:45:A:ARG:HE	18	0.6	0.29	0.68
(1,48)	1:44:A:VAL:HG11	1:45:A:ARG:HE	18	0.6	0.29	0.68
(1,48)	1:44:A:VAL:HG12	1:45:A:ARG:HE	18	0.6	0.29	0.68
(1,48)	1:44:A:VAL:HG12	1:64:A:LEU:H	18	0.6	0.29	0.68
(1,48)	1:44:A:VAL:HG12	1:43:A:GLU:H	18	0.6	0.29	0.68
(1,48)	1:44:A:VAL:HG13	1:43:A:GLU:H	18	0.6	0.29	0.68
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	18	0.23	0.2	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	18	0.23	0.2	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	18	0.23	0.2	0.14
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	17	0.23	0.09	0.21
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	17	0.23	0.09	0.21
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	17	0.23	0.09	0.21
(1,60)	1:47:A:ILE:HG22	1:74:A:SER:HB2	16	1.3	0.67	1.23
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	16	1.3	0.67	1.23
(1,60)	1:47:A:ILE:HG23	1:74:A:SER:HB2	16	1.3	0.67	1.23
(1,60)	1:58:A:ILE:HG21	1:31:A:LEU:HA	16	1.3	0.67	1.23
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	16	0.56	0.05	0.55
(1,28)	1:10:A:VAL:HG23	1:66:A:LEU:HB2	16	0.42	0.26	0.32
(1,28)	1:10:A:VAL:HG21	1:66:A:LEU:HB2	16	0.42	0.26	0.32
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	16	0.42	0.26	0.32
(1,76)	1:9:A:LEU:HD12	1:70:A:GLN:HB3	16	0.42	0.22	0.42
(1,76)	1:9:A:LEU:HD11	1:70:A:GLN:HB3	16	0.42	0.22	0.42
(1,76)	1:9:A:LEU:HD13	1:70:A:GLN:HB3	16	0.42	0.22	0.42
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD13	15	1.06	0.83	0.6
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD11	15	1.06	0.83	0.6
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD12	15	1.06	0.83	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	15	0.76	0.35	0.83
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	15	0.14	0.02	0.13
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	15	0.14	0.02	0.13
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	15	0.14	0.02	0.13
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	14	0.64	0.34	0.6
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	14	0.64	0.34	0.6
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	14	0.64	0.34	0.6
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	14	0.62	0.3	0.71
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	14	0.62	0.3	0.71
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	14	0.62	0.3	0.71
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	14	0.32	0.13	0.34
(1,52)	1:9:A:LEU:HG	1:10:A:VAL:HA	14	0.32	0.13	0.34
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	13	0.44	0.21	0.51
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	13	0.44	0.21	0.51
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	13	0.44	0.21	0.51
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	13	0.12	0.01	0.12
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	13	0.12	0.01	0.12
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	13	0.12	0.01	0.12
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	12	1.07	0.58	1.33
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	12	1.07	0.58	1.33
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	12	1.07	0.58	1.33
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	12	0.69	0.28	0.7
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	12	0.45	0.06	0.47
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	12	0.45	0.06	0.47
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	12	0.45	0.06	0.47
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	12	0.41	0.22	0.34
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	12	0.33	0.19	0.28
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	12	0.33	0.19	0.28
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	12	0.33	0.19	0.28
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	12	0.32	0.14	0.3
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	12	0.32	0.14	0.3
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	12	0.16	0.04	0.18
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	12	0.16	0.04	0.18
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	12	0.16	0.04	0.18
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	12	0.13	0.03	0.12
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	11	0.98	0.31	1.06
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	11	0.98	0.31	1.06
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	11	0.98	0.31	1.06
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	11	0.33	0.13	0.35
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	11	0.33	0.13	0.35
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	11	0.33	0.13	0.35
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	11	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	11	0.11	0.01	0.11
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	11	0.11	0.01	0.11
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	10	0.25	0.06	0.24
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	10	0.25	0.06	0.24
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	10	0.25	0.06	0.24
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	9	1.4	0.22	1.31
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	9	0.27	0.05	0.28
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	9	0.27	0.05	0.28
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	9	0.27	0.05	0.28
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	8	0.65	0.32	0.6
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	8	0.65	0.32	0.6
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	8	0.65	0.32	0.6
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	8	0.61	0.17	0.64
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	8	0.61	0.17	0.64
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	8	0.61	0.17	0.64
(1,77)	1:9:A:LEU:HD23	1:70:A:GLN:HB3	8	0.61	0.38	0.52
(1,77)	1:48:A:LEU:HD12	1:51:A:GLU:HG3	8	0.61	0.38	0.52
(1,77)	1:9:A:LEU:HD21	1:70:A:GLN:HB3	8	0.61	0.38	0.52
(1,77)	1:9:A:LEU:HD21	1:51:A:GLU:HG3	8	0.61	0.38	0.52
(1,77)	1:9:A:LEU:HD22	1:51:A:GLU:HG3	8	0.61	0.38	0.52
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG21	8	0.52	0.19	0.61
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG22	8	0.52	0.19	0.61
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG23	8	0.52	0.19	0.61
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	8	0.4	0.26	0.29
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	8	0.4	0.26	0.29
(1,56)	1:7:A:ARG:HG3	1:10:A:VAL:H	8	0.31	0.16	0.28
(1,56)	1:59:A:ARG:HG3	1:61:A:VAL:H	8	0.31	0.16	0.28
(1,56)	1:7:A:ARG:HG2	1:10:A:VAL:H	8	0.31	0.16	0.28
(1,56)	1:50:A:ARG:HG2	1:49:A:GLU:H	8	0.31	0.16	0.28
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	8	0.27	0.23	0.16
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	8	0.27	0.23	0.16
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	8	0.22	0.08	0.19
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	8	0.13	0.02	0.12
(1,1163)	1:54:A:LEU:HD11	1:51:A:GLU:HB2	7	1.51	0.57	1.72
(1,1163)	1:54:A:LEU:HD12	1:51:A:GLU:HB2	7	1.51	0.57	1.72
(1,1163)	1:54:A:LEU:HD13	1:51:A:GLU:HB2	7	1.51	0.57	1.72
(1,244)	1:31:A:LEU:HD21	1:64:A:LEU:HG	7	0.84	0.02	0.85
(1,244)	1:31:A:LEU:HD22	1:64:A:LEU:HG	7	0.84	0.02	0.85
(1,244)	1:31:A:LEU:HD23	1:64:A:LEU:HG	7	0.84	0.02	0.85
(1,233)	1:31:A:LEU:HD11	1:31:A:LEU:HA	7	0.75	0.03	0.76
(1,233)	1:31:A:LEU:HD12	1:31:A:LEU:HA	7	0.75	0.03	0.76
(1,233)	1:31:A:LEU:HD13	1:31:A:LEU:HA	7	0.75	0.03	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,72)	1:9:A:LEU:HD23	1:6:A:GLN:HE21	7	0.75	0.75	0.36
(1,72)	1:9:A:LEU:HD22	1:6:A:GLN:HE21	7	0.75	0.75	0.36
(1,72)	1:9:A:LEU:HD21	1:6:A:GLN:HE21	7	0.75	0.75	0.36
(1,72)	1:48:A:LEU:HD12	1:6:A:GLN:HE21	7	0.75	0.75	0.36
(1,240)	1:31:A:LEU:HD11	1:34:A:LEU:HB2	7	0.52	0.15	0.55
(1,240)	1:31:A:LEU:HD12	1:34:A:LEU:HB2	7	0.52	0.15	0.55
(1,240)	1:31:A:LEU:HD13	1:34:A:LEU:HB2	7	0.52	0.15	0.55
(1,1028)	1:34:A:LEU:HD21	1:33:A:ASP:H	7	0.24	0.11	0.2
(1,1028)	1:34:A:LEU:HD22	1:33:A:ASP:H	7	0.24	0.11	0.2
(1,1028)	1:34:A:LEU:HD23	1:33:A:ASP:H	7	0.24	0.11	0.2
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD11	6	0.85	0.12	0.82
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD12	6	0.85	0.12	0.82
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD13	6	0.85	0.12	0.82
(1,719)	1:63:A:GLN:HB2	1:63:A:GLN:HE21	6	0.81	0.04	0.82
(1,779)	1:52:A:HIS:HB2	1:6:A:GLN:HE21	6	0.67	0.36	0.72
(1,47)	1:22:A:LEU:HD22	1:14:A:ALA:H	6	0.55	0.31	0.48
(1,47)	1:22:A:LEU:HD21	1:14:A:ALA:H	6	0.55	0.31	0.48
(1,502)	1:19:A:ILE:HD11	1:25:A:ILE:HG13	6	0.43	0.29	0.3
(1,502)	1:19:A:ILE:HD12	1:25:A:ILE:HG13	6	0.43	0.29	0.3
(1,502)	1:19:A:ILE:HD13	1:25:A:ILE:HG13	6	0.43	0.29	0.3
(1,1303)	1:64:A:LEU:HB2	1:31:A:LEU:HB3	6	0.35	0.11	0.35
(1,294)	1:17:A:LEU:HD11	1:36:A:LEU:HB2	6	0.28	0.11	0.24
(1,294)	1:17:A:LEU:HD12	1:36:A:LEU:HB2	6	0.28	0.11	0.24
(1,294)	1:17:A:LEU:HD13	1:36:A:LEU:HB2	6	0.28	0.11	0.24
(1,294)	1:17:A:LEU:HD21	1:36:A:LEU:HB2	6	0.28	0.11	0.24
(1,294)	1:17:A:LEU:HD22	1:36:A:LEU:HB2	6	0.28	0.11	0.24
(1,294)	1:17:A:LEU:HD23	1:36:A:LEU:HB2	6	0.28	0.11	0.24
(1,1263)	1:61:A:VAL:HG11	1:62:A:ARG:HB3	6	0.2	0.08	0.18
(1,1263)	1:61:A:VAL:HG12	1:62:A:ARG:HB3	6	0.2	0.08	0.18
(1,1263)	1:61:A:VAL:HG13	1:62:A:ARG:HB3	6	0.2	0.08	0.18
(1,34)	1:34:A:LEU:HD23	1:27:A:LEU:HA	5	0.85	0.36	0.92
(1,34)	1:34:A:LEU:HD23	1:32:A:ALA:HA	5	0.85	0.36	0.92
(1,34)	1:34:A:LEU:HD22	1:66:A:LEU:HA	5	0.85	0.36	0.92
(1,499)	1:47:A:ILE:HD11	1:43:A:GLU:HG2	5	0.6	0.12	0.54
(1,499)	1:47:A:ILE:HD12	1:43:A:GLU:HG2	5	0.6	0.12	0.54
(1,499)	1:47:A:ILE:HD13	1:43:A:GLU:HG2	5	0.6	0.12	0.54
(1,700)	1:59:A:ARG:HA	1:62:A:ARG:HD2	5	0.52	0.28	0.53
(1,63)	1:47:A:ILE:HG23	1:7:A:ARG:H	5	0.4	0.18	0.41
(1,63)	1:47:A:ILE:HG21	1:7:A:ARG:H	5	0.4	0.18	0.41
(1,63)	1:47:A:ILE:HG22	1:7:A:ARG:H	5	0.4	0.18	0.41
(1,8)	1:47:A:ILE:HG23	1:7:A:ARG:H	5	0.36	0.16	0.37
(1,8)	1:47:A:ILE:HG21	1:7:A:ARG:H	5	0.36	0.16	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,8)	1:16:A:ILE:HG23	1:44:A:VAL:H	5	0.36	0.16	0.37
(1,8)	1:47:A:ILE:HG22	1:7:A:ARG:H	5	0.36	0.16	0.37
(1,549)	1:72:A:MET:HB2	1:72:A:MET:H	5	0.2	0.06	0.17
(1,662)	1:49:A:GLU:HA	1:46:A:GLN:HA	5	0.14	0.02	0.12
(1,1555)	1:34:A:LEU:HD21	1:33:A:ASP:HB3	4	1.06	0.36	0.92
(1,1555)	1:34:A:LEU:HD22	1:33:A:ASP:HB3	4	1.06	0.36	0.92
(1,1555)	1:34:A:LEU:HD23	1:33:A:ASP:HB3	4	1.06	0.36	0.92
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD21	4	0.74	0.26	0.78
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD22	4	0.74	0.26	0.78
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD23	4	0.74	0.26	0.78
(1,412)	1:45:A:ARG:HD2	1:58:A:ILE:HA	4	0.71	0.05	0.71
(1,412)	1:45:A:ARG:HD3	1:58:A:ILE:HA	4	0.71	0.05	0.71
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD21	4	0.67	0.32	0.66
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD22	4	0.67	0.32	0.66
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD23	4	0.67	0.32	0.66
(1,111)	1:55:A:VAL:HG21	1:49:A:GLU:HG3	4	0.65	0.25	0.69
(1,111)	1:55:A:VAL:HG22	1:49:A:GLU:HG3	4	0.65	0.25	0.69
(1,111)	1:55:A:VAL:HG23	1:49:A:GLU:HG3	4	0.65	0.25	0.69
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD21	4	0.42	0.16	0.44
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD22	4	0.42	0.16	0.44
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD23	4	0.42	0.16	0.44
(1,798)	1:51:A:GLU:HG2	1:50:A:ARG:HG2	4	0.42	0.11	0.43
(1,798)	1:51:A:GLU:HG3	1:50:A:ARG:HG2	4	0.42	0.11	0.43
(1,668)	1:49:A:GLU:HG2	1:46:A:GLN:HA	4	0.37	0.2	0.3
(1,787)	1:51:A:GLU:HB3	1:6:A:GLN:HE21	4	0.31	0.06	0.31
(1,1182)	1:56:A:LEU:HB3	1:57:A:PRO:HB2	4	0.3	0.26	0.17
(1,1182)	1:56:A:LEU:HB3	1:57:A:PRO:HG2	4	0.3	0.26	0.17
(1,1548)	1:19:A:ILE:HG21	1:21:A:ASP:HB2	4	0.26	0.08	0.24
(1,1548)	1:19:A:ILE:HG22	1:21:A:ASP:HB2	4	0.26	0.08	0.24
(1,1548)	1:19:A:ILE:HG23	1:21:A:ASP:HB2	4	0.26	0.08	0.24
(1,213)	1:30:A:SER:HB3	1:33:A:ASP:HA	4	0.11	0.01	0.11
(1,1545)	1:44:A:VAL:HG21	1:45:A:ARG:HE	4	0.11	0.01	0.11
(1,1545)	1:44:A:VAL:HG22	1:45:A:ARG:HE	4	0.11	0.01	0.11
(1,1545)	1:44:A:VAL:HG23	1:45:A:ARG:HE	4	0.11	0.01	0.11
(1,1123)	1:48:A:LEU:HD11	1:52:A:HIS:HB2	3	1.63	1.06	1.42
(1,1123)	1:48:A:LEU:HD12	1:52:A:HIS:HB2	3	1.63	1.06	1.42
(1,1123)	1:48:A:LEU:HD13	1:52:A:HIS:HB2	3	1.63	1.06	1.42
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD11	3	1.59	0.18	1.7
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD12	3	1.59	0.18	1.7
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD13	3	1.59	0.18	1.7
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD11	3	1.59	0.18	1.7
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD12	3	1.59	0.18	1.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD13	3	1.59	0.18	1.7
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD11	3	1.59	0.18	1.7
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD12	3	1.59	0.18	1.7
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD13	3	1.59	0.18	1.7
(1,1122)	1:48:A:LEU:HD11	1:52:A:HIS:HB3	3	1.18	0.39	1.13
(1,1122)	1:48:A:LEU:HD12	1:52:A:HIS:HB3	3	1.18	0.39	1.13
(1,1122)	1:48:A:LEU:HD13	1:52:A:HIS:HB3	3	1.18	0.39	1.13
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD11	3	1.13	0.12	1.19
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD12	3	1.13	0.12	1.19
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD13	3	1.13	0.12	1.19
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD11	3	0.83	0.0	0.83
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD12	3	0.83	0.0	0.83
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD13	3	0.83	0.0	0.83
(1,4)	1:23:A:ALA:HB2	1:25:A:ILE:HD11	3	0.79	0.38	0.93
(1,4)	1:23:A:ALA:HB3	1:25:A:ILE:HD13	3	0.79	0.38	0.93
(1,4)	1:32:A:ALA:HB2	1:36:A:LEU:HD22	3	0.79	0.38	0.93
(1,1575)	1:66:A:LEU:HD11	1:13:A:VAL:H	3	0.67	0.45	0.46
(1,1575)	1:66:A:LEU:HD12	1:13:A:VAL:H	3	0.67	0.45	0.46
(1,1575)	1:66:A:LEU:HD13	1:13:A:VAL:H	3	0.67	0.45	0.46
(1,1126)	1:48:A:LEU:HD11	1:52:A:HIS:H	3	0.58	0.21	0.45
(1,1126)	1:48:A:LEU:HD12	1:52:A:HIS:H	3	0.58	0.21	0.45
(1,1126)	1:48:A:LEU:HD13	1:52:A:HIS:H	3	0.58	0.21	0.45
(1,1012)	1:34:A:LEU:HD11	1:31:A:LEU:H	3	0.54	0.31	0.67
(1,1012)	1:34:A:LEU:HD12	1:31:A:LEU:H	3	0.54	0.31	0.67
(1,1012)	1:34:A:LEU:HD13	1:31:A:LEU:H	3	0.54	0.31	0.67
(1,5)	1:17:A:LEU:HD12	1:66:A:LEU:HB2	3	0.49	0.31	0.39
(1,5)	1:17:A:LEU:HD11	1:66:A:LEU:HB2	3	0.49	0.31	0.39
(1,1107)	1:48:A:LEU:HA	1:52:A:HIS:HB2	3	0.48	0.32	0.41
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD11	3	0.47	0.12	0.47
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD12	3	0.47	0.12	0.47
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD13	3	0.47	0.12	0.47
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD21	3	0.46	0.45	0.14
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD22	3	0.46	0.45	0.14
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD23	3	0.46	0.45	0.14
(1,593)	1:66:A:LEU:HD11	1:66:A:LEU:HA	3	0.42	0.02	0.42
(1,593)	1:66:A:LEU:HD12	1:66:A:LEU:HA	3	0.42	0.02	0.42
(1,593)	1:66:A:LEU:HD13	1:66:A:LEU:HA	3	0.42	0.02	0.42
(1,1008)	1:34:A:LEU:HD11	1:31:A:LEU:HA	3	0.34	0.1	0.36
(1,1008)	1:34:A:LEU:HD12	1:31:A:LEU:HA	3	0.34	0.1	0.36
(1,1008)	1:34:A:LEU:HD13	1:31:A:LEU:HA	3	0.34	0.1	0.36
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD11	3	0.3	0.09	0.32
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD12	3	0.3	0.09	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD13	3	0.3	0.09	0.32
(1,68)	1:57:A:PRO:HB3	1:61:A:VAL:HG21	3	0.26	0.19	0.13
(1,68)	1:57:A:PRO:HB3	1:61:A:VAL:HG22	3	0.26	0.19	0.13
(1,68)	1:57:A:PRO:HB3	1:61:A:VAL:HG23	3	0.26	0.19	0.13
(1,1576)	1:66:A:LEU:HD11	1:65:A:THR:HA	3	0.25	0.16	0.14
(1,1576)	1:66:A:LEU:HD12	1:65:A:THR:HA	3	0.25	0.16	0.14
(1,1576)	1:66:A:LEU:HD13	1:65:A:THR:HA	3	0.25	0.16	0.14
(1,81)	1:73:A:SER:HB3	1:9:A:LEU:HB3	3	0.24	0.08	0.28
(1,1698)	1:38:A:SER:H	1:39:A:LEU:H	3	0.19	0.04	0.18
(1,1091)	1:39:A:LEU:HD11	1:39:A:LEU:HA	3	0.18	0.06	0.15
(1,1091)	1:39:A:LEU:HD12	1:39:A:LEU:HA	3	0.18	0.06	0.15
(1,1091)	1:39:A:LEU:HD13	1:39:A:LEU:HA	3	0.18	0.06	0.15
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD21	3	0.15	0.03	0.14
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD22	3	0.15	0.03	0.14
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD23	3	0.15	0.03	0.14
(1,53)	1:59:A:ARG:HG2	1:58:A:ILE:H	3	0.15	0.01	0.15
(1,171)	1:22:A:LEU:HG	1:21:A:ASP:HA	3	0.13	0.03	0.11
(1,391)	1:19:A:ILE:HG21	1:21:A:ASP:HA	3	0.11	0.01	0.11
(1,391)	1:19:A:ILE:HG22	1:21:A:ASP:HA	3	0.11	0.01	0.11
(1,391)	1:19:A:ILE:HG23	1:21:A:ASP:HA	3	0.11	0.01	0.11
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD21	2	0.96	0.02	0.96
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD22	2	0.96	0.02	0.96
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD23	2	0.96	0.02	0.96
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD11	2	0.84	0.18	0.84
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD12	2	0.84	0.18	0.84
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD13	2	0.84	0.18	0.84
(1,1196)	1:56:A:LEU:HD21	1:56:A:LEU:HA	2	0.72	0.22	0.72
(1,1196)	1:56:A:LEU:HD22	1:56:A:LEU:HA	2	0.72	0.22	0.72
(1,1196)	1:56:A:LEU:HD23	1:56:A:LEU:HA	2	0.72	0.22	0.72
(1,236)	1:31:A:LEU:HD11	1:66:A:LEU:H	2	0.64	0.33	0.64
(1,236)	1:31:A:LEU:HD12	1:66:A:LEU:H	2	0.64	0.33	0.64
(1,236)	1:31:A:LEU:HD13	1:66:A:LEU:H	2	0.64	0.33	0.64
(1,1239)	1:60:A:GLU:HB3	1:56:A:LEU:HB2	2	0.61	0.06	0.61
(1,1505)	1:55:A:VAL:HG11	1:59:A:ARG:HD2	2	0.61	0.5	0.61
(1,1505)	1:55:A:VAL:HG11	1:59:A:ARG:HD3	2	0.61	0.5	0.61
(1,1505)	1:55:A:VAL:HG12	1:59:A:ARG:HD2	2	0.61	0.5	0.61
(1,1505)	1:55:A:VAL:HG12	1:59:A:ARG:HD3	2	0.61	0.5	0.61
(1,1505)	1:55:A:VAL:HG13	1:59:A:ARG:HD2	2	0.61	0.5	0.61
(1,1505)	1:55:A:VAL:HG13	1:59:A:ARG:HD3	2	0.61	0.5	0.61
(1,296)	1:17:A:LEU:HD11	1:19:A:ILE:HG13	2	0.5	0.08	0.5
(1,296)	1:17:A:LEU:HD12	1:19:A:ILE:HG13	2	0.5	0.08	0.5
(1,296)	1:17:A:LEU:HD13	1:19:A:ILE:HG13	2	0.5	0.08	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD21	2	0.5	0.3	0.5
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD22	2	0.5	0.3	0.5
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD23	2	0.5	0.3	0.5
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD21	2	0.49	0.07	0.49
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD22	2	0.49	0.07	0.49
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD23	2	0.49	0.07	0.49
(1,66)	1:58:A:ILE:HD12	1:45:A:ARG:HE	2	0.38	0.15	0.38
(1,66)	1:58:A:ILE:HD13	1:45:A:ARG:HE	2	0.38	0.15	0.38
(1,73)	1:9:A:LEU:HD12	1:69:A:LEU:HB3	2	0.36	0.16	0.36
(1,73)	1:9:A:LEU:HD13	1:69:A:LEU:HB3	2	0.36	0.16	0.36
(1,896)	1:47:A:ILE:HG21	1:6:A:GLN:HE21	2	0.25	0.14	0.25
(1,896)	1:47:A:ILE:HG22	1:6:A:GLN:HE21	2	0.25	0.14	0.25
(1,896)	1:47:A:ILE:HG23	1:6:A:GLN:HE21	2	0.25	0.14	0.25
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG21	2	0.22	0.02	0.22
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG22	2	0.22	0.02	0.22
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG23	2	0.22	0.02	0.22
(1,469)	1:17:A:LEU:HD11	1:16:A:ILE:H	2	0.22	0.08	0.22
(1,469)	1:17:A:LEU:HD12	1:16:A:ILE:H	2	0.22	0.08	0.22
(1,469)	1:17:A:LEU:HD13	1:16:A:ILE:H	2	0.22	0.08	0.22
(1,1133)	1:53:A:ASP:HA	1:53:A:ASP:H	2	0.2	0.03	0.2
(1,1415)	1:42:A:VAL:HG11	1:46:A:GLN:HE21	2	0.18	0.02	0.18
(1,1415)	1:42:A:VAL:HG12	1:46:A:GLN:HE21	2	0.18	0.02	0.18
(1,1415)	1:42:A:VAL:HG13	1:46:A:GLN:HE21	2	0.18	0.02	0.18
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD21	2	0.16	0.01	0.16
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD22	2	0.16	0.01	0.16
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD23	2	0.16	0.01	0.16
(1,844)	1:8:A:ASP:HB3	1:11:A:LYS:HB2	2	0.16	0.05	0.16
(1,844)	1:8:A:ASP:HB3	1:11:A:LYS:HB3	2	0.16	0.05	0.16
(1,1061)	1:36:A:LEU:HD21	1:38:A:SER:H	2	0.15	0.0	0.15
(1,1061)	1:36:A:LEU:HD22	1:38:A:SER:H	2	0.15	0.0	0.15
(1,1061)	1:36:A:LEU:HD23	1:38:A:SER:H	2	0.15	0.0	0.15
(1,1727)	1:86:A:LYS:H	1:85:A:PRO:HA	2	0.14	0.01	0.14
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD21	2	0.14	0.02	0.14
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD22	2	0.14	0.02	0.14
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD23	2	0.14	0.02	0.14
(1,1569)	1:10:A:VAL:HG21	1:70:A:GLN:HB2	2	0.14	0.02	0.14
(1,1569)	1:10:A:VAL:HG21	1:70:A:GLN:HB3	2	0.14	0.02	0.14
(1,1569)	1:10:A:VAL:HG22	1:70:A:GLN:HB2	2	0.14	0.02	0.14
(1,1569)	1:10:A:VAL:HG22	1:70:A:GLN:HB3	2	0.14	0.02	0.14
(1,1569)	1:10:A:VAL:HG23	1:70:A:GLN:HB2	2	0.14	0.02	0.14
(1,1569)	1:10:A:VAL:HG23	1:70:A:GLN:HB3	2	0.14	0.02	0.14
(1,1497)	1:65:A:THR:HG21	1:63:A:GLN:HB2	2	0.12	0.02	0.12

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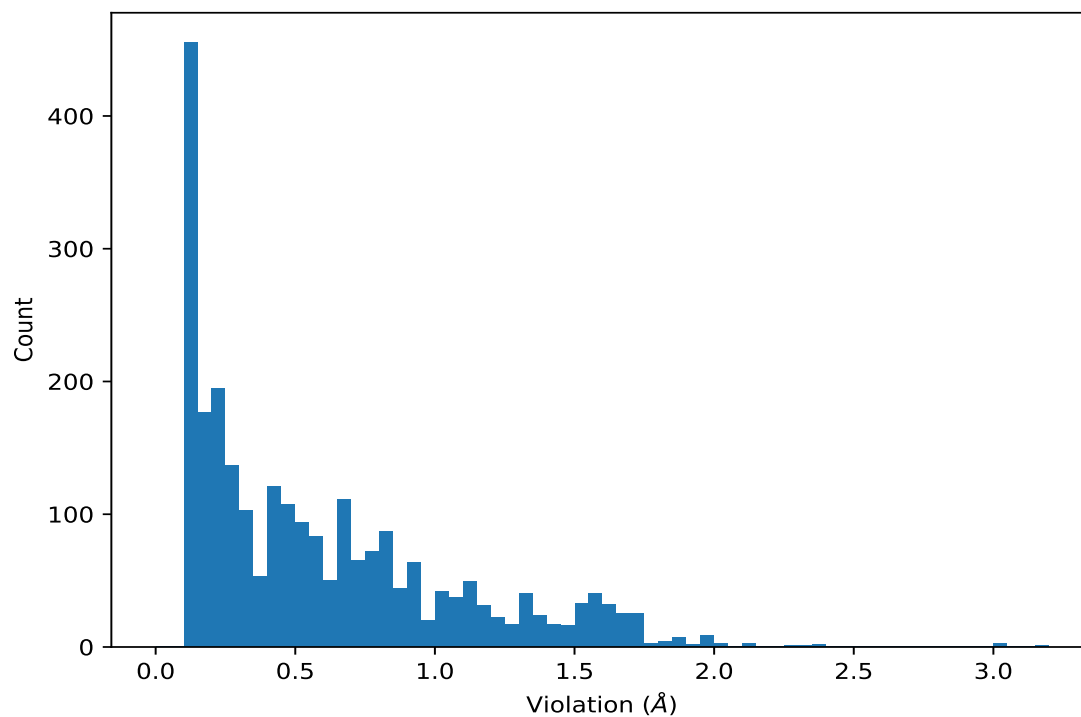
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1497)	1:65:A:THR:HG22	1:63:A:GLN:HB2	2	0.12	0.02	0.12
(1,1497)	1:65:A:THR:HG23	1:63:A:GLN:HB2	2	0.12	0.02	0.12
(1,291)	1:17:A:LEU:HG	1:17:A:LEU:H	2	0.12	0.01	0.12
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG21	2	0.12	0.02	0.12
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG22	2	0.12	0.02	0.12
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG23	2	0.12	0.02	0.12
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG21	2	0.12	0.02	0.12
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG22	2	0.12	0.02	0.12
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG23	2	0.12	0.02	0.12
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG21	2	0.12	0.02	0.12
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG22	2	0.12	0.02	0.12
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG23	2	0.12	0.02	0.12
(1,1523)	1:73:A:SER:HA	1:70:A:GLN:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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)
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD12	18	3.2
(1,1123)	1:48:A:LEU:HD11	1:52:A:HIS:HB2	2	3.01
(1,1123)	1:48:A:LEU:HD12	1:52:A:HIS:HB2	2	3.01
(1,1123)	1:48:A:LEU:HD13	1:52:A:HIS:HB2	2	3.01
(1,72)	1:9:A:LEU:HD22	1:6:A:GLN:HE21	13	2.37
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	19	2.37
(1,60)	1:58:A:ILE:HG21	1:31:A:LEU:HA	26	2.31
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	24	2.3
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	24	2.1
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	24	2.1
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	24	2.1
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	14	2.01
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	14	2.01
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	14	2.01
(1,1163)	1:54:A:LEU:HD11	1:51:A:GLU:HB2	24	1.99
(1,1163)	1:54:A:LEU:HD12	1:51:A:GLU:HB2	24	1.99
(1,1163)	1:54:A:LEU:HD13	1:51:A:GLU:HB2	24	1.99
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	27	1.98
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	27	1.98
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	27	1.98
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	26	1.96
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	26	1.96
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	26	1.96
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD12	6	1.95
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD11	13	1.93
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	17	1.89
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	17	1.89
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	17	1.89
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	18	1.88
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	13	1.87
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	13	1.87
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	13	1.87
(1,1163)	1:54:A:LEU:HD11	1:51:A:GLU:HB2	21	1.82
(1,1163)	1:54:A:LEU:HD12	1:51:A:GLU:HB2	21	1.82
(1,1163)	1:54:A:LEU:HD13	1:51:A:GLU:HB2	21	1.82
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	14	1.81
(1,60)	1:47:A:ILE:HG22	1:74:A:SER:HB2	11	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	21	1.76
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG3	2	1.75
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD11	18	1.74
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD12	18	1.74
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD13	18	1.74
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD11	18	1.74
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD12	18	1.74
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD13	18	1.74
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD11	18	1.74
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD12	18	1.74
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD13	18	1.74
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	2	1.74
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	16	1.74
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD13	24	1.74
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	19	1.73
(1,32)	1:66:A:LEU:HD12	1:70:A:GLN:HE21	12	1.73
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	19	1.72
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	19	1.72
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	19	1.72
(1,1163)	1:54:A:LEU:HD11	1:51:A:GLU:HB2	4	1.72
(1,1163)	1:54:A:LEU:HD12	1:51:A:GLU:HB2	4	1.72
(1,1163)	1:54:A:LEU:HD13	1:51:A:GLU:HB2	4	1.72
(1,1163)	1:54:A:LEU:HD11	1:51:A:GLU:HB2	29	1.72
(1,1163)	1:54:A:LEU:HD12	1:51:A:GLU:HB2	29	1.72
(1,1163)	1:54:A:LEU:HD13	1:51:A:GLU:HB2	29	1.72
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	28	1.72
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	23	1.71
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD11	2	1.7
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD12	2	1.7
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD13	2	1.7
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD11	2	1.7
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD12	2	1.7
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD13	2	1.7
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD11	2	1.7
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD12	2	1.7
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD13	2	1.7
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	28	1.69
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	28	1.69
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	28	1.69
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE2	8	1.69
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	17	1.68
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	17	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	17	1.68
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	29	1.67
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	29	1.67
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	29	1.67
(1,1122)	1:48:A:LEU:HD11	1:52:A:HIS:HB3	22	1.67
(1,1122)	1:48:A:LEU:HD12	1:52:A:HIS:HB3	22	1.67
(1,1122)	1:48:A:LEU:HD13	1:52:A:HIS:HB3	22	1.67
(1,60)	1:47:A:ILE:HG23	1:74:A:SER:HB2	13	1.67
(1,60)	1:47:A:ILE:HG23	1:74:A:SER:HB2	20	1.67
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	16	1.66
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	16	1.65
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	16	1.65
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	16	1.65
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	15	1.65
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	9	1.64
(1,1555)	1:34:A:LEU:HD21	1:33:A:ASP:HB3	27	1.64
(1,1555)	1:34:A:LEU:HD22	1:33:A:ASP:HB3	27	1.64
(1,1555)	1:34:A:LEU:HD23	1:33:A:ASP:HB3	27	1.64
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	5	1.62
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	5	1.62
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	5	1.62
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	8	1.62
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	8	1.62
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	8	1.62
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	11	1.62
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	11	1.62
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	11	1.62
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	19	1.62
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	19	1.62
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	19	1.62
(1,1163)	1:54:A:LEU:HD11	1:51:A:GLU:HB2	2	1.61
(1,1163)	1:54:A:LEU:HD12	1:51:A:GLU:HB2	2	1.61
(1,1163)	1:54:A:LEU:HD13	1:51:A:GLU:HB2	2	1.61
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	19	1.61
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	20	1.61
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	25	1.61
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	28	1.61
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	18	1.6
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	18	1.6
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	18	1.6
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	26	1.6
(1,64)	1:12:A:ALA:HB1	1:6:A:GLN:HG2	24	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	25	1.59
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	25	1.59
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	25	1.59
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	1	1.58
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	1	1.58
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	1	1.58
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	9	1.57
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	9	1.57
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	9	1.57
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	22	1.57
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	22	1.57
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	22	1.57
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	30	1.57
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	30	1.57
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	30	1.57
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	9	1.57
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	9	1.57
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	9	1.57
(1,9)	1:16:A:ILE:HG22	1:43:A:GLU:H	23	1.57
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	6	1.56
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	6	1.56
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	6	1.56
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	27	1.56
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	27	1.56
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	27	1.56
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	14	1.56
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	14	1.56
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	14	1.56
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	3	1.56
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	1	1.56
(1,49)	1:47:A:ILE:HG22	1:43:A:GLU:HG3	6	1.56
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE2	14	1.56
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	29	1.56
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	23	1.55
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	23	1.55
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	23	1.55
(1,1163)	1:54:A:LEU:HD11	1:51:A:GLU:HB2	1	1.55
(1,1163)	1:54:A:LEU:HD12	1:51:A:GLU:HB2	1	1.55
(1,1163)	1:54:A:LEU:HD13	1:51:A:GLU:HB2	1	1.55
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE3	19	1.55
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	17	1.54
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	17	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	17	1.54
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	5	1.54
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	12	1.54
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	4	1.52
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	4	1.52
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	4	1.52
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	12	1.52
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	12	1.52
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	12	1.52
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	26	1.52
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	26	1.52
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	26	1.52
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	29	1.52
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	29	1.52
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	29	1.52
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	13	1.52
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	5	1.52
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	10	1.51
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	10	1.51
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	10	1.51
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	13	1.51
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	13	1.51
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	13	1.51
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	20	1.51
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	20	1.51
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	20	1.51
(1,49)	1:47:A:ILE:HG21	1:43:A:GLU:HG3	18	1.51
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE3	29	1.51
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	21	1.5
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	21	1.5
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	21	1.5
(1,64)	1:12:A:ALA:HB2	1:6:A:GLN:HG2	22	1.49
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	19	1.49
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	24	1.48
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	24	1.48
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	24	1.48
(1,32)	1:27:A:LEU:HD11	1:70:A:GLN:HE21	22	1.48
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	22	1.47
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	19	1.47
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	14	1.46
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	14	1.46
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	14	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	26	1.46
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	26	1.46
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	26	1.46
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	14	1.46
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD13	1	1.46
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	2	1.45
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	2	1.45
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	2	1.45
(1,64)	1:12:A:ALA:HB2	1:6:A:GLN:HG3	8	1.44
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	26	1.44
(1,9)	1:16:A:ILE:HG23	1:43:A:GLU:H	4	1.44
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	10	1.43
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	15	1.43
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	15	1.43
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	15	1.43
(1,1123)	1:48:A:LEU:HD11	1:52:A:HIS:HB2	22	1.42
(1,1123)	1:48:A:LEU:HD12	1:52:A:HIS:HB2	22	1.42
(1,1123)	1:48:A:LEU:HD13	1:52:A:HIS:HB2	22	1.42
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE2	23	1.42
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	10	1.42
(1,67)	1:58:A:ILE:HD12	1:42:A:VAL:HG23	28	1.41
(1,43)	1:13:A:VAL:HG23	1:17:A:LEU:H	6	1.41
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	10	1.4
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG3	26	1.4
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	8	1.4
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	19	1.39
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	19	1.39
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	19	1.39
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	7	1.39
(1,77)	1:9:A:LEU:HD23	1:70:A:GLN:HB3	22	1.39
(1,64)	1:12:A:ALA:HB2	1:6:A:GLN:HG2	6	1.39
(1,50)	1:16:A:ILE:HG23	1:39:A:LEU:HA	22	1.39
(1,64)	1:12:A:ALA:HB1	1:6:A:GLN:HG3	1	1.38
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	6	1.38
(1,34)	1:34:A:LEU:HD23	1:32:A:ALA:HA	11	1.38
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD11	8	1.38
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	15	1.37
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	20	1.37
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	3	1.36
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	20	1.36
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	20	1.36
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	20	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	1	1.36
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	14	1.35
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	21	1.35
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	27	1.35
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	18	1.34
(1,60)	1:47:A:ILE:HG23	1:74:A:SER:HB2	14	1.34
(1,49)	1:16:A:ILE:HG21	1:43:A:GLU:HG3	5	1.34
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	20	1.33
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	20	1.33
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	20	1.33
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD11	22	1.33
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD12	22	1.33
(1,900)	1:47:A:ILE:HG21	1:48:A:LEU:HD13	22	1.33
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD11	22	1.33
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD12	22	1.33
(1,900)	1:47:A:ILE:HG22	1:48:A:LEU:HD13	22	1.33
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD11	22	1.33
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD12	22	1.33
(1,900)	1:47:A:ILE:HG23	1:48:A:LEU:HD13	22	1.33
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	24	1.33
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	20	1.32
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	20	1.32
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	20	1.32
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	28	1.32
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	28	1.32
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	28	1.32
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	20	1.32
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	15	1.32
(1,50)	1:16:A:ILE:HG22	1:39:A:LEU:HA	15	1.32
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	14	1.31
(1,64)	1:12:A:ALA:HB1	1:6:A:GLN:HG3	4	1.31
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	14	1.31
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	16	1.31
(1,43)	1:13:A:VAL:HG23	1:17:A:LEU:H	13	1.31
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	14	1.3
(1,1575)	1:66:A:LEU:HD11	1:13:A:VAL:H	18	1.3
(1,1575)	1:66:A:LEU:HD12	1:13:A:VAL:H	18	1.3
(1,1575)	1:66:A:LEU:HD13	1:13:A:VAL:H	18	1.3
(1,1202)	1:56:A:LEU:HD21	1:55:A:VAL:HB	14	1.3
(1,1202)	1:56:A:LEU:HD22	1:55:A:VAL:HB	14	1.3
(1,1202)	1:56:A:LEU:HD23	1:55:A:VAL:HB	14	1.3
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	4	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	29	1.3
(1,49)	1:47:A:ILE:HG21	1:43:A:GLU:HG3	3	1.3
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	13	1.29
(1,43)	1:13:A:VAL:HG23	1:17:A:LEU:H	22	1.29
(1,43)	1:13:A:VAL:HG23	1:17:A:LEU:H	23	1.29
(1,9)	1:16:A:ILE:HG21	1:43:A:GLU:H	20	1.29
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	13	1.28
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	2	1.28
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	12	1.28
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	12	1.27
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	17	1.27
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	14	1.26
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	14	1.26
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	14	1.26
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	25	1.26
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	7	1.25
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD11	18	1.25
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD12	18	1.25
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD13	18	1.25
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	22	1.24
(1,43)	1:13:A:VAL:HG23	1:17:A:LEU:H	25	1.24
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	24	1.24
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	3	1.23
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	3	1.23
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	3	1.23
(1,64)	1:12:A:ALA:HB2	1:6:A:GLN:HG2	29	1.23
(1,49)	1:47:A:ILE:HG23	1:43:A:GLU:HG3	12	1.23
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE3	22	1.23
(1,32)	1:66:A:LEU:HD13	1:70:A:GLN:HE21	9	1.23
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	23	1.22
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	23	1.22
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	23	1.22
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	18	1.22
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	6	1.21
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	11	1.21
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE2	1	1.21
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE3	17	1.21
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	3	1.21
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	29	1.21
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	9	1.21
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	23	1.21
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	30	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	30	1.2
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	30	1.2
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	18	1.2
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	18	1.2
(1,49)	1:47:A:ILE:HG21	1:43:A:GLU:HG3	22	1.2
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	7	1.2
(1,9)	1:16:A:ILE:HG22	1:43:A:GLU:H	29	1.2
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	24	1.19
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	24	1.19
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	24	1.19
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	20	1.19
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD11	2	1.19
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD12	2	1.19
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD13	2	1.19
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG3	5	1.19
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	23	1.19
(1,9)	1:16:A:ILE:HG21	1:43:A:GLU:H	10	1.19
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	13	1.18
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	5	1.18
(1,779)	1:52:A:HIS:HB2	1:6:A:GLN:HE21	13	1.18
(1,64)	1:12:A:ALA:HB1	1:6:A:GLN:HG2	23	1.18
(1,58)	1:66:A:LEU:HD22	1:10:A:VAL:HB	3	1.18
(1,49)	1:47:A:ILE:HG23	1:43:A:GLU:HG3	2	1.18
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	28	1.17
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	22	1.17
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	1	1.17
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	8	1.16
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD13	27	1.16
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	14	1.16
(1,4)	1:23:A:ALA:HB3	1:25:A:ILE:HD13	18	1.16
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	29	1.15
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	16	1.15
(1,49)	1:47:A:ILE:HG21	1:43:A:GLU:HG3	10	1.15
(1,49)	1:47:A:ILE:HG22	1:43:A:GLU:HG3	20	1.15
(1,47)	1:22:A:LEU:HD21	1:14:A:ALA:H	18	1.15
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	1	1.14
(1,1200)	1:56:A:LEU:HD21	1:55:A:VAL:H	14	1.14
(1,1200)	1:56:A:LEU:HD22	1:55:A:VAL:H	14	1.14
(1,1200)	1:56:A:LEU:HD23	1:55:A:VAL:H	14	1.14
(1,70)	1:9:A:LEU:HD22	1:72:A:MET:H	30	1.14
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	24	1.14
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE2	10	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	29	1.14
(1,28)	1:10:A:VAL:HG23	1:66:A:LEU:HB2	3	1.14
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	13	1.13
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	13	1.13
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	13	1.13
(1,1122)	1:48:A:LEU:HD11	1:52:A:HIS:HB3	2	1.13
(1,1122)	1:48:A:LEU:HD12	1:52:A:HIS:HB3	2	1.13
(1,1122)	1:48:A:LEU:HD13	1:52:A:HIS:HB3	2	1.13
(1,444)	1:47:A:ILE:HA	1:50:A:ARG:HB3	25	1.13
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG3	20	1.13
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	21	1.13
(1,60)	1:47:A:ILE:HG22	1:74:A:SER:HB2	23	1.13
(1,58)	1:66:A:LEU:HD22	1:10:A:VAL:HB	8	1.13
(1,58)	1:66:A:LEU:HD22	1:10:A:VAL:HB	9	1.13
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	30	1.13
(1,59)	1:66:A:LEU:HD22	1:64:A:LEU:HB2	11	1.12
(1,50)	1:16:A:ILE:HG21	1:36:A:LEU:HA	5	1.12
(1,49)	1:47:A:ILE:HG23	1:43:A:GLU:HG3	19	1.12
(1,1505)	1:55:A:VAL:HG11	1:59:A:ARG:HD2	1	1.11
(1,1505)	1:55:A:VAL:HG11	1:59:A:ARG:HD3	1	1.11
(1,1505)	1:55:A:VAL:HG12	1:59:A:ARG:HD2	1	1.11
(1,1505)	1:55:A:VAL:HG12	1:59:A:ARG:HD3	1	1.11
(1,1505)	1:55:A:VAL:HG13	1:59:A:ARG:HD2	1	1.11
(1,1505)	1:55:A:VAL:HG13	1:59:A:ARG:HD3	1	1.11
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	15	1.11
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	21	1.11
(1,76)	1:9:A:LEU:HD11	1:70:A:GLN:HB3	3	1.11
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	11	1.11
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	5	1.11
(1,50)	1:16:A:ILE:HG22	1:36:A:LEU:HA	2	1.11
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE3	18	1.11
(1,40)	1:64:A:LEU:HD23	1:63:A:GLN:HB2	24	1.11
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	20	1.11
(1,9)	1:16:A:ILE:HG22	1:43:A:GLU:H	18	1.11
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	1	1.1
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	6	1.1
(1,49)	1:47:A:ILE:HG22	1:43:A:GLU:HG3	26	1.1
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	20	1.09
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD21	14	1.09
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD22	14	1.09
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD23	14	1.09
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	20	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:29:A:SER:HB3	1:33:A:ASP:HB3	27	1.08
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD21	28	1.07
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD22	28	1.07
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD23	28	1.07
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	10	1.07
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	15	1.07
(1,43)	1:13:A:VAL:HG23	1:17:A:LEU:H	28	1.07
(1,1)	1:55:A:VAL:HG22	1:54:A:LEU:H	1	1.07
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	26	1.06
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	26	1.06
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	26	1.06
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	1	1.06
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE3	3	1.06
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE3	13	1.06
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	24	1.06
(1,9)	1:16:A:ILE:HG21	1:43:A:GLU:H	8	1.06
(1,9)	1:16:A:ILE:HG22	1:43:A:GLU:H	13	1.06
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	14	1.05
(1,1555)	1:34:A:LEU:HD21	1:33:A:ASP:HB3	3	1.05
(1,1555)	1:34:A:LEU:HD22	1:33:A:ASP:HB3	3	1.05
(1,1555)	1:34:A:LEU:HD23	1:33:A:ASP:HB3	3	1.05
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	3	1.05
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	13	1.05
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	23	1.05
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD11	30	1.05
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD12	30	1.05
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD13	30	1.05
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD21	28	1.05
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD22	28	1.05
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD23	28	1.05
(1,72)	1:9:A:LEU:HD21	1:6:A:GLN:HE21	18	1.05
(1,58)	1:66:A:LEU:HD22	1:10:A:VAL:HB	25	1.05
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	25	1.04
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	25	1.04
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	25	1.04
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	11	1.04
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	30	1.04
(1,1544)	1:44:A:VAL:HG21	1:44:A:VAL:H	18	1.03
(1,1544)	1:44:A:VAL:HG22	1:44:A:VAL:H	18	1.03
(1,1544)	1:44:A:VAL:HG23	1:44:A:VAL:H	18	1.03
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	28	1.03
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	20	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	20	1.03
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	20	1.03
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE3	6	1.03
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE2	7	1.03
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE3	12	1.03
(1,32)	1:27:A:LEU:HD11	1:70:A:GLN:HE21	30	1.03
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD11	13	1.02
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD12	13	1.02
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD13	13	1.02
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	7	1.02
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	8	1.02
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	17	1.02
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	22	1.02
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	7	1.02
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	28	1.02
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE3	28	1.02
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	29	1.01
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	29	1.01
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	29	1.01
(1,64)	1:12:A:ALA:HB1	1:6:A:GLN:HG2	30	1.01
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	26	1.01
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	16	1.01
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	23	1.01
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	4	1.0
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	30	1.0
(1,502)	1:19:A:ILE:HD11	1:25:A:ILE:HG13	22	1.0
(1,502)	1:19:A:ILE:HD12	1:25:A:ILE:HG13	22	1.0
(1,502)	1:19:A:ILE:HD13	1:25:A:ILE:HG13	22	1.0
(1,49)	1:47:A:ILE:HG21	1:43:A:GLU:HG3	7	1.0
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE3	15	1.0
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	20	1.0
(1,9)	1:47:A:ILE:HG22	1:50:A:ARG:HE	22	1.0
(1,34)	1:34:A:LEU:HD23	1:32:A:ALA:HA	16	0.99
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD21	14	0.98
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD22	14	0.98
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD23	14	0.98
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	4	0.98
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	30	0.97
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	6	0.97
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	6	0.97
(1,779)	1:52:A:HIS:HB2	1:6:A:GLN:HE21	18	0.97
(1,236)	1:31:A:LEU:HD11	1:66:A:LEU:H	19	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:31:A:LEU:HD12	1:66:A:LEU:H	19	0.97
(1,236)	1:31:A:LEU:HD13	1:66:A:LEU:H	19	0.97
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	1	0.97
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	22	0.96
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD11	22	0.96
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD12	22	0.96
(1,461)	1:47:A:ILE:HG12	1:48:A:LEU:HD13	22	0.96
(1,77)	1:9:A:LEU:HD21	1:70:A:GLN:HB3	11	0.96
(1,72)	1:9:A:LEU:HD22	1:6:A:GLN:HE21	30	0.96
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	3	0.96
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	22	0.95
(1,1196)	1:56:A:LEU:HD21	1:56:A:LEU:HA	14	0.95
(1,1196)	1:56:A:LEU:HD22	1:56:A:LEU:HA	14	0.95
(1,1196)	1:56:A:LEU:HD23	1:56:A:LEU:HA	14	0.95
(1,1065)	1:36:A:LEU:HD11	1:38:A:SER:H	5	0.95
(1,1065)	1:36:A:LEU:HD12	1:38:A:SER:H	5	0.95
(1,1065)	1:36:A:LEU:HD13	1:38:A:SER:H	5	0.95
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD11	5	0.95
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD12	5	0.95
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD13	5	0.95
(1,111)	1:55:A:VAL:HG21	1:49:A:GLU:HG3	18	0.95
(1,111)	1:55:A:VAL:HG22	1:49:A:GLU:HG3	18	0.95
(1,111)	1:55:A:VAL:HG23	1:49:A:GLU:HG3	18	0.95
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	12	0.95
(1,32)	1:66:A:LEU:HD13	1:70:A:GLN:HE21	13	0.95
(1,1648)	1:74:A:SER:HB3	1:54:A:LEU:HD21	18	0.94
(1,1648)	1:74:A:SER:HB3	1:54:A:LEU:HD22	18	0.94
(1,1648)	1:74:A:SER:HB3	1:54:A:LEU:HD23	18	0.94
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	15	0.94
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD21	20	0.94
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD22	20	0.94
(1,928)	1:57:A:PRO:HG2	1:56:A:LEU:HD23	20	0.94
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	15	0.94
(1,50)	1:16:A:ILE:HG22	1:39:A:LEU:HA	29	0.94
(1,49)	1:47:A:ILE:HG22	1:43:A:GLU:HG3	4	0.94
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	23	0.93
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	3	0.93
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	3	0.93
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	3	0.93
(1,49)	1:47:A:ILE:HG21	1:43:A:GLU:HG3	23	0.93
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE3	24	0.93
(1,43)	1:13:A:VAL:HG21	1:17:A:LEU:H	4	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:23:A:ALA:HB2	1:25:A:ILE:HD11	13	0.93
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	27	0.92
(1,58)	1:66:A:LEU:HD22	1:10:A:VAL:HB	2	0.92
(1,48)	1:44:A:VAL:HG13	1:43:A:GLU:H	10	0.92
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE2	21	0.92
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	17	0.92
(1,34)	1:34:A:LEU:HD23	1:27:A:LEU:HA	30	0.92
(1,32)	1:66:A:LEU:HD11	1:70:A:GLN:HE21	2	0.92
(1,9)	1:16:A:ILE:HG23	1:43:A:GLU:H	17	0.92
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	27	0.91
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	27	0.91
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	27	0.91
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	8	0.91
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	8	0.91
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	8	0.91
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	29	0.91
(1,49)	1:47:A:ILE:HG22	1:43:A:GLU:HG3	14	0.91
(1,48)	1:44:A:VAL:HG11	1:45:A:ARG:HE	2	0.91
(1,48)	1:44:A:VAL:HG13	1:45:A:ARG:HE	17	0.91
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	15	0.91
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	3	0.9
(1,1107)	1:48:A:LEU:HA	1:52:A:HIS:HB2	2	0.9
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	28	0.9
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	28	0.9
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	28	0.9
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	18	0.9
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	18	0.9
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	18	0.9
(1,64)	1:12:A:ALA:HB1	1:6:A:GLN:HG2	15	0.9
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	17	0.9
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	17	0.9
(1,5)	1:17:A:LEU:HD11	1:66:A:LEU:HB2	14	0.9
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	3	0.89
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	3	0.89
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	3	0.89
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	11	0.89
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	19	0.89
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	28	0.89
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD21	24	0.89
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD22	24	0.89
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD23	24	0.89
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD21	24	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD22	24	0.89
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD23	24	0.89
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	19	0.89
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	6	0.89
(1,9)	1:16:A:ILE:HG22	1:43:A:GLU:H	28	0.89
(1,48)	1:44:A:VAL:HG12	1:45:A:ARG:HE	19	0.88
(1,1126)	1:48:A:LEU:HD11	1:52:A:HIS:H	2	0.87
(1,1126)	1:48:A:LEU:HD12	1:52:A:HIS:H	2	0.87
(1,1126)	1:48:A:LEU:HD13	1:52:A:HIS:H	2	0.87
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	19	0.87
(1,48)	1:44:A:VAL:HG12	1:43:A:GLU:H	14	0.87
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD11	16	0.86
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD12	16	0.86
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD13	16	0.86
(1,700)	1:59:A:ARG:HA	1:62:A:ARG:HD2	28	0.86
(1,244)	1:31:A:LEU:HD21	1:64:A:LEU:HG	15	0.86
(1,244)	1:31:A:LEU:HD22	1:64:A:LEU:HG	15	0.86
(1,244)	1:31:A:LEU:HD23	1:64:A:LEU:HG	15	0.86
(1,244)	1:31:A:LEU:HD21	1:64:A:LEU:HG	17	0.86
(1,244)	1:31:A:LEU:HD22	1:64:A:LEU:HG	17	0.86
(1,244)	1:31:A:LEU:HD23	1:64:A:LEU:HG	17	0.86
(1,244)	1:31:A:LEU:HD21	1:64:A:LEU:HG	19	0.86
(1,244)	1:31:A:LEU:HD22	1:64:A:LEU:HG	19	0.86
(1,244)	1:31:A:LEU:HD23	1:64:A:LEU:HG	19	0.86
(1,229)	1:31:A:LEU:HA	1:36:A:LEU:HD21	5	0.86
(1,229)	1:31:A:LEU:HA	1:36:A:LEU:HD22	5	0.86
(1,229)	1:31:A:LEU:HA	1:36:A:LEU:HD23	5	0.86
(1,59)	1:66:A:LEU:HD22	1:64:A:LEU:HB2	2	0.86
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	1	0.86
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	26	0.86
(1,58)	1:66:A:LEU:HD23	1:10:A:VAL:HB	27	0.86
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	3	0.86
(1,49)	1:47:A:ILE:HG21	1:43:A:GLU:HG3	28	0.86
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	2	0.86
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	14	0.85
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	14	0.85
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	14	0.85
(1,719)	1:63:A:GLN:HB2	1:63:A:GLN:HE21	29	0.85
(1,244)	1:31:A:LEU:HD21	1:64:A:LEU:HG	13	0.85
(1,244)	1:31:A:LEU:HD22	1:64:A:LEU:HG	13	0.85
(1,244)	1:31:A:LEU:HD23	1:64:A:LEU:HG	13	0.85
(1,102)	1:55:A:VAL:HG21	1:55:A:VAL:H	1	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:55:A:VAL:HG22	1:55:A:VAL:H	1	0.85
(1,102)	1:55:A:VAL:HG23	1:55:A:VAL:H	1	0.85
(1,64)	1:12:A:ALA:HB2	1:6:A:GLN:HG3	16	0.85
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	9	0.85
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	13	0.85
(1,48)	1:44:A:VAL:HG12	1:43:A:GLU:H	22	0.85
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HG2	14	0.84
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD11	22	0.84
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD12	22	0.84
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD13	22	0.84
(1,1012)	1:34:A:LEU:HD11	1:31:A:LEU:H	5	0.84
(1,1012)	1:34:A:LEU:HD12	1:31:A:LEU:H	5	0.84
(1,1012)	1:34:A:LEU:HD13	1:31:A:LEU:H	5	0.84
(1,719)	1:63:A:GLN:HB2	1:63:A:GLN:HE21	24	0.84
(1,59)	1:66:A:LEU:HD21	1:64:A:LEU:HB2	4	0.84
(1,58)	1:36:A:LEU:HD13	1:43:A:GLU:HB2	21	0.84
(1,43)	1:13:A:VAL:HG22	1:17:A:LEU:H	16	0.84
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	10	0.84
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	13	0.84
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	30	0.83
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD11	2	0.83
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD12	2	0.83
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD13	2	0.83
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD11	18	0.83
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD12	18	0.83
(1,1117)	1:48:A:LEU:HA	1:48:A:LEU:HD13	18	0.83
(1,719)	1:63:A:GLN:HB2	1:63:A:GLN:HE21	10	0.83
(1,244)	1:31:A:LEU:HD21	1:64:A:LEU:HG	5	0.83
(1,244)	1:31:A:LEU:HD22	1:64:A:LEU:HG	5	0.83
(1,244)	1:31:A:LEU:HD23	1:64:A:LEU:HG	5	0.83
(1,244)	1:31:A:LEU:HD21	1:64:A:LEU:HG	16	0.83
(1,244)	1:31:A:LEU:HD22	1:64:A:LEU:HG	16	0.83
(1,244)	1:31:A:LEU:HD23	1:64:A:LEU:HG	16	0.83
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	6	0.83
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	6	0.83
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	6	0.83
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	30	0.83
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	17	0.83
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	24	0.82
(1,499)	1:47:A:ILE:HD11	1:43:A:GLU:HG2	21	0.82
(1,499)	1:47:A:ILE:HD12	1:43:A:GLU:HG2	21	0.82
(1,499)	1:47:A:ILE:HD13	1:43:A:GLU:HG2	21	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:44:A:VAL:HG13	1:43:A:GLU:H	15	0.82
(1,9)	1:16:A:ILE:HG21	1:43:A:GLU:H	30	0.82
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	18	0.81
(1,719)	1:63:A:GLN:HB2	1:63:A:GLN:HE21	5	0.81
(1,244)	1:31:A:LEU:HD21	1:64:A:LEU:HG	30	0.81
(1,244)	1:31:A:LEU:HD22	1:64:A:LEU:HG	30	0.81
(1,244)	1:31:A:LEU:HD23	1:64:A:LEU:HG	30	0.81
(1,65)	1:31:A:LEU:HD13	1:36:A:LEU:HB3	18	0.81
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	14	0.81
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	20	0.81
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE3	25	0.81
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	25	0.81
(1,32)	1:27:A:LEU:HD11	1:70:A:GLN:HE21	7	0.81
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	17	0.8
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	17	0.8
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	17	0.8
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	24	0.8
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	24	0.8
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	24	0.8
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	13	0.8
(1,1555)	1:34:A:LEU:HD21	1:33:A:ASP:HB3	20	0.8
(1,1555)	1:34:A:LEU:HD22	1:33:A:ASP:HB3	20	0.8
(1,1555)	1:34:A:LEU:HD23	1:33:A:ASP:HB3	20	0.8
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	13	0.8
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	13	0.8
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	13	0.8
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	24	0.8
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	24	0.8
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	13	0.8
(1,233)	1:31:A:LEU:HD11	1:31:A:LEU:HA	30	0.8
(1,233)	1:31:A:LEU:HD12	1:31:A:LEU:HA	30	0.8
(1,233)	1:31:A:LEU:HD13	1:31:A:LEU:HA	30	0.8
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	3	0.8
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	27	0.8
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	20	0.8
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	1	0.8
(1,32)	1:27:A:LEU:HD12	1:70:A:GLN:HE21	21	0.8
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	7	0.79
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD21	14	0.79
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD22	14	0.79
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD23	14	0.79
(1,719)	1:63:A:GLN:HB2	1:63:A:GLN:HE21	30	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	21	0.79
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	21	0.79
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	21	0.79
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	20	0.79
(1,58)	1:66:A:LEU:HD22	1:10:A:VAL:HB	10	0.79
(1,49)	1:47:A:ILE:HG23	1:43:A:GLU:HG3	15	0.79
(1,48)	1:44:A:VAL:HG12	1:43:A:GLU:H	9	0.79
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	17	0.78
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	17	0.78
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	17	0.78
(1,779)	1:52:A:HIS:HB2	1:6:A:GLN:HE21	30	0.78
(1,700)	1:59:A:ARG:HA	1:62:A:ARG:HD2	19	0.78
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	28	0.78
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD11	2	0.78
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	11	0.77
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	11	0.77
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	11	0.77
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	15	0.77
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	18	0.77
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	22	0.77
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD11	15	0.77
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD12	15	0.77
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD13	15	0.77
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD11	19	0.77
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD12	19	0.77
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD13	19	0.77
(1,233)	1:31:A:LEU:HD11	1:31:A:LEU:HA	5	0.77
(1,233)	1:31:A:LEU:HD12	1:31:A:LEU:HA	5	0.77
(1,233)	1:31:A:LEU:HD13	1:31:A:LEU:HA	5	0.77
(1,233)	1:31:A:LEU:HD11	1:31:A:LEU:HA	15	0.77
(1,233)	1:31:A:LEU:HD12	1:31:A:LEU:HA	15	0.77
(1,233)	1:31:A:LEU:HD13	1:31:A:LEU:HA	15	0.77
(1,60)	1:47:A:ILE:HG22	1:74:A:SER:HB2	2	0.77
(1,43)	1:13:A:VAL:HG23	1:17:A:LEU:H	11	0.77
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	16	0.77
(1,9)	1:16:A:ILE:HG21	1:43:A:GLU:H	5	0.77
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	2	0.76
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HG2	28	0.76
(1,572)	1:43:A:GLU:HB2	1:44:A:VAL:HG21	18	0.76
(1,572)	1:43:A:GLU:HB2	1:44:A:VAL:HG22	18	0.76
(1,572)	1:43:A:GLU:HB2	1:44:A:VAL:HG23	18	0.76
(1,412)	1:45:A:ARG:HD2	1:58:A:ILE:HA	11	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:45:A:ARG:HD3	1:58:A:ILE:HA	11	0.76
(1,412)	1:45:A:ARG:HD2	1:58:A:ILE:HA	30	0.76
(1,412)	1:45:A:ARG:HD3	1:58:A:ILE:HA	30	0.76
(1,233)	1:31:A:LEU:HD11	1:31:A:LEU:HA	13	0.76
(1,233)	1:31:A:LEU:HD12	1:31:A:LEU:HA	13	0.76
(1,233)	1:31:A:LEU:HD13	1:31:A:LEU:HA	13	0.76
(1,233)	1:31:A:LEU:HD11	1:31:A:LEU:HA	16	0.76
(1,233)	1:31:A:LEU:HD12	1:31:A:LEU:HA	16	0.76
(1,233)	1:31:A:LEU:HD13	1:31:A:LEU:HA	16	0.76
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	27	0.76
(1,54)	1:7:A:ARG:HG3	1:10:A:VAL:HA	7	0.76
(1,48)	1:44:A:VAL:HG12	1:64:A:LEU:H	25	0.76
(1,1566)	1:68:A:LYS:HD2	1:64:A:LEU:H	13	0.75
(1,1566)	1:68:A:LYS:HD3	1:64:A:LEU:H	13	0.75
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	27	0.75
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	12	0.75
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	15	0.75
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	8	0.75
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	8	0.75
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	8	0.75
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	19	0.75
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	19	0.75
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	19	0.75
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE2	4	0.75
(1,9)	1:47:A:ILE:HG23	1:50:A:ARG:HE	15	0.75
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	21	0.74
(1,1182)	1:56:A:LEU:HB3	1:57:A:PRO:HG2	14	0.74
(1,719)	1:63:A:GLN:HB2	1:63:A:GLN:HE21	15	0.74
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	28	0.74
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	28	0.74
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	28	0.74
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE3	5	0.74
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	26	0.74
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	16	0.73
(1,1555)	1:34:A:LEU:HD21	1:33:A:ASP:HB3	29	0.73
(1,1555)	1:34:A:LEU:HD22	1:33:A:ASP:HB3	29	0.73
(1,1555)	1:34:A:LEU:HD23	1:33:A:ASP:HB3	29	0.73
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	9	0.73
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	2	0.73
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	11	0.73
(1,1122)	1:48:A:LEU:HD11	1:52:A:HIS:HB3	18	0.73
(1,1122)	1:48:A:LEU:HD12	1:52:A:HIS:HB3	18	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:48:A:LEU:HD13	1:52:A:HIS:HB3	18	0.73
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	9	0.73
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	9	0.73
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	9	0.73
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	25	0.73
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	25	0.73
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	25	0.73
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	2	0.73
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	2	0.73
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	2	0.73
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	23	0.73
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	23	0.73
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	23	0.73
(1,233)	1:31:A:LEU:HD11	1:31:A:LEU:HA	17	0.73
(1,233)	1:31:A:LEU:HD12	1:31:A:LEU:HA	17	0.73
(1,233)	1:31:A:LEU:HD13	1:31:A:LEU:HA	17	0.73
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	10	0.73
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	2	0.73
(1,9)	1:16:A:ILE:HG22	1:43:A:GLU:H	1	0.73
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	18	0.72
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	18	0.72
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	18	0.72
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	12	0.72
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HG2	17	0.72
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	24	0.72
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	12	0.72
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	12	0.72
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	12	0.72
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	5	0.72
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	5	0.72
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	5	0.72
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	3	0.72
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	3	0.72
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	3	0.72
(1,111)	1:55:A:VAL:HG21	1:49:A:GLU:HG3	2	0.72
(1,111)	1:55:A:VAL:HG22	1:49:A:GLU:HG3	2	0.72
(1,111)	1:55:A:VAL:HG23	1:49:A:GLU:HG3	2	0.72
(1,82)	1:73:A:SER:HB2	1:7:A:ARG:HG2	29	0.72
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	11	0.72
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	11	0.71
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	11	0.71
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	19	0.71
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	22	0.71
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	22	0.71
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	22	0.71
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	19	0.71
(1,32)	1:66:A:LEU:HD12	1:70:A:GLN:HE21	10	0.71
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	13	0.7
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	13	0.7
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	13	0.7
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	27	0.7
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	29	0.7
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	1	0.7
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	1	0.7
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	1	0.7
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD11	17	0.7
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD12	17	0.7
(1,801)	1:65:A:THR:HA	1:31:A:LEU:HD13	17	0.7
(1,668)	1:49:A:GLU:HG2	1:46:A:GLN:HA	2	0.7
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	1	0.7
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	1	0.7
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	1	0.7
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	8	0.7
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	8	0.7
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	8	0.7
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	17	0.7
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	17	0.7
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	17	0.7
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD13	16	0.7
(1,77)	1:9:A:LEU:HD23	1:70:A:GLN:HB3	2	0.7
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	11	0.69
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	11	0.69
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	11	0.69
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	21	0.69
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	21	0.69
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	21	0.69
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	23	0.69
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	23	0.69
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	23	0.69
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	7	0.69
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	7	0.69
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	7	0.69
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	18	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:31:A:LEU:HD11	1:31:A:LEU:HA	19	0.69
(1,233)	1:31:A:LEU:HD12	1:31:A:LEU:HA	19	0.69
(1,233)	1:31:A:LEU:HD13	1:31:A:LEU:HA	19	0.69
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	8	0.69
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	14	0.69
(1,9)	1:47:A:ILE:HG21	1:50:A:ARG:HE	2	0.69
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	19	0.68
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	19	0.68
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	19	0.68
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	23	0.68
(1,9)	1:16:A:ILE:HG21	1:43:A:GLU:H	19	0.68
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	14	0.67
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	14	0.67
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	14	0.67
(1,1239)	1:60:A:GLU:HB3	1:56:A:LEU:HB2	10	0.67
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	6	0.67
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	16	0.67
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	25	0.67
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	26	0.67
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	30	0.67
(1,1012)	1:34:A:LEU:HD11	1:31:A:LEU:H	28	0.67
(1,1012)	1:34:A:LEU:HD12	1:31:A:LEU:H	28	0.67
(1,1012)	1:34:A:LEU:HD13	1:31:A:LEU:H	28	0.67
(1,566)	1:72:A:MET:HG2	1:68:A:LYS:HB2	11	0.67
(1,566)	1:72:A:MET:HG2	1:68:A:LYS:HB3	11	0.67
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	7	0.67
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	7	0.67
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	7	0.67
(1,82)	1:73:A:SER:HB2	1:7:A:ARG:HG3	1	0.67
(1,82)	1:73:A:SER:HB2	1:7:A:ARG:HG3	2	0.67
(1,59)	1:36:A:LEU:HD11	1:64:A:LEU:HB2	18	0.67
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	8	0.67
(1,32)	1:27:A:LEU:HD12	1:70:A:GLN:HE21	26	0.67
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG21	17	0.67
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG23	27	0.67
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	26	0.66
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD11	6	0.66
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD12	6	0.66
(1,1509)	1:72:A:MET:HG2	1:9:A:LEU:HD13	6	0.66
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	5	0.66
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	20	0.66
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	25	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	25	0.66
(1,779)	1:52:A:HIS:HB2	1:6:A:GLN:HE21	5	0.66
(1,412)	1:45:A:ARG:HD2	1:58:A:ILE:HA	28	0.66
(1,412)	1:45:A:ARG:HD3	1:58:A:ILE:HA	28	0.66
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD21	27	0.66
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD22	27	0.66
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD23	27	0.66
(1,111)	1:55:A:VAL:HG21	1:49:A:GLU:HG3	29	0.66
(1,111)	1:55:A:VAL:HG22	1:49:A:GLU:HG3	29	0.66
(1,111)	1:55:A:VAL:HG23	1:49:A:GLU:HG3	29	0.66
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG3	9	0.66
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	25	0.66
(1,50)	1:16:A:ILE:HG22	1:39:A:LEU:HA	12	0.66
(1,50)	1:16:A:ILE:HG23	1:39:A:LEU:HA	27	0.66
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	21	0.65
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	21	0.65
(1,1445)	1:44:A:VAL:HG11	1:47:A:ILE:HG13	18	0.65
(1,1445)	1:44:A:VAL:HG12	1:47:A:ILE:HG13	18	0.65
(1,1445)	1:44:A:VAL:HG13	1:47:A:ILE:HG13	18	0.65
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	19	0.65
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	6	0.65
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	7	0.65
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	7	0.65
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	7	0.65
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	5	0.65
(1,412)	1:45:A:ARG:HD2	1:58:A:ILE:HA	16	0.65
(1,412)	1:45:A:ARG:HD3	1:58:A:ILE:HA	16	0.65
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	5	0.65
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	24	0.65
(1,50)	1:16:A:ILE:HG23	1:39:A:LEU:HA	9	0.65
(1,47)	1:22:A:LEU:HD21	1:14:A:ALA:H	14	0.65
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	13	0.65
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG23	20	0.65
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	15	0.64
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	15	0.64
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	15	0.64
(1,499)	1:47:A:ILE:HD11	1:43:A:GLU:HG2	16	0.64
(1,499)	1:47:A:ILE:HD12	1:43:A:GLU:HG2	16	0.64
(1,499)	1:47:A:ILE:HD13	1:43:A:GLU:HG2	16	0.64
(1,77)	1:9:A:LEU:HD22	1:51:A:GLU:HG3	30	0.64
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	8	0.64
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	17	0.63
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	3	0.63
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD21	28	0.63
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD22	28	0.63
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD23	28	0.63
(1,240)	1:31:A:LEU:HD11	1:34:A:LEU:HB2	15	0.63
(1,240)	1:31:A:LEU:HD12	1:34:A:LEU:HB2	15	0.63
(1,240)	1:31:A:LEU:HD13	1:34:A:LEU:HB2	15	0.63
(1,240)	1:31:A:LEU:HD11	1:34:A:LEU:HB2	19	0.63
(1,240)	1:31:A:LEU:HD12	1:34:A:LEU:HB2	19	0.63
(1,240)	1:31:A:LEU:HD13	1:34:A:LEU:HB2	19	0.63
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	2	0.63
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	14	0.63
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	22	0.63
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	15	0.62
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	15	0.62
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	15	0.62
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	1	0.62
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	20	0.62
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	20	0.62
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	20	0.62
(1,240)	1:31:A:LEU:HD11	1:34:A:LEU:HB2	30	0.62
(1,240)	1:31:A:LEU:HD12	1:34:A:LEU:HB2	30	0.62
(1,240)	1:31:A:LEU:HD13	1:34:A:LEU:HB2	30	0.62
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	17	0.62
(1,75)	1:9:A:LEU:HD13	1:75:A:LYS:HB3	6	0.62
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG21	29	0.62
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	8	0.61
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	20	0.61
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD11	18	0.61
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD12	18	0.61
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD13	18	0.61
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	7	0.61
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	7	0.61
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	7	0.61
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	11	0.61
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	26	0.61
(1,63)	1:47:A:ILE:HG22	1:7:A:ARG:H	30	0.61
(1,48)	1:44:A:VAL:HG12	1:45:A:ARG:HE	4	0.61
(1,34)	1:34:A:LEU:HD22	1:66:A:LEU:HA	18	0.61
(1,8)	1:47:A:ILE:HG22	1:7:A:ARG:H	30	0.61
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	20	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	20	0.6
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	20	0.6
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	16	0.6
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	25	0.6
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG21	3	0.6
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD12	25	0.6
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD13	26	0.6
(1,1610)	1:13:A:VAL:HG21	1:9:A:LEU:HD11	13	0.59
(1,1610)	1:13:A:VAL:HG21	1:9:A:LEU:HD12	13	0.59
(1,1610)	1:13:A:VAL:HG21	1:9:A:LEU:HD13	13	0.59
(1,1610)	1:13:A:VAL:HG22	1:9:A:LEU:HD11	13	0.59
(1,1610)	1:13:A:VAL:HG22	1:9:A:LEU:HD12	13	0.59
(1,1610)	1:13:A:VAL:HG22	1:9:A:LEU:HD13	13	0.59
(1,1610)	1:13:A:VAL:HG23	1:9:A:LEU:HD11	13	0.59
(1,1610)	1:13:A:VAL:HG23	1:9:A:LEU:HD12	13	0.59
(1,1610)	1:13:A:VAL:HG23	1:9:A:LEU:HD13	13	0.59
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	12	0.59
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	15	0.59
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	11	0.59
(1,1128)	1:36:A:LEU:HD11	1:37:A:ASP:H	5	0.59
(1,1128)	1:36:A:LEU:HD12	1:37:A:ASP:H	5	0.59
(1,1128)	1:36:A:LEU:HD13	1:37:A:ASP:H	5	0.59
(1,502)	1:19:A:ILE:HD11	1:25:A:ILE:HG13	2	0.59
(1,502)	1:19:A:ILE:HD12	1:25:A:ILE:HG13	2	0.59
(1,502)	1:19:A:ILE:HD13	1:25:A:ILE:HG13	2	0.59
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	22	0.59
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	22	0.59
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	22	0.59
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG3	12	0.59
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	24	0.59
(1,50)	1:16:A:ILE:HG21	1:39:A:LEU:HA	3	0.59
(1,50)	1:16:A:ILE:HG21	1:36:A:LEU:HA	8	0.59
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE2	9	0.59
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD11	19	0.59
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	28	0.58
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	26	0.58
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	26	0.58
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	10	0.58
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	3	0.58
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	15	0.58
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	23	0.58
(1,296)	1:17:A:LEU:HD11	1:19:A:ILE:HG13	16	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:17:A:LEU:HD12	1:19:A:ILE:HG13	16	0.58
(1,296)	1:17:A:LEU:HD13	1:19:A:ILE:HG13	16	0.58
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	10	0.58
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	10	0.58
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	10	0.58
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	20	0.58
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	20	0.58
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	20	0.58
(1,59)	1:66:A:LEU:HD22	1:64:A:LEU:HB2	9	0.58
(1,54)	1:7:A:ARG:HG3	1:10:A:VAL:HA	26	0.58
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG22	13	0.58
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	2	0.57
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	9	0.57
(1,63)	1:47:A:ILE:HG21	1:7:A:ARG:H	11	0.57
(1,59)	1:66:A:LEU:HD21	1:64:A:LEU:HB2	16	0.57
(1,59)	1:66:A:LEU:HD21	1:64:A:LEU:HB2	28	0.57
(1,56)	1:59:A:ARG:HG3	1:61:A:VAL:H	8	0.57
(1,48)	1:44:A:VAL:HG12	1:64:A:LEU:H	8	0.57
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	5	0.57
(1,1303)	1:64:A:LEU:HB2	1:31:A:LEU:HB3	28	0.56
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD21	28	0.56
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD22	28	0.56
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD23	28	0.56
(1,798)	1:51:A:GLU:HG2	1:50:A:ARG:HG2	23	0.56
(1,798)	1:51:A:GLU:HG3	1:50:A:ARG:HG2	23	0.56
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	6	0.56
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	18	0.55
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	18	0.55
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	22	0.55
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	4	0.55
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	18	0.55
(1,1239)	1:60:A:GLU:HB3	1:56:A:LEU:HB2	8	0.55
(1,240)	1:31:A:LEU:HD11	1:34:A:LEU:HB2	16	0.55
(1,240)	1:31:A:LEU:HD12	1:34:A:LEU:HB2	16	0.55
(1,240)	1:31:A:LEU:HD13	1:34:A:LEU:HB2	16	0.55
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	24	0.55
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	24	0.55
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	24	0.55
(1,76)	1:9:A:LEU:HD11	1:70:A:GLN:HB3	23	0.55
(1,76)	1:9:A:LEU:HD13	1:70:A:GLN:HB3	29	0.55
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	5	0.54
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	13	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	4	0.54
(1,499)	1:47:A:ILE:HD11	1:43:A:GLU:HG2	11	0.54
(1,499)	1:47:A:ILE:HD12	1:43:A:GLU:HG2	11	0.54
(1,499)	1:47:A:ILE:HD13	1:43:A:GLU:HG2	11	0.54
(1,240)	1:31:A:LEU:HD11	1:34:A:LEU:HB2	17	0.54
(1,240)	1:31:A:LEU:HD12	1:34:A:LEU:HB2	17	0.54
(1,240)	1:31:A:LEU:HD13	1:34:A:LEU:HB2	17	0.54
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	21	0.54
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	24	0.54
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD13	12	0.54
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	8	0.53
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	8	0.53
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	1	0.53
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	17	0.53
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	8	0.53
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	8	0.53
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	8	0.53
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	27	0.53
(1,700)	1:59:A:ARG:HA	1:62:A:ARG:HD2	10	0.53
(1,240)	1:31:A:LEU:HD11	1:34:A:LEU:HB2	13	0.53
(1,240)	1:31:A:LEU:HD12	1:34:A:LEU:HB2	13	0.53
(1,240)	1:31:A:LEU:HD13	1:34:A:LEU:HB2	13	0.53
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	8	0.53
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD13	13	0.53
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	26	0.53
(1,68)	1:57:A:PRO:HB3	1:61:A:VAL:HG23	20	0.53
(1,58)	1:66:A:LEU:HD22	1:10:A:VAL:HB	29	0.53
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	13	0.53
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD11	20	0.53
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	5	0.52
(1,499)	1:47:A:ILE:HD11	1:43:A:GLU:HG2	24	0.52
(1,499)	1:47:A:ILE:HD12	1:43:A:GLU:HG2	24	0.52
(1,499)	1:47:A:ILE:HD13	1:43:A:GLU:HG2	24	0.52
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	7	0.52
(1,73)	1:9:A:LEU:HD12	1:69:A:LEU:HB3	13	0.52
(1,66)	1:58:A:ILE:HD13	1:45:A:ARG:HE	15	0.52
(1,59)	1:66:A:LEU:HD22	1:64:A:LEU:HB2	3	0.52
(1,32)	1:27:A:LEU:HD11	1:70:A:GLN:HE21	1	0.52
(1,32)	1:27:A:LEU:HD12	1:70:A:GLN:HE21	16	0.52
(1,28)	1:10:A:VAL:HG21	1:66:A:LEU:HB2	5	0.52
(1,28)	1:10:A:VAL:HG23	1:66:A:LEU:HB2	6	0.52
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	13	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	13	0.51
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	28	0.51
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	28	0.51
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	21	0.51
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	29	0.51
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	29	0.51
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	29	0.51
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	10	0.51
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	10	0.51
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	10	0.51
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	29	0.51
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	29	0.51
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	29	0.51
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD13	23	0.51
(1,76)	1:9:A:LEU:HD12	1:70:A:GLN:HB3	21	0.51
(1,59)	1:66:A:LEU:HD22	1:64:A:LEU:HB2	29	0.51
(1,48)	1:44:A:VAL:HG12	1:45:A:ARG:HE	26	0.51
(1,32)	1:27:A:LEU:HD13	1:70:A:GLN:HE21	19	0.51
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	15	0.5
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	15	0.5
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	14	0.5
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	14	0.5
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	19	0.5
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	19	0.5
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	22	0.5
(1,1196)	1:56:A:LEU:HD21	1:56:A:LEU:HA	20	0.5
(1,1196)	1:56:A:LEU:HD22	1:56:A:LEU:HA	20	0.5
(1,1196)	1:56:A:LEU:HD23	1:56:A:LEU:HA	20	0.5
(1,1183)	1:56:A:LEU:HB2	1:57:A:PRO:HB2	8	0.5
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	13	0.5
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	13	0.5
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	13	0.5
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	24	0.5
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	24	0.5
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	24	0.5
(1,499)	1:47:A:ILE:HD11	1:43:A:GLU:HG2	27	0.5
(1,499)	1:47:A:ILE:HD12	1:43:A:GLU:HG2	27	0.5
(1,499)	1:47:A:ILE:HD13	1:43:A:GLU:HG2	27	0.5
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	12	0.5
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	12	0.5
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	12	0.5
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD13	29	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:9:A:LEU:HG	1:10:A:VAL:HA	30	0.5
(1,50)	1:16:A:ILE:HG23	1:39:A:LEU:HA	4	0.5
(1,50)	1:16:A:ILE:HG21	1:39:A:LEU:HA	10	0.5
(1,50)	1:16:A:ILE:HG21	1:39:A:LEU:HA	19	0.5
(1,50)	1:16:A:ILE:HG21	1:36:A:LEU:HA	26	0.5
(1,47)	1:22:A:LEU:HD22	1:14:A:ALA:H	1	0.5
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE3	11	0.5
(1,32)	1:66:A:LEU:HD13	1:70:A:GLN:HE21	4	0.5
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	17	0.49
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	17	0.49
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	3	0.49
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	3	0.49
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	14	0.49
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	14	0.49
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	14	0.49
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	19	0.49
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	19	0.49
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	19	0.49
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	4	0.49
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	4	0.49
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	4	0.49
(1,60)	1:47:A:ILE:HG21	1:74:A:SER:HB2	12	0.49
(1,59)	1:66:A:LEU:HD22	1:64:A:LEU:HB2	10	0.49
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	30	0.49
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	4	0.49
(1,32)	1:27:A:LEU:HD11	1:70:A:GLN:HE21	27	0.49
(1,28)	1:10:A:VAL:HG23	1:66:A:LEU:HB2	23	0.49
(1,9)	1:16:A:ILE:HG21	1:43:A:GLU:H	6	0.49
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	10	0.48
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	10	0.48
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	10	0.48
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	23	0.48
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	23	0.48
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	9	0.48
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	9	0.48
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	24	0.48
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	24	0.48
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	27	0.48
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	27	0.48
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	27	0.48
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	12	0.48
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	1	0.48
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	1	0.48
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	27	0.48
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	27	0.48
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	27	0.48
(1,76)	1:9:A:LEU:HD12	1:70:A:GLN:HB3	2	0.48
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	13	0.48
(1,1576)	1:66:A:LEU:HD11	1:65:A:THR:HA	11	0.47
(1,1576)	1:66:A:LEU:HD12	1:65:A:THR:HA	11	0.47
(1,1576)	1:66:A:LEU:HD13	1:65:A:THR:HA	11	0.47
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	24	0.47
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	13	0.47
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	11	0.47
(1,1248)	1:61:A:VAL:HA	1:62:A:ARG:HB3	7	0.47
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	17	0.47
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	17	0.47
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	17	0.47
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	20	0.47
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	20	0.47
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	20	0.47
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	29	0.47
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	29	0.47
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	29	0.47
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD11	2	0.47
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD12	2	0.47
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD13	2	0.47
(1,294)	1:17:A:LEU:HD11	1:36:A:LEU:HB2	26	0.47
(1,294)	1:17:A:LEU:HD12	1:36:A:LEU:HB2	26	0.47
(1,294)	1:17:A:LEU:HD13	1:36:A:LEU:HB2	26	0.47
(1,294)	1:17:A:LEU:HD21	1:36:A:LEU:HB2	26	0.47
(1,294)	1:17:A:LEU:HD22	1:36:A:LEU:HB2	26	0.47
(1,294)	1:17:A:LEU:HD23	1:36:A:LEU:HB2	26	0.47
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	11	0.47
(1,47)	1:22:A:LEU:HD22	1:14:A:ALA:H	19	0.47
(1,38)	1:58:A:ILE:HG22	1:32:A:ALA:HA	3	0.47
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	12	0.46
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	1	0.46
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	1	0.46
(1,1575)	1:66:A:LEU:HD11	1:13:A:VAL:H	30	0.46
(1,1575)	1:66:A:LEU:HD12	1:13:A:VAL:H	30	0.46
(1,1575)	1:66:A:LEU:HD13	1:13:A:VAL:H	30	0.46
(1,1508)	1:72:A:MET:HG3	1:9:A:LEU:HD11	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1508)	1:72:A:MET:HG3	1:9:A:LEU:HD12	13	0.46
(1,1508)	1:72:A:MET:HG3	1:9:A:LEU:HD13	13	0.46
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	1	0.46
(1,76)	1:9:A:LEU:HD12	1:70:A:GLN:HB3	19	0.46
(1,56)	1:7:A:ARG:HG3	1:10:A:VAL:H	18	0.46
(1,56)	1:59:A:ARG:HG3	1:61:A:VAL:H	24	0.46
(1,52)	1:9:A:LEU:HG	1:10:A:VAL:HA	7	0.46
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE3	26	0.46
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	22	0.45
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	22	0.45
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	26	0.45
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	26	0.45
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	26	0.45
(1,1126)	1:48:A:LEU:HD11	1:52:A:HIS:H	22	0.45
(1,1126)	1:48:A:LEU:HD12	1:52:A:HIS:H	22	0.45
(1,1126)	1:48:A:LEU:HD13	1:52:A:HIS:H	22	0.45
(1,1123)	1:48:A:LEU:HD11	1:52:A:HIS:HB2	18	0.45
(1,1123)	1:48:A:LEU:HD12	1:52:A:HIS:HB2	18	0.45
(1,1123)	1:48:A:LEU:HD13	1:52:A:HIS:HB2	18	0.45
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	18	0.45
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	18	0.45
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	18	0.45
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	12	0.45
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	12	0.45
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	12	0.45
(1,798)	1:51:A:GLU:HG2	1:50:A:ARG:HG2	12	0.45
(1,798)	1:51:A:GLU:HG3	1:50:A:ARG:HG2	12	0.45
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	22	0.45
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	22	0.45
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	22	0.45
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	11	0.45
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	5	0.44
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	5	0.44
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	5	0.44
(1,1221)	1:58:A:ILE:HG21	1:57:A:PRO:HB3	14	0.44
(1,1221)	1:58:A:ILE:HG22	1:57:A:PRO:HB3	14	0.44
(1,1221)	1:58:A:ILE:HG23	1:57:A:PRO:HB3	14	0.44
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	16	0.44
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	16	0.44
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	16	0.44
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	3	0.44
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	3	0.44
(1,1008)	1:34:A:LEU:HD11	1:31:A:LEU:HA	5	0.44
(1,1008)	1:34:A:LEU:HD12	1:31:A:LEU:HA	5	0.44
(1,1008)	1:34:A:LEU:HD13	1:31:A:LEU:HA	5	0.44
(1,1006)	1:33:A:ASP:HB2	1:30:A:SER:H	27	0.44
(1,593)	1:66:A:LEU:HD11	1:66:A:LEU:HA	30	0.44
(1,593)	1:66:A:LEU:HD12	1:66:A:LEU:HA	30	0.44
(1,593)	1:66:A:LEU:HD13	1:66:A:LEU:HA	30	0.44
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	24	0.44
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	24	0.44
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	24	0.44
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD21	24	0.44
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD22	24	0.44
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD23	24	0.44
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD21	27	0.44
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD22	27	0.44
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD23	27	0.44
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD13	17	0.44
(1,76)	1:9:A:LEU:HD12	1:70:A:GLN:HB3	16	0.44
(1,50)	1:16:A:ILE:HG23	1:39:A:LEU:HA	17	0.44
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	16	0.44
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	21	0.44
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	3	0.43
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	3	0.43
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	3	0.43
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD21	27	0.43
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD22	27	0.43
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD23	27	0.43
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	19	0.43
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	19	0.43
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	19	0.43
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	26	0.43
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	26	0.43
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	26	0.43
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	30	0.43
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	30	0.43
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	30	0.43
(1,847)	1:8:A:ASP:HB2	1:11:A:LYS:HD2	25	0.43
(1,847)	1:8:A:ASP:HB2	1:11:A:LYS:HD3	25	0.43
(1,76)	1:9:A:LEU:HD13	1:70:A:GLN:HB3	9	0.43
(1,59)	1:66:A:LEU:HD21	1:64:A:LEU:HB2	8	0.43
(1,59)	1:66:A:LEU:HD21	1:64:A:LEU:HB2	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	19	0.43
(1,52)	1:9:A:LEU:HG	1:10:A:VAL:HA	16	0.43
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	22	0.42
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	22	0.42
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	25	0.42
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD21	24	0.42
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD22	24	0.42
(1,1100)	1:40:A:MET:HG2	1:39:A:LEU:HD23	24	0.42
(1,739)	1:70:A:GLN:HA	1:71:A:GLU:HB2	15	0.42
(1,593)	1:66:A:LEU:HD11	1:66:A:LEU:HA	18	0.42
(1,593)	1:66:A:LEU:HD12	1:66:A:LEU:HA	18	0.42
(1,593)	1:66:A:LEU:HD13	1:66:A:LEU:HA	18	0.42
(1,296)	1:17:A:LEU:HD11	1:19:A:ILE:HG13	7	0.42
(1,296)	1:17:A:LEU:HD12	1:19:A:ILE:HG13	7	0.42
(1,296)	1:17:A:LEU:HD13	1:19:A:ILE:HG13	7	0.42
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD13	20	0.42
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	28	0.42
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	29	0.41
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	29	0.41
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	29	0.41
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	12	0.41
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	12	0.41
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	12	0.41
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	22	0.41
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	22	0.41
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	22	0.41
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	26	0.41
(1,1241)	1:60:A:GLU:HB2	1:61:A:VAL:HG21	2	0.41
(1,1241)	1:60:A:GLU:HB2	1:61:A:VAL:HG22	2	0.41
(1,1241)	1:60:A:GLU:HB2	1:61:A:VAL:HG23	2	0.41
(1,1126)	1:48:A:LEU:HD11	1:52:A:HIS:H	18	0.41
(1,1126)	1:48:A:LEU:HD12	1:52:A:HIS:H	18	0.41
(1,1126)	1:48:A:LEU:HD13	1:52:A:HIS:H	18	0.41
(1,1107)	1:48:A:LEU:HA	1:52:A:HIS:HB2	1	0.41
(1,1028)	1:34:A:LEU:HD21	1:33:A:ASP:H	27	0.41
(1,1028)	1:34:A:LEU:HD22	1:33:A:ASP:H	27	0.41
(1,1028)	1:34:A:LEU:HD23	1:33:A:ASP:H	27	0.41
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	24	0.41
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	24	0.41
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	24	0.41
(1,798)	1:51:A:GLU:HG2	1:50:A:ARG:HG2	25	0.41
(1,798)	1:51:A:GLU:HG3	1:50:A:ARG:HG2	25	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	7	0.41
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	7	0.41
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	7	0.41
(1,222)	1:31:A:LEU:HB3	1:36:A:LEU:HD21	5	0.41
(1,222)	1:31:A:LEU:HB3	1:36:A:LEU:HD22	5	0.41
(1,222)	1:31:A:LEU:HB3	1:36:A:LEU:HD23	5	0.41
(1,77)	1:48:A:LEU:HD12	1:51:A:GLU:HG3	20	0.41
(1,76)	1:9:A:LEU:HD13	1:70:A:GLN:HB3	27	0.41
(1,63)	1:47:A:ILE:HG22	1:7:A:ARG:H	19	0.41
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	7	0.41
(1,8)	1:47:A:ILE:HG22	1:7:A:ARG:H	19	0.41
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	20	0.4
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	2	0.4
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	2	0.4
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	2	0.4
(1,1028)	1:34:A:LEU:HD21	1:33:A:ASP:H	3	0.4
(1,1028)	1:34:A:LEU:HD22	1:33:A:ASP:H	3	0.4
(1,1028)	1:34:A:LEU:HD23	1:33:A:ASP:H	3	0.4
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	28	0.4
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	28	0.4
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	28	0.4
(1,787)	1:51:A:GLU:HB3	1:6:A:GLN:HE21	5	0.4
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD11	18	0.4
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD12	18	0.4
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD13	18	0.4
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	12	0.4
(1,1592)	1:34:A:LEU:HD21	1:30:A:SER:H	17	0.39
(1,1592)	1:34:A:LEU:HD22	1:30:A:SER:H	17	0.39
(1,1592)	1:34:A:LEU:HD23	1:30:A:SER:H	17	0.39
(1,1548)	1:19:A:ILE:HG21	1:21:A:ASP:HB2	22	0.39
(1,1548)	1:19:A:ILE:HG22	1:21:A:ASP:HB2	22	0.39
(1,1548)	1:19:A:ILE:HG23	1:21:A:ASP:HB2	22	0.39
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	6	0.39
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	6	0.39
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	6	0.39
(1,1303)	1:64:A:LEU:HB2	1:31:A:LEU:HB3	7	0.39
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	30	0.39
(1,1179)	1:55:A:VAL:HG11	1:56:A:LEU:HB3	1	0.39
(1,1179)	1:55:A:VAL:HG12	1:56:A:LEU:HB3	1	0.39
(1,1179)	1:55:A:VAL:HG13	1:56:A:LEU:HB3	1	0.39
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	27	0.39
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	27	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	27	0.39
(1,896)	1:47:A:ILE:HG21	1:6:A:GLN:HE21	12	0.39
(1,896)	1:47:A:ILE:HG22	1:6:A:GLN:HE21	12	0.39
(1,896)	1:47:A:ILE:HG23	1:6:A:GLN:HE21	12	0.39
(1,593)	1:66:A:LEU:HD11	1:66:A:LEU:HA	11	0.39
(1,593)	1:66:A:LEU:HD12	1:66:A:LEU:HA	11	0.39
(1,593)	1:66:A:LEU:HD13	1:66:A:LEU:HA	11	0.39
(1,116)	1:55:A:VAL:HG21	1:54:A:LEU:HB3	1	0.39
(1,116)	1:55:A:VAL:HG22	1:54:A:LEU:HB3	1	0.39
(1,116)	1:55:A:VAL:HG23	1:54:A:LEU:HB3	1	0.39
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	1	0.39
(1,32)	1:27:A:LEU:HD11	1:70:A:GLN:HE21	5	0.39
(1,9)	1:16:A:ILE:HG23	1:43:A:GLU:H	27	0.39
(1,5)	1:17:A:LEU:HD12	1:66:A:LEU:HB2	2	0.39
(1,1589)	1:20:A:ARG:HG3	1:67:A:ARG:HE	21	0.38
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	6	0.38
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	10	0.38
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	28	0.37
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	28	0.37
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	28	0.37
(1,114)	1:55:A:VAL:HG11	1:57:A:PRO:HG3	1	0.37
(1,114)	1:55:A:VAL:HG12	1:57:A:PRO:HG3	1	0.37
(1,114)	1:55:A:VAL:HG13	1:57:A:PRO:HG3	1	0.37
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	10	0.37
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	22	0.37
(1,48)	1:44:A:VAL:HG13	1:45:A:ARG:HE	30	0.37
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	29	0.37
(1,8)	1:16:A:ILE:HG23	1:44:A:VAL:H	11	0.37
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	7	0.36
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	24	0.36
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	7	0.36
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	7	0.36
(1,1008)	1:34:A:LEU:HD11	1:31:A:LEU:HA	28	0.36
(1,1008)	1:34:A:LEU:HD12	1:31:A:LEU:HA	28	0.36
(1,1008)	1:34:A:LEU:HD13	1:31:A:LEU:HA	28	0.36
(1,72)	1:48:A:LEU:HD12	1:6:A:GLN:HE21	28	0.36
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	23	0.36
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	1	0.35
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	1	0.35
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	1	0.35
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	19	0.35
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	16	0.35
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	16	0.35
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	19	0.35
(1,1303)	1:64:A:LEU:HB2	1:31:A:LEU:HB3	19	0.35
(1,1303)	1:64:A:LEU:HB2	1:31:A:LEU:HB3	22	0.35
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	16	0.35
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD21	8	0.35
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD22	8	0.35
(1,315)	1:40:A:MET:HB3	1:39:A:LEU:HD23	8	0.35
(1,294)	1:17:A:LEU:HD11	1:36:A:LEU:HB2	11	0.35
(1,294)	1:17:A:LEU:HD12	1:36:A:LEU:HB2	11	0.35
(1,294)	1:17:A:LEU:HD13	1:36:A:LEU:HB2	11	0.35
(1,294)	1:17:A:LEU:HD21	1:36:A:LEU:HB2	11	0.35
(1,294)	1:17:A:LEU:HD22	1:36:A:LEU:HB2	11	0.35
(1,294)	1:17:A:LEU:HD23	1:36:A:LEU:HB2	11	0.35
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	3	0.35
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	3	0.35
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	3	0.35
(1,70)	1:9:A:LEU:HD21	1:72:A:MET:H	16	0.35
(1,56)	1:7:A:ARG:HG2	1:10:A:VAL:H	16	0.35
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	13	0.35
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	11	0.35
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	10	0.34
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	27	0.34
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	27	0.34
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	27	0.34
(1,787)	1:51:A:GLU:HB3	1:6:A:GLN:HE21	3	0.34
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	7	0.34
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	7	0.34
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	7	0.34
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	12	0.34
(1,47)	1:22:A:LEU:HD22	1:14:A:ALA:H	6	0.34
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	4	0.34
(1,1389)	1:12:A:ALA:HB1	1:9:A:LEU:HD21	13	0.33
(1,1389)	1:12:A:ALA:HB1	1:9:A:LEU:HD22	13	0.33
(1,1389)	1:12:A:ALA:HB1	1:9:A:LEU:HD23	13	0.33
(1,1389)	1:12:A:ALA:HB2	1:9:A:LEU:HD21	13	0.33
(1,1389)	1:12:A:ALA:HB2	1:9:A:LEU:HD22	13	0.33
(1,1389)	1:12:A:ALA:HB2	1:9:A:LEU:HD23	13	0.33
(1,1389)	1:12:A:ALA:HB3	1:9:A:LEU:HD21	13	0.33
(1,1389)	1:12:A:ALA:HB3	1:9:A:LEU:HD22	13	0.33
(1,1389)	1:12:A:ALA:HB3	1:9:A:LEU:HD23	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	28	0.33
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	20	0.33
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	20	0.33
(1,502)	1:19:A:ILE:HD11	1:25:A:ILE:HG13	1	0.33
(1,502)	1:19:A:ILE:HD12	1:25:A:ILE:HG13	1	0.33
(1,502)	1:19:A:ILE:HD13	1:25:A:ILE:HG13	1	0.33
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD11	5	0.33
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	28	0.33
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	23	0.33
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE3	27	0.33
(1,34)	1:34:A:LEU:HD23	1:27:A:LEU:HA	7	0.33
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	18	0.33
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	27	0.32
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	13	0.32
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	13	0.32
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	13	0.32
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	20	0.32
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	20	0.32
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	20	0.32
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	3	0.32
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	3	0.32
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	3	0.32
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	14	0.32
(1,668)	1:49:A:GLU:HG2	1:46:A:GLN:HA	18	0.32
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD11	22	0.32
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD12	22	0.32
(1,468)	1:47:A:ILE:HA	1:48:A:LEU:HD13	22	0.32
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD11	2	0.32
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD12	2	0.32
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD13	2	0.32
(1,89)	1:32:A:ALA:H	1:36:A:LEU:HD22	5	0.32
(1,77)	1:48:A:LEU:HD12	1:51:A:GLU:HG3	10	0.32
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	23	0.32
(1,64)	1:12:A:ALA:HB2	1:6:A:GLN:HG2	25	0.32
(1,52)	1:9:A:LEU:HG	1:10:A:VAL:HA	8	0.32
(1,32)	1:66:A:LEU:HD13	1:70:A:GLN:HE21	11	0.32
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	8	0.32
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	22	0.32
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	28	0.32
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	8	0.32
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	20	0.32
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	14	0.31
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	21	0.31
(1,1220)	1:58:A:ILE:HG21	1:62:A:ARG:HD2	26	0.31
(1,1220)	1:58:A:ILE:HG22	1:62:A:ARG:HD2	26	0.31
(1,1220)	1:58:A:ILE:HG23	1:62:A:ARG:HD2	26	0.31
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	14	0.31
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	14	0.31
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	14	0.31
(1,236)	1:31:A:LEU:HD11	1:66:A:LEU:H	13	0.31
(1,236)	1:31:A:LEU:HD12	1:66:A:LEU:H	13	0.31
(1,236)	1:31:A:LEU:HD13	1:66:A:LEU:H	13	0.31
(1,81)	1:73:A:SER:HB3	1:9:A:LEU:HB3	19	0.31
(1,76)	1:9:A:LEU:HD12	1:70:A:GLN:HB3	5	0.31
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	1	0.31
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	9	0.3
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	9	0.3
(1,1542)	1:44:A:VAL:HG21	1:40:A:MET:HB2	18	0.3
(1,1542)	1:44:A:VAL:HG22	1:40:A:MET:HB2	18	0.3
(1,1542)	1:44:A:VAL:HG23	1:40:A:MET:HB2	18	0.3
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	25	0.3
(1,1263)	1:61:A:VAL:HG11	1:62:A:ARG:HB3	22	0.3
(1,1263)	1:61:A:VAL:HG12	1:62:A:ARG:HB3	22	0.3
(1,1263)	1:61:A:VAL:HG13	1:62:A:ARG:HB3	22	0.3
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	26	0.3
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	26	0.3
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	26	0.3
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	17	0.3
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	17	0.3
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	17	0.3
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	3	0.3
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	3	0.3
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	19	0.3
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	19	0.3
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	19	0.3
(1,469)	1:17:A:LEU:HD11	1:16:A:ILE:H	16	0.3
(1,469)	1:17:A:LEU:HD12	1:16:A:ILE:H	16	0.3
(1,469)	1:17:A:LEU:HD13	1:16:A:ILE:H	16	0.3
(1,294)	1:17:A:LEU:HD11	1:36:A:LEU:HB2	3	0.3
(1,294)	1:17:A:LEU:HD12	1:36:A:LEU:HB2	3	0.3
(1,294)	1:17:A:LEU:HD13	1:36:A:LEU:HB2	3	0.3
(1,294)	1:17:A:LEU:HD21	1:36:A:LEU:HB2	3	0.3
(1,294)	1:17:A:LEU:HD22	1:36:A:LEU:HB2	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:17:A:LEU:HD23	1:36:A:LEU:HB2	3	0.3
(1,76)	1:9:A:LEU:HD11	1:70:A:GLN:HB3	15	0.3
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE3	16	0.3
(1,45)	1:22:A:LEU:HD21	1:11:A:LYS:HE2	30	0.3
(1,25)	1:52:A:HIS:HB2	1:48:A:LEU:HA	2	0.3
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	12	0.3
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	25	0.3
(1,1263)	1:61:A:VAL:HG11	1:62:A:ARG:HB3	7	0.29
(1,1263)	1:61:A:VAL:HG12	1:62:A:ARG:HB3	7	0.29
(1,1263)	1:61:A:VAL:HG13	1:62:A:ARG:HB3	7	0.29
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD21	8	0.29
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD22	8	0.29
(1,1099)	1:40:A:MET:HG3	1:39:A:LEU:HD23	8	0.29
(1,1019)	1:34:A:LEU:HD21	1:34:A:LEU:HA	5	0.29
(1,1019)	1:34:A:LEU:HD22	1:34:A:LEU:HA	5	0.29
(1,1019)	1:34:A:LEU:HD23	1:34:A:LEU:HA	5	0.29
(1,668)	1:49:A:GLU:HG2	1:46:A:GLN:HA	29	0.29
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	1	0.29
(1,77)	1:9:A:LEU:HD21	1:51:A:GLU:HG3	18	0.29
(1,74)	1:9:A:LEU:HD11	1:47:A:ILE:HB	13	0.29
(1,58)	1:66:A:LEU:HD21	1:10:A:VAL:HB	12	0.29
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	28	0.29
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	27	0.29
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD11	9	0.29
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	4	0.28
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	4	0.28
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	4	0.28
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	24	0.28
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	24	0.28
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	24	0.28
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	13	0.28
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	13	0.28
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	13	0.28
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	14	0.28
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	14	0.28
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	14	0.28
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	30	0.28
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	30	0.28
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	18	0.28
(1,81)	1:73:A:SER:HB3	1:9:A:LEU:HB3	9	0.28
(1,76)	1:9:A:LEU:HD11	1:70:A:GLN:HB3	20	0.28
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	22	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1548)	1:19:A:ILE:HG21	1:21:A:ASP:HB2	25	0.27
(1,1548)	1:19:A:ILE:HG22	1:21:A:ASP:HB2	25	0.27
(1,1548)	1:19:A:ILE:HG23	1:21:A:ASP:HB2	25	0.27
(1,1540)	1:44:A:VAL:HG21	1:40:A:MET:HA	18	0.27
(1,1540)	1:44:A:VAL:HG22	1:40:A:MET:HA	18	0.27
(1,1540)	1:44:A:VAL:HG23	1:40:A:MET:HA	18	0.27
(1,1180)	1:55:A:VAL:HG21	1:53:A:ASP:HA	1	0.27
(1,1180)	1:55:A:VAL:HG22	1:53:A:ASP:HA	1	0.27
(1,1180)	1:55:A:VAL:HG23	1:53:A:ASP:HA	1	0.27
(1,787)	1:51:A:GLU:HB3	1:6:A:GLN:HE21	26	0.27
(1,549)	1:72:A:MET:HB2	1:72:A:MET:H	18	0.27
(1,502)	1:19:A:ILE:HD11	1:25:A:ILE:HG13	24	0.27
(1,502)	1:19:A:ILE:HD12	1:25:A:ILE:HG13	24	0.27
(1,502)	1:19:A:ILE:HD13	1:25:A:ILE:HG13	24	0.27
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	14	0.27
(1,76)	1:9:A:LEU:HD12	1:70:A:GLN:HB3	26	0.27
(1,70)	1:9:A:LEU:HD23	1:72:A:MET:H	7	0.27
(1,63)	1:47:A:ILE:HG23	1:7:A:ARG:H	1	0.27
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	23	0.27
(1,38)	1:58:A:ILE:HG23	1:32:A:ALA:HA	27	0.27
(1,32)	1:66:A:LEU:HD12	1:70:A:GLN:HE21	18	0.27
(1,8)	1:47:A:ILE:HG23	1:7:A:ARG:H	1	0.27
(1,4)	1:32:A:ALA:HB2	1:36:A:LEU:HD22	5	0.27
(1,1643)	1:9:A:LEU:HD11	1:72:A:MET:H	13	0.26
(1,1643)	1:9:A:LEU:HD12	1:72:A:MET:H	13	0.26
(1,1643)	1:9:A:LEU:HD13	1:72:A:MET:H	13	0.26
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	1	0.26
(1,1575)	1:66:A:LEU:HD11	1:13:A:VAL:H	11	0.26
(1,1575)	1:66:A:LEU:HD12	1:13:A:VAL:H	11	0.26
(1,1575)	1:66:A:LEU:HD13	1:13:A:VAL:H	11	0.26
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	24	0.26
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	24	0.26
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	24	0.26
(1,1091)	1:39:A:LEU:HD11	1:39:A:LEU:HA	8	0.26
(1,1091)	1:39:A:LEU:HD12	1:39:A:LEU:HA	8	0.26
(1,1091)	1:39:A:LEU:HD13	1:39:A:LEU:HA	8	0.26
(1,1020)	1:34:A:LEU:HD21	1:33:A:ASP:HB2	29	0.26
(1,1020)	1:34:A:LEU:HD22	1:33:A:ASP:HB2	29	0.26
(1,1020)	1:34:A:LEU:HD23	1:33:A:ASP:HB2	29	0.26
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	24	0.26
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	24	0.26
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	24	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:72:A:MET:HB2	1:72:A:MET:H	6	0.26
(1,111)	1:55:A:VAL:HG21	1:49:A:GLU:HG3	25	0.26
(1,111)	1:55:A:VAL:HG22	1:49:A:GLU:HG3	25	0.26
(1,111)	1:55:A:VAL:HG23	1:49:A:GLU:HG3	25	0.26
(1,76)	1:9:A:LEU:HD12	1:70:A:GLN:HB3	18	0.26
(1,59)	1:66:A:LEU:HD22	1:64:A:LEU:HB2	25	0.26
(1,59)	1:66:A:LEU:HD21	1:64:A:LEU:HB2	30	0.26
(1,50)	1:16:A:ILE:HG22	1:39:A:LEU:HA	18	0.26
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	10	0.26
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	17	0.26
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	15	0.25
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	15	0.25
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	29	0.25
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	24	0.25
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	24	0.25
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	28	0.25
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	28	0.25
(1,798)	1:51:A:GLU:HG2	1:50:A:ARG:HG2	15	0.25
(1,798)	1:51:A:GLU:HG3	1:50:A:ARG:HG2	15	0.25
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	1	0.25
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	1	0.25
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	1	0.25
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	9	0.25
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	26	0.25
(1,50)	1:16:A:ILE:HG21	1:39:A:LEU:HA	30	0.25
(1,1698)	1:38:A:SER:H	1:39:A:LEU:H	22	0.24
(1,1642)	1:9:A:LEU:HD11	1:6:A:GLN:HE21	7	0.24
(1,1642)	1:9:A:LEU:HD12	1:6:A:GLN:HE21	7	0.24
(1,1642)	1:9:A:LEU:HD13	1:6:A:GLN:HE21	7	0.24
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	26	0.24
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	26	0.24
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	26	0.24
(1,787)	1:51:A:GLU:HB3	1:6:A:GLN:HE21	15	0.24
(1,779)	1:52:A:HIS:HB2	1:6:A:GLN:HE21	11	0.24
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	17	0.24
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG21	15	0.24
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG22	15	0.24
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG23	15	0.24
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	15	0.24
(1,49)	1:47:A:ILE:HG22	1:43:A:GLU:HG3	24	0.24
(1,48)	1:44:A:VAL:HG12	1:45:A:ARG:HE	6	0.24
(1,48)	1:44:A:VAL:HG11	1:45:A:ARG:HE	23	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	23	0.24
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	5	0.23
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	5	0.23
(1,1303)	1:64:A:LEU:HB2	1:31:A:LEU:HB3	15	0.23
(1,1263)	1:61:A:VAL:HG11	1:62:A:ARG:HB3	21	0.23
(1,1263)	1:61:A:VAL:HG12	1:62:A:ARG:HB3	21	0.23
(1,1263)	1:61:A:VAL:HG13	1:62:A:ARG:HB3	21	0.23
(1,1133)	1:53:A:ASP:HA	1:53:A:ASP:H	12	0.23
(1,1082)	1:39:A:LEU:HB3	1:39:A:LEU:H	17	0.23
(1,1028)	1:34:A:LEU:HD21	1:33:A:ASP:H	26	0.23
(1,1028)	1:34:A:LEU:HD22	1:33:A:ASP:H	26	0.23
(1,1028)	1:34:A:LEU:HD23	1:33:A:ASP:H	26	0.23
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	3	0.23
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	3	0.23
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	3	0.23
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	15	0.23
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	15	0.23
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	15	0.23
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	26	0.23
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	26	0.23
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	26	0.23
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	2	0.23
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	2	0.23
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	2	0.23
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	30	0.23
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	11	0.23
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	30	0.23
(1,66)	1:58:A:ILE:HD12	1:45:A:ARG:HE	30	0.23
(1,64)	1:12:A:ALA:HB3	1:6:A:GLN:HG2	28	0.23
(1,45)	1:22:A:LEU:HD23	1:11:A:LYS:HE2	20	0.23
(1,28)	1:10:A:VAL:HG23	1:66:A:LEU:HB2	7	0.23
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG22	26	0.23
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	12	0.22
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	12	0.22
(1,1303)	1:64:A:LEU:HB2	1:31:A:LEU:HB3	18	0.22
(1,1271)	1:62:A:ARG:HA	1:58:A:ILE:HG12	14	0.22
(1,1182)	1:56:A:LEU:HB3	1:57:A:PRO:HG2	13	0.22
(1,774)	1:6:A:GLN:HA	1:6:A:GLN:HG3	16	0.22
(1,700)	1:59:A:ARG:HA	1:62:A:ARG:HD2	30	0.22
(1,502)	1:19:A:ILE:HD11	1:25:A:ILE:HG13	7	0.22
(1,502)	1:19:A:ILE:HD12	1:25:A:ILE:HG13	7	0.22
(1,502)	1:19:A:ILE:HD13	1:25:A:ILE:HG13	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	9	0.22
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	9	0.22
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	9	0.22
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	18	0.22
(1,76)	1:9:A:LEU:HD11	1:70:A:GLN:HB3	30	0.22
(1,72)	1:9:A:LEU:HD22	1:6:A:GLN:HE21	7	0.22
(1,52)	1:9:A:LEU:HG	1:10:A:VAL:HA	24	0.22
(1,50)	1:16:A:ILE:HG22	1:39:A:LEU:HA	25	0.22
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	25	0.22
(1,1593)	1:34:A:LEU:HD21	1:29:A:SER:HA	28	0.21
(1,1593)	1:34:A:LEU:HD22	1:29:A:SER:HA	28	0.21
(1,1593)	1:34:A:LEU:HD23	1:29:A:SER:HA	28	0.21
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	11	0.21
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	11	0.21
(1,1302)	1:64:A:LEU:HB3	1:31:A:LEU:HB3	5	0.21
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	16	0.21
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	16	0.21
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	16	0.21
(1,1049)	1:36:A:LEU:HD21	1:40:A:MET:HB3	9	0.21
(1,1049)	1:36:A:LEU:HD22	1:40:A:MET:HB3	9	0.21
(1,1049)	1:36:A:LEU:HD23	1:40:A:MET:HB3	9	0.21
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	17	0.21
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	17	0.21
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	17	0.21
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	19	0.21
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	19	0.21
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	19	0.21
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	28	0.21
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	28	0.21
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	28	0.21
(1,1008)	1:34:A:LEU:HD11	1:31:A:LEU:HA	19	0.21
(1,1008)	1:34:A:LEU:HD12	1:31:A:LEU:HA	19	0.21
(1,1008)	1:34:A:LEU:HD13	1:31:A:LEU:HA	19	0.21
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	20	0.21
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	20	0.21
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	20	0.21
(1,952)	1:11:A:LYS:HG2	1:11:A:LYS:H	8	0.21
(1,844)	1:8:A:ASP:HB3	1:11:A:LYS:HB2	18	0.21
(1,844)	1:8:A:ASP:HB3	1:11:A:LYS:HB3	18	0.21
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	13	0.21
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	13	0.21
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	14	0.21
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	14	0.21
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	14	0.21
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	4	0.21
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	4	0.21
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	4	0.21
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	1	0.21
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	3	0.21
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	8	0.21
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	13	0.21
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	16	0.21
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	24	0.21
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	17	0.21
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	17	0.21
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	17	0.21
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	26	0.21
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	26	0.21
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	26	0.21
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	28	0.21
(1,60)	1:47:A:ILE:HG22	1:74:A:SER:HB2	7	0.21
(1,56)	1:50:A:ARG:HG2	1:49:A:GLU:H	25	0.21
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	19	0.2
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	19	0.2
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	15	0.2
(1,1554)	1:34:A:LEU:HD21	1:26:A:ASN:HB3	27	0.2
(1,1554)	1:34:A:LEU:HD22	1:26:A:ASN:HB3	27	0.2
(1,1554)	1:34:A:LEU:HD23	1:26:A:ASN:HB3	27	0.2
(1,1548)	1:19:A:ILE:HG21	1:21:A:ASP:HB2	1	0.2
(1,1548)	1:19:A:ILE:HG22	1:21:A:ASP:HB2	1	0.2
(1,1548)	1:19:A:ILE:HG23	1:21:A:ASP:HB2	1	0.2
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	20	0.2
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	20	0.2
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	20	0.2
(1,1415)	1:42:A:VAL:HG11	1:46:A:GLN:HE21	6	0.2
(1,1415)	1:42:A:VAL:HG12	1:46:A:GLN:HE21	6	0.2
(1,1415)	1:42:A:VAL:HG13	1:46:A:GLN:HE21	6	0.2
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	12	0.2
(1,1354)	1:69:A:LEU:HD21	1:67:A:ARG:HD3	9	0.2
(1,1354)	1:69:A:LEU:HD22	1:67:A:ARG:HD3	9	0.2
(1,1354)	1:69:A:LEU:HD23	1:67:A:ARG:HD3	9	0.2
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	13	0.2
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	13	0.2
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	17	0.2
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	17	0.2
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	17	0.2
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	5	0.2
(1,1028)	1:34:A:LEU:HD21	1:33:A:ASP:H	17	0.2
(1,1028)	1:34:A:LEU:HD22	1:33:A:ASP:H	17	0.2
(1,1028)	1:34:A:LEU:HD23	1:33:A:ASP:H	17	0.2
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	29	0.2
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	29	0.2
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	29	0.2
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD21	20	0.2
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD22	20	0.2
(1,927)	1:57:A:PRO:HG3	1:56:A:LEU:HD23	20	0.2
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG21	25	0.2
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG22	25	0.2
(1,664)	1:49:A:GLU:HG2	1:55:A:VAL:HG23	25	0.2
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	2	0.2
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	2	0.2
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	2	0.2
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	8	0.2
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	8	0.2
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	8	0.2
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	22	0.2
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	22	0.2
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	22	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	4	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	5	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	6	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	7	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	9	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	11	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	12	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	20	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	21	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	23	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	26	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	27	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	29	0.2
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	30	0.2
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	11	0.2
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	11	0.2
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD21	24	0.2
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD22	24	0.2
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD23	24	0.2
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	12	0.2
(1,82)	1:73:A:SER:HB2	1:7:A:ARG:HG3	27	0.2
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	27	0.2
(1,45)	1:22:A:LEU:HD22	1:11:A:LYS:HE2	2	0.2
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	26	0.2
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD12	14	0.2
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	16	0.19
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	16	0.19
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	21	0.19
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	21	0.19
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	21	0.19
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	15	0.19
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	15	0.19
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	15	0.19
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	20	0.19
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	20	0.19
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	20	0.19
(1,700)	1:59:A:ARG:HA	1:62:A:ARG:HD2	27	0.19
(1,571)	1:43:A:GLU:HB3	1:44:A:VAL:HG21	18	0.19
(1,571)	1:43:A:GLU:HB3	1:44:A:VAL:HG22	18	0.19
(1,571)	1:43:A:GLU:HB3	1:44:A:VAL:HG23	18	0.19
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	2	0.19
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	10	0.19
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	15	0.19
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	18	0.19
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	19	0.19
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	22	0.19
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	25	0.19
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	28	0.19
(1,294)	1:17:A:LEU:HD11	1:36:A:LEU:HB2	4	0.19
(1,294)	1:17:A:LEU:HD12	1:36:A:LEU:HB2	4	0.19
(1,294)	1:17:A:LEU:HD13	1:36:A:LEU:HB2	4	0.19
(1,294)	1:17:A:LEU:HD21	1:36:A:LEU:HB2	4	0.19
(1,294)	1:17:A:LEU:HD22	1:36:A:LEU:HB2	4	0.19
(1,294)	1:17:A:LEU:HD23	1:36:A:LEU:HB2	4	0.19
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	4	0.19
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	11	0.19
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	25	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	26	0.19
(1,73)	1:9:A:LEU:HD13	1:69:A:LEU:HB3	6	0.19
(1,72)	1:9:A:LEU:HD23	1:6:A:GLN:HE21	11	0.19
(1,28)	1:10:A:VAL:HG23	1:66:A:LEU:HB2	26	0.19
(1,1698)	1:38:A:SER:H	1:39:A:LEU:H	17	0.18
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	6	0.18
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	6	0.18
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	13	0.18
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	3	0.18
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	3	0.18
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	3	0.18
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	24	0.18
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	24	0.18
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	24	0.18
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	18	0.18
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	18	0.18
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	18	0.18
(1,1071)	1:36:A:LEU:HG	1:38:A:SER:H	18	0.18
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD21	29	0.18
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD22	29	0.18
(1,994)	1:33:A:ASP:HA	1:34:A:LEU:HD23	29	0.18
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	2	0.18
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	2	0.18
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	2	0.18
(1,779)	1:52:A:HIS:HB2	1:6:A:GLN:HE21	7	0.18
(1,668)	1:49:A:GLU:HG2	1:46:A:GLN:HA	19	0.18
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD11	22	0.18
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD12	22	0.18
(1,460)	1:47:A:ILE:HG13	1:48:A:LEU:HD13	22	0.18
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	29	0.18
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	29	0.18
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	29	0.18
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	14	0.18
(1,323)	1:45:A:ARG:HB2	1:45:A:ARG:HG2	17	0.18
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD21	8	0.18
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD22	8	0.18
(1,316)	1:40:A:MET:HB2	1:39:A:LEU:HD23	8	0.18
(1,294)	1:17:A:LEU:HD11	1:36:A:LEU:HB2	16	0.18
(1,294)	1:17:A:LEU:HD12	1:36:A:LEU:HB2	16	0.18
(1,294)	1:17:A:LEU:HD13	1:36:A:LEU:HB2	16	0.18
(1,294)	1:17:A:LEU:HD21	1:36:A:LEU:HB2	16	0.18
(1,294)	1:17:A:LEU:HD22	1:36:A:LEU:HB2	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:17:A:LEU:HD23	1:36:A:LEU:HB2	16	0.18
(1,294)	1:17:A:LEU:HD11	1:36:A:LEU:HB2	22	0.18
(1,294)	1:17:A:LEU:HD12	1:36:A:LEU:HB2	22	0.18
(1,294)	1:17:A:LEU:HD13	1:36:A:LEU:HB2	22	0.18
(1,294)	1:17:A:LEU:HD21	1:36:A:LEU:HB2	22	0.18
(1,294)	1:17:A:LEU:HD22	1:36:A:LEU:HB2	22	0.18
(1,294)	1:17:A:LEU:HD23	1:36:A:LEU:HB2	22	0.18
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	23	0.18
(1,77)	1:48:A:LEU:HD12	1:51:A:GLU:HG3	28	0.18
(1,48)	1:44:A:VAL:HG13	1:45:A:ARG:HE	1	0.18
(1,47)	1:22:A:LEU:HD22	1:14:A:ALA:H	9	0.18
(1,32)	1:66:A:LEU:HD12	1:70:A:GLN:HE21	28	0.18
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	15	0.18
(1,9)	1:16:A:ILE:HG23	1:43:A:GLU:H	24	0.18
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	17	0.17
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	17	0.17
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	27	0.17
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	27	0.17
(1,1548)	1:19:A:ILE:HG21	1:21:A:ASP:HB2	10	0.17
(1,1548)	1:19:A:ILE:HG22	1:21:A:ASP:HB2	10	0.17
(1,1548)	1:19:A:ILE:HG23	1:21:A:ASP:HB2	10	0.17
(1,1491)	1:42:A:VAL:HG21	1:46:A:GLN:HG2	27	0.17
(1,1491)	1:42:A:VAL:HG22	1:46:A:GLN:HG2	27	0.17
(1,1491)	1:42:A:VAL:HG23	1:46:A:GLN:HG2	27	0.17
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	7	0.17
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	7	0.17
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	7	0.17
(1,1133)	1:53:A:ASP:HA	1:53:A:ASP:H	19	0.17
(1,1028)	1:34:A:LEU:HD21	1:33:A:ASP:H	24	0.17
(1,1028)	1:34:A:LEU:HD22	1:33:A:ASP:H	24	0.17
(1,1028)	1:34:A:LEU:HD23	1:33:A:ASP:H	24	0.17
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD21	13	0.17
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD22	13	0.17
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD23	13	0.17
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	20	0.17
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	20	0.17
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	20	0.17
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	22	0.17
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	22	0.17
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	22	0.17
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	29	0.17
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	29	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	29	0.17
(1,662)	1:49:A:GLU:HA	1:46:A:GLN:HA	5	0.17
(1,662)	1:49:A:GLU:HA	1:46:A:GLN:HA	8	0.17
(1,549)	1:72:A:MET:HB2	1:72:A:MET:H	13	0.17
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	5	0.17
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	5	0.17
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	5	0.17
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	17	0.17
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	17	0.17
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	17	0.17
(1,240)	1:31:A:LEU:HD11	1:34:A:LEU:HB2	5	0.17
(1,240)	1:31:A:LEU:HD12	1:34:A:LEU:HB2	5	0.17
(1,240)	1:31:A:LEU:HD13	1:34:A:LEU:HB2	5	0.17
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	6	0.17
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	6	0.17
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	6	0.17
(1,171)	1:22:A:LEU:HG	1:21:A:ASP:HA	23	0.17
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	22	0.17
(1,56)	1:7:A:ARG:HG3	1:10:A:VAL:H	3	0.17
(1,48)	1:44:A:VAL:HG12	1:45:A:ARG:HE	11	0.17
(1,28)	1:10:A:VAL:HG22	1:66:A:LEU:HB2	19	0.17
(1,26)	1:51:A:GLU:HA	1:47:A:ILE:HG22	14	0.17
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	16	0.17
(1,5)	1:17:A:LEU:HD12	1:66:A:LEU:HB2	18	0.17
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	3	0.16
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	3	0.16
(1,1415)	1:42:A:VAL:HG11	1:46:A:GLN:HE21	15	0.16
(1,1415)	1:42:A:VAL:HG12	1:46:A:GLN:HE21	15	0.16
(1,1415)	1:42:A:VAL:HG13	1:46:A:GLN:HE21	15	0.16
(1,1394)	1:44:A:VAL:HA	1:44:A:VAL:HG11	18	0.16
(1,1394)	1:44:A:VAL:HA	1:44:A:VAL:HG12	18	0.16
(1,1394)	1:44:A:VAL:HA	1:44:A:VAL:HG13	18	0.16
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	6	0.16
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	6	0.16
(1,1314)	1:64:A:LEU:HD21	1:68:A:LYS:HD2	12	0.16
(1,1314)	1:64:A:LEU:HD21	1:68:A:LYS:HD3	12	0.16
(1,1314)	1:64:A:LEU:HD22	1:68:A:LYS:HD2	12	0.16
(1,1314)	1:64:A:LEU:HD22	1:68:A:LYS:HD3	12	0.16
(1,1314)	1:64:A:LEU:HD23	1:68:A:LYS:HD2	12	0.16
(1,1314)	1:64:A:LEU:HD23	1:68:A:LYS:HD3	12	0.16
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD21	13	0.16
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD22	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD23	13	0.16
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	2	0.16
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	2	0.16
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	2	0.16
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	4	0.16
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	4	0.16
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	4	0.16
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	8	0.16
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	8	0.16
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	8	0.16
(1,549)	1:72:A:MET:HB2	1:72:A:MET:H	24	0.16
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	6	0.16
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	6	0.16
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	6	0.16
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	18	0.16
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	24	0.16
(1,53)	1:59:A:ARG:HG2	1:58:A:ILE:H	8	0.16
(1,48)	1:44:A:VAL:HG13	1:45:A:ARG:HE	21	0.16
(1,28)	1:10:A:VAL:HG21	1:66:A:LEU:HB2	9	0.16
(1,1727)	1:86:A:LYS:H	1:85:A:PRO:HA	5	0.15
(1,1698)	1:38:A:SER:H	1:39:A:LEU:H	30	0.15
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	16	0.15
(1,1569)	1:10:A:VAL:HG21	1:70:A:GLN:HB2	7	0.15
(1,1569)	1:10:A:VAL:HG21	1:70:A:GLN:HB3	7	0.15
(1,1569)	1:10:A:VAL:HG22	1:70:A:GLN:HB2	7	0.15
(1,1569)	1:10:A:VAL:HG22	1:70:A:GLN:HB3	7	0.15
(1,1569)	1:10:A:VAL:HG23	1:70:A:GLN:HB2	7	0.15
(1,1569)	1:10:A:VAL:HG23	1:70:A:GLN:HB3	7	0.15
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	19	0.15
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	19	0.15
(1,1163)	1:54:A:LEU:HD11	1:51:A:GLU:HB2	18	0.15
(1,1163)	1:54:A:LEU:HD12	1:51:A:GLU:HB2	18	0.15
(1,1163)	1:54:A:LEU:HD13	1:51:A:GLU:HB2	18	0.15
(1,1091)	1:39:A:LEU:HD11	1:39:A:LEU:HA	12	0.15
(1,1091)	1:39:A:LEU:HD12	1:39:A:LEU:HA	12	0.15
(1,1091)	1:39:A:LEU:HD13	1:39:A:LEU:HA	12	0.15
(1,1061)	1:36:A:LEU:HD21	1:38:A:SER:H	7	0.15
(1,1061)	1:36:A:LEU:HD22	1:38:A:SER:H	7	0.15
(1,1061)	1:36:A:LEU:HD23	1:38:A:SER:H	7	0.15
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	29	0.15
(1,1028)	1:34:A:LEU:HD21	1:33:A:ASP:H	14	0.15
(1,1028)	1:34:A:LEU:HD22	1:33:A:ASP:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	1:34:A:LEU:HD23	1:33:A:ASP:H	14	0.15
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD21	6	0.15
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD22	6	0.15
(1,851)	1:9:A:LEU:HA	1:9:A:LEU:HD23	6	0.15
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	9	0.15
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	12	0.15
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	14	0.15
(1,502)	1:19:A:ILE:HD11	1:25:A:ILE:HG13	9	0.15
(1,502)	1:19:A:ILE:HD12	1:25:A:ILE:HG13	9	0.15
(1,502)	1:19:A:ILE:HD13	1:25:A:ILE:HG13	9	0.15
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	16	0.15
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	16	0.15
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	16	0.15
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	6	0.15
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	6	0.15
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	6	0.15
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	6	0.15
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	15	0.15
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	21	0.15
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	8	0.15
(1,53)	1:59:A:ARG:HG2	1:58:A:ILE:H	10	0.15
(1,38)	1:58:A:ILE:HG21	1:32:A:ALA:HA	18	0.15
(1,28)	1:10:A:VAL:HG23	1:66:A:LEU:HB2	15	0.15
(1,9)	1:47:A:ILE:HG21	1:50:A:ARG:HE	3	0.15
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	12	0.14
(1,1584)	1:59:A:ARG:HG3	1:58:A:ILE:H	23	0.14
(1,1576)	1:66:A:LEU:HD11	1:65:A:THR:HA	14	0.14
(1,1576)	1:66:A:LEU:HD12	1:65:A:THR:HA	14	0.14
(1,1576)	1:66:A:LEU:HD13	1:65:A:THR:HA	14	0.14
(1,1576)	1:66:A:LEU:HD11	1:65:A:THR:HA	18	0.14
(1,1576)	1:66:A:LEU:HD12	1:65:A:THR:HA	18	0.14
(1,1576)	1:66:A:LEU:HD13	1:65:A:THR:HA	18	0.14
(1,1497)	1:65:A:THR:HG21	1:63:A:GLN:HB2	13	0.14
(1,1497)	1:65:A:THR:HG22	1:63:A:GLN:HB2	13	0.14
(1,1497)	1:65:A:THR:HG23	1:63:A:GLN:HB2	13	0.14
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	9	0.14
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	9	0.14
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	9	0.14
(1,1376)	1:12:A:ALA:HB1	1:7:A:ARG:HD2	5	0.14
(1,1376)	1:12:A:ALA:HB1	1:7:A:ARG:HD3	5	0.14
(1,1376)	1:12:A:ALA:HB2	1:7:A:ARG:HD2	5	0.14
(1,1376)	1:12:A:ALA:HB2	1:7:A:ARG:HD3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1376)	1:12:A:ALA:HB3	1:7:A:ARG:HD2	5	0.14
(1,1376)	1:12:A:ALA:HB3	1:7:A:ARG:HD3	5	0.14
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	7	0.14
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	18	0.14
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	18	0.14
(1,1308)	1:64:A:LEU:HA	1:63:A:GLN:HE21	16	0.14
(1,1263)	1:61:A:VAL:HG11	1:62:A:ARG:HB3	4	0.14
(1,1263)	1:61:A:VAL:HG12	1:62:A:ARG:HB3	4	0.14
(1,1263)	1:61:A:VAL:HG13	1:62:A:ARG:HB3	4	0.14
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD21	17	0.14
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD22	17	0.14
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD23	17	0.14
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD21	26	0.14
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD22	26	0.14
(1,1168)	1:54:A:LEU:HG	1:56:A:LEU:HD23	26	0.14
(1,1061)	1:36:A:LEU:HD21	1:38:A:SER:H	11	0.14
(1,1061)	1:36:A:LEU:HD22	1:38:A:SER:H	11	0.14
(1,1061)	1:36:A:LEU:HD23	1:38:A:SER:H	11	0.14
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	21	0.14
(1,1028)	1:34:A:LEU:HD21	1:33:A:ASP:H	20	0.14
(1,1028)	1:34:A:LEU:HD22	1:33:A:ASP:H	20	0.14
(1,1028)	1:34:A:LEU:HD23	1:33:A:ASP:H	20	0.14
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB2	14	0.14
(1,845)	1:8:A:ASP:HB2	1:11:A:LYS:HB3	14	0.14
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	6	0.14
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	6	0.14
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	6	0.14
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	19	0.14
(1,475)	1:22:A:LEU:HD21	1:20:A:ARG:HB2	18	0.14
(1,475)	1:22:A:LEU:HD22	1:20:A:ARG:HB2	18	0.14
(1,475)	1:22:A:LEU:HD23	1:20:A:ARG:HB2	18	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	6	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	6	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	6	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	7	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	7	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	7	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	21	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	21	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	21	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	30	0.14
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	30	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	30	0.14
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD21	20	0.14
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD22	20	0.14
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD23	20	0.14
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	28	0.14
(1,63)	1:47:A:ILE:HG21	1:7:A:ARG:H	7	0.14
(1,56)	1:7:A:ARG:HG2	1:10:A:VAL:H	17	0.14
(1,53)	1:59:A:ARG:HG2	1:58:A:ILE:H	11	0.14
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	19	0.14
(1,50)	1:16:A:ILE:HG22	1:39:A:LEU:HA	13	0.14
(1,31)	1:27:A:LEU:HD23	1:67:A:ARG:HA	15	0.14
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	30	0.14
(1,8)	1:47:A:ILE:HG21	1:7:A:ARG:H	7	0.14
(1,1727)	1:86:A:LYS:H	1:85:A:PRO:HA	22	0.13
(1,1638)	1:57:A:PRO:HB3	1:59:A:ARG:HB2	9	0.13
(1,1595)	1:68:A:LYS:HB2	1:64:A:LEU:H	10	0.13
(1,1595)	1:68:A:LYS:HB3	1:64:A:LEU:H	10	0.13
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	1	0.13
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	1	0.13
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	1	0.13
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	4	0.13
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	4	0.13
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	4	0.13
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	12	0.13
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	12	0.13
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	12	0.13
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	18	0.13
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	18	0.13
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	18	0.13
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	25	0.13
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	25	0.13
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	25	0.13
(1,1263)	1:61:A:VAL:HG11	1:62:A:ARG:HB3	18	0.13
(1,1263)	1:61:A:VAL:HG12	1:62:A:ARG:HB3	18	0.13
(1,1263)	1:61:A:VAL:HG13	1:62:A:ARG:HB3	18	0.13
(1,1107)	1:48:A:LEU:HA	1:52:A:HIS:HB2	17	0.13
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG21	18	0.13
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG22	18	0.13
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG23	18	0.13
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG21	18	0.13
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG22	18	0.13
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG23	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG21	18	0.13
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG22	18	0.13
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG23	18	0.13
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	6	0.13
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	26	0.13
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	27	0.13
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	28	0.13
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	28	0.13
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	28	0.13
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	1	0.13
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	1	0.13
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	1	0.13
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	3	0.13
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	3	0.13
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	3	0.13
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	5	0.13
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	5	0.13
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	5	0.13
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	7	0.13
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	7	0.13
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	7	0.13
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	28	0.13
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	28	0.13
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	28	0.13
(1,549)	1:72:A:MET:HB2	1:72:A:MET:H	8	0.13
(1,479)	1:23:A:ALA:HA	1:21:A:ASP:HA	19	0.13
(1,469)	1:17:A:LEU:HD11	1:16:A:ILE:H	7	0.13
(1,469)	1:17:A:LEU:HD12	1:16:A:ILE:H	7	0.13
(1,469)	1:17:A:LEU:HD13	1:16:A:ILE:H	7	0.13
(1,291)	1:17:A:LEU:HG	1:17:A:LEU:H	7	0.13
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	12	0.13
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	12	0.13
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	12	0.13
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	29	0.13
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	29	0.13
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	29	0.13
(1,213)	1:30:A:SER:HB3	1:33:A:ASP:HA	27	0.13
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	2	0.13
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	22	0.13
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	27	0.13
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	25	0.13
(1,81)	1:73:A:SER:HB3	1:9:A:LEU:HB3	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:57:A:PRO:HB3	1:61:A:VAL:HG21	28	0.13
(1,56)	1:7:A:ARG:HG3	1:10:A:VAL:H	22	0.13
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	4	0.13
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	7	0.13
(1,18)	1:71:A:GLU:HA	1:74:A:SER:H	22	0.13
(1,17)	1:72:A:MET:HB3	1:48:A:LEU:HD11	10	0.13
(1,9)	1:16:A:ILE:HG22	1:43:A:GLU:H	25	0.13
(1,1581)	1:14:A:ALA:HB1	1:70:A:GLN:HG3	7	0.12
(1,1581)	1:14:A:ALA:HB2	1:70:A:GLN:HG3	7	0.12
(1,1581)	1:14:A:ALA:HB3	1:70:A:GLN:HG3	7	0.12
(1,1569)	1:10:A:VAL:HG21	1:70:A:GLN:HB2	3	0.12
(1,1569)	1:10:A:VAL:HG21	1:70:A:GLN:HB3	3	0.12
(1,1569)	1:10:A:VAL:HG22	1:70:A:GLN:HB2	3	0.12
(1,1569)	1:10:A:VAL:HG22	1:70:A:GLN:HB3	3	0.12
(1,1569)	1:10:A:VAL:HG23	1:70:A:GLN:HB2	3	0.12
(1,1569)	1:10:A:VAL:HG23	1:70:A:GLN:HB3	3	0.12
(1,1545)	1:44:A:VAL:HG21	1:45:A:ARG:HE	9	0.12
(1,1545)	1:44:A:VAL:HG22	1:45:A:ARG:HE	9	0.12
(1,1545)	1:44:A:VAL:HG23	1:45:A:ARG:HE	9	0.12
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	21	0.12
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	21	0.12
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	21	0.12
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	28	0.12
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	28	0.12
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	28	0.12
(1,1400)	1:44:A:VAL:HB	1:45:A:ARG:HE	18	0.12
(1,1369)	1:71:A:GLU:HG2	1:72:A:MET:H	5	0.12
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	8	0.12
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	8	0.12
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	5	0.12
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	5	0.12
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	5	0.12
(1,1263)	1:61:A:VAL:HG11	1:62:A:ARG:HB3	20	0.12
(1,1263)	1:61:A:VAL:HG12	1:62:A:ARG:HB3	20	0.12
(1,1263)	1:61:A:VAL:HG13	1:62:A:ARG:HB3	20	0.12
(1,1182)	1:56:A:LEU:HB3	1:57:A:PRO:HB2	18	0.12
(1,1091)	1:39:A:LEU:HD11	1:39:A:LEU:HA	27	0.12
(1,1091)	1:39:A:LEU:HD12	1:39:A:LEU:HA	27	0.12
(1,1091)	1:39:A:LEU:HD13	1:39:A:LEU:HA	27	0.12
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	22	0.12
(1,1018)	1:34:A:LEU:HD21	1:29:A:SER:HB2	3	0.12
(1,1018)	1:34:A:LEU:HD22	1:29:A:SER:HB2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:34:A:LEU:HD23	1:29:A:SER:HB2	3	0.12
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	19	0.12
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	19	0.12
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	19	0.12
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	21	0.12
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	21	0.12
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	21	0.12
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	30	0.12
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	30	0.12
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	30	0.12
(1,1012)	1:34:A:LEU:HD11	1:31:A:LEU:H	19	0.12
(1,1012)	1:34:A:LEU:HD12	1:31:A:LEU:H	19	0.12
(1,1012)	1:34:A:LEU:HD13	1:31:A:LEU:H	19	0.12
(1,972)	1:27:A:LEU:HD21	1:70:A:GLN:HE21	21	0.12
(1,972)	1:27:A:LEU:HD22	1:70:A:GLN:HE21	21	0.12
(1,972)	1:27:A:LEU:HD23	1:70:A:GLN:HE21	21	0.12
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	10	0.12
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	10	0.12
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	10	0.12
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	12	0.12
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	12	0.12
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	12	0.12
(1,778)	1:52:A:HIS:HB3	1:6:A:GLN:HE21	22	0.12
(1,662)	1:49:A:GLU:HA	1:46:A:GLN:HA	10	0.12
(1,662)	1:49:A:GLU:HA	1:46:A:GLN:HA	18	0.12
(1,662)	1:49:A:GLU:HA	1:46:A:GLN:HA	21	0.12
(1,391)	1:19:A:ILE:HG21	1:21:A:ASP:HA	25	0.12
(1,391)	1:19:A:ILE:HG22	1:21:A:ASP:HA	25	0.12
(1,391)	1:19:A:ILE:HG23	1:21:A:ASP:HA	25	0.12
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	2	0.12
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	2	0.12
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	2	0.12
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	18	0.12
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	18	0.12
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	18	0.12
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	9	0.12
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	9	0.12
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	9	0.12
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	29	0.12
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	29	0.12
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	29	0.12
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD21	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD22	3	0.12
(1,192)	1:29:A:SER:HB3	1:34:A:LEU:HD23	3	0.12
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	24	0.12
(1,72)	1:9:A:LEU:HD23	1:6:A:GLN:HE21	1	0.12
(1,68)	1:57:A:PRO:HB3	1:61:A:VAL:HG22	12	0.12
(1,59)	1:66:A:LEU:HD23	1:64:A:LEU:HB2	15	0.12
(1,52)	1:19:A:ILE:HG13	1:10:A:VAL:HA	29	0.12
(1,1732)	1:32:A:ALA:H	1:65:A:THR:HG21	17	0.11
(1,1732)	1:32:A:ALA:H	1:65:A:THR:HG22	17	0.11
(1,1732)	1:32:A:ALA:H	1:65:A:THR:HG23	17	0.11
(1,1646)	1:9:A:LEU:HG	1:9:A:LEU:H	3	0.11
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD2	20	0.11
(1,1618)	1:58:A:ILE:HG12	1:59:A:ARG:HD3	20	0.11
(1,1553)	1:19:A:ILE:HG21	1:26:A:ASN:H	6	0.11
(1,1553)	1:19:A:ILE:HG22	1:26:A:ASN:H	6	0.11
(1,1553)	1:19:A:ILE:HG23	1:26:A:ASN:H	6	0.11
(1,1546)	1:44:A:VAL:HG11	1:42:A:VAL:HA	11	0.11
(1,1546)	1:44:A:VAL:HG12	1:42:A:VAL:HA	11	0.11
(1,1546)	1:44:A:VAL:HG13	1:42:A:VAL:HA	11	0.11
(1,1545)	1:44:A:VAL:HG21	1:45:A:ARG:HE	8	0.11
(1,1545)	1:44:A:VAL:HG22	1:45:A:ARG:HE	8	0.11
(1,1545)	1:44:A:VAL:HG23	1:45:A:ARG:HE	8	0.11
(1,1545)	1:44:A:VAL:HG21	1:45:A:ARG:HE	15	0.11
(1,1545)	1:44:A:VAL:HG22	1:45:A:ARG:HE	15	0.11
(1,1545)	1:44:A:VAL:HG23	1:45:A:ARG:HE	15	0.11
(1,1525)	1:73:A:SER:HA	1:9:A:LEU:HD21	13	0.11
(1,1525)	1:73:A:SER:HA	1:9:A:LEU:HD22	13	0.11
(1,1525)	1:73:A:SER:HA	1:9:A:LEU:HD23	13	0.11
(1,1523)	1:73:A:SER:HA	1:70:A:GLN:H	3	0.11
(1,1523)	1:73:A:SER:HA	1:70:A:GLN:H	22	0.11
(1,1505)	1:55:A:VAL:HG11	1:59:A:ARG:HD2	25	0.11
(1,1505)	1:55:A:VAL:HG11	1:59:A:ARG:HD3	25	0.11
(1,1505)	1:55:A:VAL:HG12	1:59:A:ARG:HD2	25	0.11
(1,1505)	1:55:A:VAL:HG12	1:59:A:ARG:HD3	25	0.11
(1,1505)	1:55:A:VAL:HG13	1:59:A:ARG:HD2	25	0.11
(1,1505)	1:55:A:VAL:HG13	1:59:A:ARG:HD3	25	0.11
(1,1402)	1:42:A:VAL:HA	1:45:A:ARG:HB3	15	0.11
(1,1332)	1:68:A:LYS:HE2	1:69:A:LEU:H	20	0.11
(1,1332)	1:68:A:LYS:HE3	1:69:A:LEU:H	20	0.11
(1,1327)	1:68:A:LYS:HD2	1:71:A:GLU:HB2	15	0.11
(1,1327)	1:68:A:LYS:HD3	1:71:A:GLU:HB2	15	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	4	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	4	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	6	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	6	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	6	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	22	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	22	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	22	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB1	23	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB2	23	0.11
(1,1276)	1:62:A:ARG:HB3	1:32:A:ALA:HB3	23	0.11
(1,1182)	1:56:A:LEU:HB3	1:57:A:PRO:HG2	22	0.11
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	2	0.11
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	3	0.11
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	28	0.11
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	2	0.11
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	2	0.11
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	2	0.11
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	15	0.11
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	15	0.11
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	15	0.11
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	16	0.11
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	16	0.11
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	16	0.11
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	17	0.11
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	17	0.11
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	17	0.11
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	26	0.11
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	26	0.11
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	26	0.11
(1,896)	1:47:A:ILE:HG21	1:6:A:GLN:HE21	6	0.11
(1,896)	1:47:A:ILE:HG22	1:6:A:GLN:HE21	6	0.11
(1,896)	1:47:A:ILE:HG23	1:6:A:GLN:HE21	6	0.11
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD21	8	0.11
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD22	8	0.11
(1,862)	1:10:A:VAL:HA	1:9:A:LEU:HD23	8	0.11
(1,841)	1:8:A:ASP:HB2	1:11:A:LYS:H	25	0.11
(1,813)	1:65:A:THR:HG21	1:69:A:LEU:H	27	0.11
(1,813)	1:65:A:THR:HG22	1:69:A:LEU:H	27	0.11
(1,813)	1:65:A:THR:HG23	1:69:A:LEU:H	27	0.11
(1,806)	1:65:A:THR:HG21	1:67:A:ARG:HB2	2	0.11
(1,806)	1:65:A:THR:HG21	1:67:A:ARG:HB3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:65:A:THR:HG22	1:67:A:ARG:HB2	2	0.11
(1,806)	1:65:A:THR:HG22	1:67:A:ARG:HB3	2	0.11
(1,806)	1:65:A:THR:HG23	1:67:A:ARG:HB2	2	0.11
(1,806)	1:65:A:THR:HG23	1:67:A:ARG:HB3	2	0.11
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	7	0.11
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	15	0.11
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	3	0.11
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	3	0.11
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	3	0.11
(1,391)	1:19:A:ILE:HG21	1:21:A:ASP:HA	17	0.11
(1,391)	1:19:A:ILE:HG22	1:21:A:ASP:HA	17	0.11
(1,391)	1:19:A:ILE:HG23	1:21:A:ASP:HA	17	0.11
(1,291)	1:17:A:LEU:HG	1:17:A:LEU:H	16	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	8	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	8	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	8	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	20	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	20	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	20	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	22	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	22	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	22	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD11	25	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD12	25	0.11
(1,264)	1:32:A:ALA:HA	1:34:A:LEU:HD13	25	0.11
(1,213)	1:30:A:SER:HB3	1:33:A:ASP:HA	26	0.11
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	14	0.11
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	14	0.11
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	14	0.11
(1,171)	1:22:A:LEU:HG	1:21:A:ASP:HA	27	0.11
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	3	0.11
(1,83)	1:73:A:SER:HB3	1:69:A:LEU:HD12	10	0.11
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	4	0.11
(1,82)	1:73:A:SER:HB2	1:9:A:LEU:HB3	23	0.11
(1,76)	1:9:A:LEU:HD11	1:70:A:GLN:HB3	11	0.11
(1,59)	1:66:A:LEU:HD21	1:64:A:LEU:HB2	24	0.11
(1,1701)	1:47:A:ILE:H	1:48:A:LEU:H	14	0.1
(1,1545)	1:44:A:VAL:HG21	1:45:A:ARG:HE	11	0.1
(1,1545)	1:44:A:VAL:HG22	1:45:A:ARG:HE	11	0.1
(1,1545)	1:44:A:VAL:HG23	1:45:A:ARG:HE	11	0.1
(1,1497)	1:65:A:THR:HG21	1:63:A:GLN:HB2	14	0.1
(1,1497)	1:65:A:THR:HG22	1:63:A:GLN:HB2	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1497)	1:65:A:THR:HG23	1:63:A:GLN:HB2	14	0.1
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	10	0.1
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	10	0.1
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	10	0.1
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	15	0.1
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	15	0.1
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	15	0.1
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	16	0.1
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	16	0.1
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	16	0.1
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	23	0.1
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	23	0.1
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	23	0.1
(1,1484)	1:14:A:ALA:HB1	1:19:A:ILE:HB	27	0.1
(1,1484)	1:14:A:ALA:HB2	1:19:A:ILE:HB	27	0.1
(1,1484)	1:14:A:ALA:HB3	1:19:A:ILE:HB	27	0.1
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG21	23	0.1
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG22	23	0.1
(1,1050)	1:36:A:LEU:HD11	1:44:A:VAL:HG23	23	0.1
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG21	23	0.1
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG22	23	0.1
(1,1050)	1:36:A:LEU:HD12	1:44:A:VAL:HG23	23	0.1
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG21	23	0.1
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG22	23	0.1
(1,1050)	1:36:A:LEU:HD13	1:44:A:VAL:HG23	23	0.1
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	4	0.1
(1,1037)	1:36:A:LEU:HB3	1:40:A:MET:HA	25	0.1
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	10	0.1
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	10	0.1
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	10	0.1
(1,1017)	1:34:A:LEU:HD21	1:31:A:LEU:HA	29	0.1
(1,1017)	1:34:A:LEU:HD22	1:31:A:LEU:HA	29	0.1
(1,1017)	1:34:A:LEU:HD23	1:31:A:LEU:HA	29	0.1
(1,844)	1:8:A:ASP:HB3	1:11:A:LYS:HB2	11	0.1
(1,844)	1:8:A:ASP:HB3	1:11:A:LYS:HB3	11	0.1
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	23	0.1
(1,704)	1:59:A:ARG:HB2	1:59:A:ARG:H	24	0.1
(1,394)	1:19:A:ILE:HG21	1:25:A:ILE:HG13	28	0.1
(1,394)	1:19:A:ILE:HG22	1:25:A:ILE:HG13	28	0.1
(1,394)	1:19:A:ILE:HG23	1:25:A:ILE:HG13	28	0.1
(1,391)	1:19:A:ILE:HG21	1:21:A:ASP:HA	5	0.1
(1,391)	1:19:A:ILE:HG22	1:21:A:ASP:HA	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:19:A:ILE:HG23	1:21:A:ASP:HA	5	0.1
(1,239)	1:31:A:LEU:HD11	1:62:A:ARG:HG3	25	0.1
(1,239)	1:31:A:LEU:HD12	1:62:A:ARG:HG3	25	0.1
(1,239)	1:31:A:LEU:HD13	1:62:A:ARG:HG3	25	0.1
(1,213)	1:30:A:SER:HB3	1:33:A:ASP:HA	11	0.1
(1,213)	1:30:A:SER:HB3	1:33:A:ASP:HA	28	0.1
(1,177)	1:22:A:LEU:HD11	1:24:A:GLY:HA2	13	0.1
(1,177)	1:22:A:LEU:HD12	1:24:A:GLY:HA2	13	0.1
(1,177)	1:22:A:LEU:HD13	1:24:A:GLY:HA2	13	0.1
(1,171)	1:22:A:LEU:HG	1:21:A:ASP:HA	24	0.1
(1,85)	1:24:A:GLY:H	1:23:A:ALA:HA	5	0.1
(1,54)	1:20:A:ARG:HG3	1:10:A:VAL:HA	6	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found